

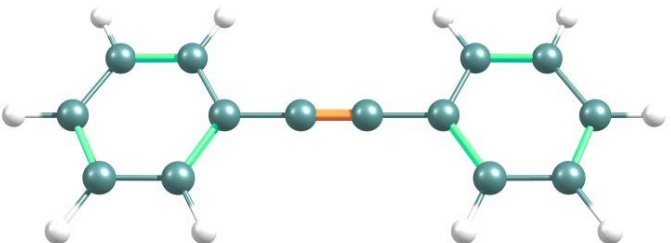
## Supporting Information for

### The role of the metal in the dual-metal catalysed hydrophenoxylation of diphenylacetylene

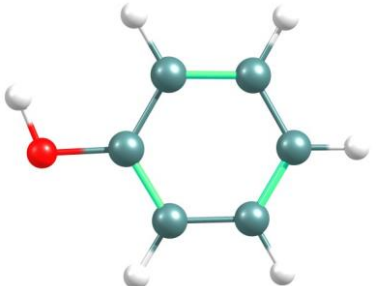
Oscar F. González-Belman,<sup>a,b</sup> J. Oscar C. Jiménez-Halla,<sup>b</sup> Fady Nahra,<sup>c</sup> Catherine S. J. Cazin,<sup>c</sup> and Albert Poater<sup>a,\*</sup>

**Table S1.** xyz coordinate data sets, absolute energies in a.u., and 3D sketches for all DFT optimized complexes.

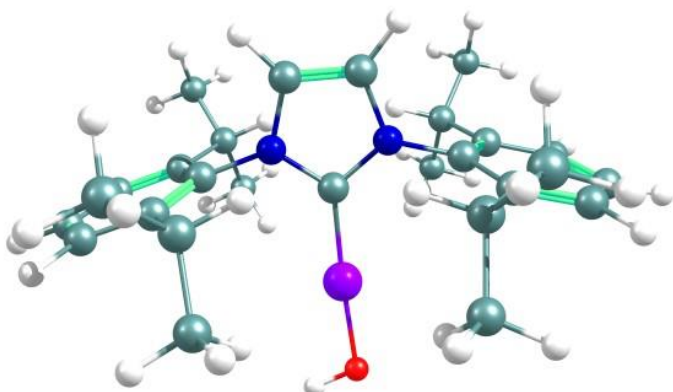
#### PhCCPh

	<p>Zero-point correction= 0.186056 (Hartree/Particle)            Thermal correction to Energy= 0.197410            Thermal correction to Enthalpy= 0.198354            Thermal correction to Gibbs Free Energy= 0.147419            Sum of electronic and zero-point Energies= -538.881794            Sum of electronic and thermal Energies= -538.870441            Sum of electronic and thermal Enthalpies= -538.869496            Sum of electronic and thermal Free Energies= -538.920432</p>	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr><td>6</td><td>0.000002000</td><td>-0.616839000</td><td>-0.000034000</td></tr> <tr><td>6</td><td>-0.000002000</td><td>0.616839000</td><td>-0.000034000</td></tr> <tr><td>6</td><td>0.000004000</td><td>-2.044448000</td><td>-0.000017000</td></tr> <tr><td>6</td><td>0.000272000</td><td>-2.771012000</td><td>-1.222759000</td></tr> <tr><td>6</td><td>-0.000268000</td><td>-2.770977000</td><td>1.222747000</td></tr> <tr><td>6</td><td>0.000274000</td><td>-4.172465000</td><td>-1.216816000</td></tr> <tr><td>1</td><td>0.000482000</td><td>-2.216621000</td><td>-2.173614000</td></tr> <tr><td>6</td><td>-0.000272000</td><td>-4.172431000</td><td>1.216844000</td></tr> <tr><td>1</td><td>-0.000480000</td><td>-2.216559000</td><td>2.173586000</td></tr> <tr><td>6</td><td>0.000002000</td><td>-4.879440000</td><td>0.000024000</td></tr> <tr><td>1</td><td>0.000485000</td><td>-4.720346000</td><td>-2.172649000</td></tr> <tr><td>1</td><td>-0.000484000</td><td>-4.720284000</td><td>2.172693000</td></tr> <tr><td>1</td><td>0.000000000</td><td>-5.980915000</td><td>0.000040000</td></tr> <tr><td>6</td><td>-0.000004000</td><td>2.044448000</td><td>-0.000017000</td></tr> <tr><td>6</td><td>-0.000272000</td><td>2.771012000</td><td>-1.222759000</td></tr> <tr><td>6</td><td>0.000268000</td><td>2.770977000</td><td>1.222747000</td></tr> <tr><td>6</td><td>-0.000274000</td><td>4.172465000</td><td>-1.216816000</td></tr> <tr><td>1</td><td>-0.000482000</td><td>2.216621000</td><td>-2.173614000</td></tr> <tr><td>6</td><td>0.000272000</td><td>4.172431000</td><td>1.216844000</td></tr> <tr><td>1</td><td>0.000480000</td><td>2.216559000</td><td>2.173586000</td></tr> <tr><td>6</td><td>-0.000002000</td><td>4.879440000</td><td>0.000024000</td></tr> <tr><td>1</td><td>-0.000485000</td><td>4.720346000</td><td>-2.172649000</td></tr> <tr><td>1</td><td>0.000484000</td><td>4.720284000</td><td>2.172693000</td></tr> <tr><td>1</td><td>0.000000000</td><td>5.980915000</td><td>0.000040000</td></tr> </table>	6	0.000002000	-0.616839000	-0.000034000	6	-0.000002000	0.616839000	-0.000034000	6	0.000004000	-2.044448000	-0.000017000	6	0.000272000	-2.771012000	-1.222759000	6	-0.000268000	-2.770977000	1.222747000	6	0.000274000	-4.172465000	-1.216816000	1	0.000482000	-2.216621000	-2.173614000	6	-0.000272000	-4.172431000	1.216844000	1	-0.000480000	-2.216559000	2.173586000	6	0.000002000	-4.879440000	0.000024000	1	0.000485000	-4.720346000	-2.172649000	1	-0.000484000	-4.720284000	2.172693000	1	0.000000000	-5.980915000	0.000040000	6	-0.000004000	2.044448000	-0.000017000	6	-0.000272000	2.771012000	-1.222759000	6	0.000268000	2.770977000	1.222747000	6	-0.000274000	4.172465000	-1.216816000	1	-0.000482000	2.216621000	-2.173614000	6	0.000272000	4.172431000	1.216844000	1	0.000480000	2.216559000	2.173586000	6	-0.000002000	4.879440000	0.000024000	1	-0.000485000	4.720346000	-2.172649000	1	0.000484000	4.720284000	2.172693000	1	0.000000000	5.980915000	0.000040000
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#### PhOH

	<p>Zero-point correction= 0.101760 (Hartree/Particle)            Thermal correction to Energy= 0.107379            Thermal correction to Enthalpy= 0.108323            Thermal correction to Gibbs Free Energy= 0.072713            Sum of electronic and zero-point Energies= -307.146137            Sum of electronic and thermal Energies= -307.140517            Sum of electronic and thermal Enthalpies= -307.139573            Sum of electronic and thermal Free Energies= -307.175184</p>	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr><td>6</td><td>0.954476000</td><td>-0.027497000</td><td>0.000187000</td></tr> <tr><td>6</td><td>0.221164000</td><td>-1.234028000</td><td>0.000095000</td></tr> <tr><td>6</td><td>0.268261000</td><td>1.206180000</td><td>0.000019000</td></tr> <tr><td>6</td><td>-1.180870000</td><td>-1.197322000</td><td>-0.000016000</td></tr> <tr><td>1</td><td>0.771878000</td><td>-2.187010000</td><td>0.000159000</td></tr> <tr><td>6</td><td>-1.136832000</td><td>1.228971000</td><td>0.000007000</td></tr> <tr><td>1</td><td>0.839898000</td><td>2.150706000</td><td>-0.000146000</td></tr> <tr><td>6</td><td>-1.870580000</td><td>0.030263000</td><td>-0.000039000</td></tr> <tr><td>1</td><td>-1.743585000</td><td>-2.144767000</td><td>-0.000042000</td></tr> <tr><td>1</td><td>-1.659913000</td><td>2.198785000</td><td>-0.000070000</td></tr> <tr><td>1</td><td>-2.971167000</td><td>0.051554000</td><td>-0.000178000</td></tr> <tr><td>8</td><td>2.318184000</td><td>-0.112678000</td><td>-0.000297000</td></tr> <tr><td>1</td><td>2.683709000</td><td>0.792754000</td><td>0.001142000</td></tr> </table>	6	0.954476000	-0.027497000	0.000187000	6	0.221164000	-1.234028000	0.000095000	6	0.268261000	1.206180000	0.000019000	6	-1.180870000	-1.197322000	-0.000016000	1	0.771878000	-2.187010000	0.000159000	6	-1.136832000	1.228971000	0.000007000	1	0.839898000	2.150706000	-0.000146000	6	-1.870580000	0.030263000	-0.000039000	1	-1.743585000	-2.144767000	-0.000042000	1	-1.659913000	2.198785000	-0.000070000	1	-2.971167000	0.051554000	-0.000178000	8	2.318184000	-0.112678000	-0.000297000	1	2.683709000	0.792754000	0.001142000
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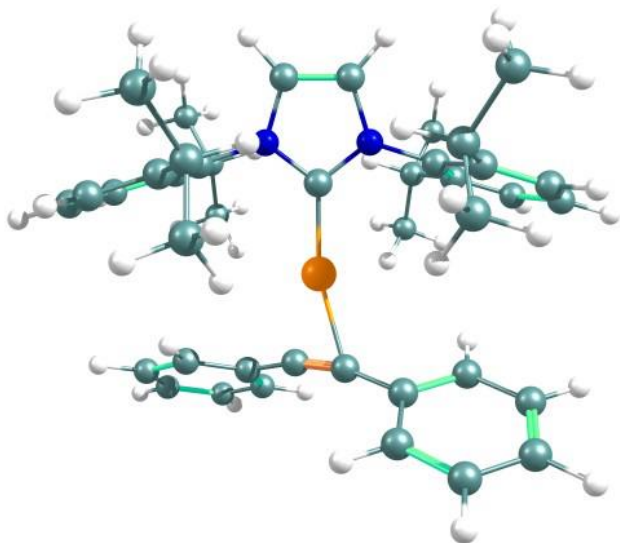
# I [Au(OH)(IPr)]



Zero-point correction= 0.565396 (Hartree/Particle)  
 Thermal correction to Energy= 0.600785  
 Thermal correction to Enthalpy= 0.601730  
 Thermal correction to Gibbs Free Energy= 0.494345  
 Sum of electronic and zero-point Energies= -1370.341437  
 Sum of electronic and thermal Energies= -1370.306047  
 Sum of electronic and thermal Enthalpies= -1370.305103  
 Sum of electronic and thermal Free Energies= -1370.412488

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7	-1.077757000	0.041050000	-1.256054000
6	0.701235000	0.090690000	-2.583303000
6	-0.668589000	0.082041000	-2.589736000
6	2.481793000	0.043263000	-0.817911000
6	-2.462995000	0.024056000	-0.834815000
1	1.427467000	0.117663000	-3.401374000
1	-1.387128000	0.100757000	-3.414871000
6	3.140512000	-1.206243000	-0.673174000
6	4.497334000	-1.184728000	-0.289517000
6	5.167997000	0.024450000	-0.059188000
6	4.489811000	1.242950000	-0.202151000
6	3.132712000	1.283234000	-0.583233000
6	2.424357000	-2.542137000	-0.872108000
1	5.036187000	-2.137036000	-0.163342000
1	6.228111000	0.016935000	0.240561000
1	5.022634000	2.187291000	-0.008007000
6	2.406963000	2.624487000	-0.686399000
6	-3.130023000	1.262662000	-0.641755000
6	-4.485559000	1.217594000	-0.256518000
6	-5.146610000	-0.004115000	-0.068733000
6	-4.460339000	-1.211317000	-0.258939000
6	-3.104224000	-1.228429000	-0.645113000
6	-2.422529000	2.609457000	-0.791384000
1	-5.030243000	2.160721000	-0.091952000
1	-6.205034000	-0.015395000	0.236597000
1	-4.985353000	-2.165846000	-0.096226000
6	-2.374502000	-2.561904000	-0.806451000
1	1.405495000	-2.323786000	-1.254697000
6	2.255827000	-3.275996000	0.476768000
6	3.126154000	-3.430993000	-1.920072000
1	1.392984000	2.428097000	-1.092880000
6	2.220201000	3.250263000	0.713624000
6	3.109414000	3.595762000	-1.657658000
1	-1.404003000	2.412684000	-1.186540000
6	-3.134232000	3.533480000	-1.801465000
6	-2.251555000	3.291231000	0.584240000
1	-1.350655000	-2.342386000	-1.174892000
6	-2.224727000	-3.274738000	0.555811000
6	-3.053473000	-3.471086000	-1.852534000
1	1.681629000	-4.216451000	0.339528000
1	3.240106000	-3.543511000	0.916924000
1	1.712651000	-2.643162000	1.209469000
1	2.552271000	-4.367948000	-2.079354000
1	3.219486000	-2.916839000	-2.899285000
1	4.147555000	-3.722702000	-1.595906000
1	1.637410000	4.192956000	0.644946000
1	1.677883000	2.556291000	1.389765000
1	3.198288000	3.492023000	1.181785000
1	2.525147000	4.534580000	-1.756855000
1	4.122856000	3.875995000	-1.300160000
1	3.221502000	3.154382000	-2.669868000
1	-2.565894000	4.478622000	-1.929495000
1	-3.231307000	3.055142000	-2.798335000
1	-4.155035000	3.807665000	-1.460709000
1	-1.681875000	4.238923000	0.481124000
1	-3.234823000	3.537353000	1.038641000
1	-1.705401000	2.632420000	1.291056000
1	-1.643928000	-4.214183000	0.440522000
1	-1.698151000	-2.629905000	1.290263000
1	-3.214223000	-3.541984000	0.983947000
1	-2.473545000	-4.408431000	-1.985960000
1	-4.079514000	-3.760504000	-1.541218000
1	-3.131572000	-2.973538000	-2.841641000
79	-0.018034000	-0.062176000	1.568881000
1	0.758225000	-0.187207000	3.923464000
8	-0.150573000	-0.183463000	3.561940000

## II [Cu(PhCCPh)(IPr)]<sup>+</sup>



Zero-point correction= 0.740841 (Hartree/Particle)  
 Thermal correction to Energy= 0.787238  
 Thermal correction to Enthalpy= 0.788182  
 Thermal correction to Gibbs Free Energy= 0.653023  
 Sum of electronic and zero-point Energies= -1894.864172  
 Sum of electronic and thermal Energies= -1894.817775  
 Sum of electronic and thermal Enthalpies= -1894.816831  
 Sum of electronic and thermal Free Energies= -1894.951991

6	0.000124000	-1.177682000	0.000107000
7	-1.012716000	-2.015386000	-0.391186000
7	1.013091000	-2.015289000	0.391249000
6	-0.640378000	-3.348090000	-0.247144000
6	0.640982000	-3.348032000	0.246936000
6	-2.306613000	-1.578112000	-0.882414000
6	2.306984000	-1.577918000	0.882410000
1	-1.314157000	-4.170783000	-0.506432000
1	1.314878000	-4.170662000	0.506120000
6	-2.452782000	-1.319540000	-2.271943000
6	-3.727531000	-0.913618000	-2.719818000
6	-4.802689000	-0.781543000	-1.829173000
6	-4.626345000	-1.050920000	-0.464524000
6	-3.375671000	-1.457833000	0.045323000
6	-1.308125000	-1.483911000	-3.272836000
1	-3.882944000	-0.708587000	-3.790700000
1	-5.791298000	-0.473891000	-2.204937000
1	-5.480556000	-0.949467000	0.223058000
6	-3.221433000	-1.761187000	1.536429000
6	2.453312000	-1.319630000	2.271970000
6	3.728074000	-0.913674000	2.719776000
6	4.803112000	-0.781313000	1.829031000
6	4.626621000	-1.050437000	0.464351000
6	3.375922000	-1.457353000	-0.045430000
6	1.308711000	-1.483936000	3.272940000
1	3.883582000	-0.708846000	3.790683000
1	5.791738000	-0.473644000	2.204736000
1	5.480741000	-0.948789000	-0.223317000
6	3.221589000	-1.760555000	-1.536557000
1	-0.404933000	-1.795973000	-2.707421000
6	-0.966710000	-0.150332000	-3.971515000
6	-1.613296000	-2.596489000	-4.299837000
1	-2.163778000	-2.046759000	1.718386000
6	-3.510174000	-0.516520000	2.402351000
6	-4.098767000	-2.959154000	1.961686000
1	0.405876000	-1.797555000	2.707814000
6	1.614588000	-2.594897000	4.301439000
6	0.966061000	-0.149684000	3.969768000
1	2.163819000	-2.045689000	-1.718547000
6	3.510876000	-0.515988000	-2.402447000
6	4.098456000	-2.958857000	-1.961825000
1	-0.102678000	-0.279364000	-4.655785000
1	-1.816937000	0.225135000	-4.578706000
1	-0.703676000	0.638049000	-3.235040000
1	-0.748193000	-2.747145000	-4.978420000
1	-1.830013000	-3.564560000	-3.803324000
1	-2.489974000	-2.340543000	-4.930848000
1	-3.338482000	-0.742703000	3.475167000
1	-2.858636000	0.336474000	2.120523000
1	-4.563236000	-0.181302000	2.299049000
1	-3.930499000	-3.203667000	3.030982000
1	-5.179490000	-2.737649000	1.837629000
1	-3.873953000	-3.866690000	1.364545000
1	0.749365000	-2.745466000	4.979886000
1	1.832342000	-3.563393000	3.806210000
1	2.490765000	-2.337431000	4.932532000
1	0.102139000	-0.278497000	4.654223000
1	1.816007000	0.227381000	4.576372000
1	0.702345000	0.637417000	3.232159000
1	3.339073000	-0.742075000	-3.475265000
1	2.859734000	0.337300000	-2.120606000
1	4.564094000	-0.181255000	-2.299160000
1	3.930150000	-3.203250000	-3.031144000
1	5.179261000	-2.737791000	-1.837690000
1	3.873247000	-3.866333000	-1.364743000
29	-0.000088000	0.725615000	0.000230000
6	-0.610880000	2.678822000	0.155353000
6	0.610452000	2.678831000	-0.154819000
6	-1.939252000	3.004420000	0.612088000
6	-2.108256000	3.657887000	1.863003000
6	-3.076296000	2.717706000	-0.188454000

	6	-3.390485000	4.028733000	2.288955000
	1	-1.226041000	3.880476000	2.481912000
	6	-4.352227000	3.098216000	0.249429000
	1	-2.946602000	2.205352000	-1.153768000
	6	-4.512514000	3.752798000	1.484687000
	1	-3.515663000	4.544047000	3.253870000
	1	-5.229409000	2.884457000	-0.380229000
	1	-5.517011000	4.051925000	1.822578000
	6	1.938663000	3.004776000	-0.611817000
	6	3.076020000	2.717868000	0.188202000
	6	2.107148000	3.658751000	-1.862538000
	6	4.351756000	3.098680000	-0.249993000
	1	2.946727000	2.205136000	1.153369000
	6	3.389187000	4.029888000	-2.288811000
	1	1.224688000	3.881491000	-2.481042000
	6	4.511534000	3.753750000	-1.485056000
	1	5.229186000	2.884771000	0.379269000
	1	3.513964000	4.545592000	-3.253569000
	1	5.515879000	4.053105000	-1.823195000

### III [(IPr)Cu(OH)Au(IPr)]

	79	-1.652397000	-0.400502000	-0.111949000
	8	0.301535000	-1.076293000	-0.344852000
	1	0.272861000	-2.046375000	-0.447003000
	29	2.060552000	-0.470389000	-0.178673000
	6	-3.543426000	0.137036000	0.072780000
	7	-4.631415000	-0.678621000	-0.113798000
	6	-5.814389000	0.028349000	0.089356000
	1	-6.794712000	-0.447159000	-0.012293000
	6	-5.458974000	1.313177000	0.410512000
	1	-6.064790000	2.193240000	0.647160000
	7	-4.065717000	1.362721000	0.396854000
	6	-4.574748000	-2.082741000	-0.476574000
	6	-4.571935000	-2.426457000	-1.854463000
	6	-4.536231000	-3.799529000	-2.174833000
	1	-4.532435000	-4.106624000	-3.232614000
	6	-4.509570000	-4.779712000	-1.172917000
	1	-4.486024000	-5.845820000	-1.448577000
	6	-4.518121000	-4.407319000	0.178560000
	1	-4.500331000	-5.187388000	0.955928000
	6	-4.552874000	-3.050496000	0.562386000
	6	-4.596427000	-1.383477000	-2.972587000
	1	-4.652642000	-0.379746000	-2.501076000
	6	-3.293905000	-1.422805000	-3.800913000
	1	-2.403498000	-1.267482000	-3.156470000
	1	-3.301413000	-0.627943000	-4.575564000
	1	-3.172362000	-2.395675000	-4.321979000
	6	-5.843296000	-1.536751000	-3.870264000
	1	-6.782358000	-1.481598000	-3.282016000
	1	-5.843454000	-2.506852000	-4.410147000
	1	-5.871705000	-0.732901000	-4.634974000
	6	-4.551136000	-2.677266000	2.045460000
	1	-4.635293000	-1.572485000	2.118570000
	6	-5.761404000	-3.278406000	2.791434000
	1	-5.770367000	-2.943200000	3.849422000
	1	-5.730497000	-4.388108000	2.797026000
	1	-6.722207000	-2.973361000	2.328173000
	6	-3.217710000	-3.074685000	2.715249000
	1	-3.204092000	-2.754080000	3.777813000
	1	-2.355790000	-2.601060000	2.200448000
	1	-3.064752000	-4.174298000	2.695454000
	6	-3.298678000	2.559006000	0.686472000

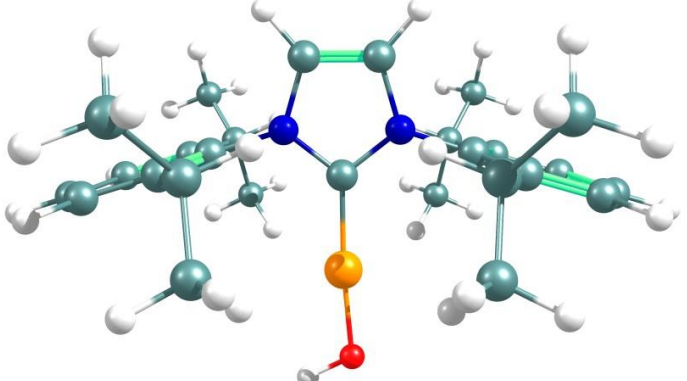
  

Zero-point correction=	1.121686
(Hartree/Particle)	
Thermal correction to Energy=	1.191946
Thermal correction to Enthalpy=	1.192890
Thermal correction to Gibbs Free Energy=	1.005238
Sum of electronic and zero-point Energies=	-2726.365190
Sum of electronic and thermal Energies=	-2726.294930
Sum of electronic and thermal Enthalpies=	-2726.293986
Sum of electronic and thermal Free Energies=	-
2726.481638	

6	-2.957085000	2.833174000	2.037282000
6	-2.241042000	4.021291000	2.291188000
1	-1.958714000	4.269528000	3.326174000
6	-1.888659000	4.893050000	1.251195000
1	-1.336183000	5.819174000	1.475331000
6	-2.244032000	4.594695000	-0.071448000
1	-1.964928000	5.291136000	-0.877812000
6	-2.961406000	3.422674000	-0.388753000
6	-3.310485000	1.890442000	3.188587000
1	-3.987085000	1.105589000	2.789814000
6	-2.047894000	1.175106000	3.717991000
1	-1.537442000	0.611346000	2.909060000
1	-2.313927000	0.459410000	4.523767000
1	-1.320879000	1.901248000	4.138914000
6	-4.070331000	2.610840000	4.322219000
1	-4.982397000	3.118853000	3.947064000
1	-3.440346000	3.376590000	4.821294000
1	-4.379968000	1.883724000	5.101223000
6	-3.340427000	3.128044000	-1.840665000
1	-3.933758000	2.189622000	-1.853090000
6	-2.086275000	2.881775000	-2.706510000
1	-2.376742000	2.622376000	-3.745934000
1	-1.474332000	2.049454000	-2.301012000
1	-1.441468000	3.784219000	-2.754618000
6	-4.231524000	4.239134000	-2.436103000
1	-4.545098000	3.973816000	-3.467150000
1	-3.694622000	5.209161000	-2.493322000
1	-5.147784000	4.399074000	-1.831282000
6	3.859650000	-0.035357000	-0.040887000
7	4.871410000	-0.912851000	0.272650000
6	6.108283000	-0.272871000	0.277157000
1	7.037335000	-0.805478000	0.502985000
6	5.872098000	1.040683000	-0.041157000
1	6.552921000	1.890346000	-0.152240000
7	4.497413000	1.166775000	-0.231108000
6	4.675930000	-2.322260000	0.551964000
6	4.773147000	-3.245859000	-0.523219000
6	4.579058000	-4.610087000	-0.222397000
1	4.645174000	-5.355330000	-1.030596000
6	4.307481000	-5.034195000	1.086100000
1	4.163337000	-6.105524000	1.297336000
6	4.226283000	-4.099168000	2.127506000
1	4.018633000	-4.445838000	3.151996000
6	4.410880000	-2.721206000	1.889317000
6	5.057636000	-2.813809000	-1.962519000
1	5.252251000	-1.720834000	-1.956125000
6	3.827333000	-3.050792000	-2.865120000
1	2.937302000	-2.509280000	-2.480880000
1	3.569562000	-4.129135000	-2.925768000
1	4.024852000	-2.695055000	-3.897788000
6	6.318084000	-3.497937000	-2.533218000
1	7.207731000	-3.313908000	-1.896530000
1	6.540181000	-3.113076000	-3.550180000
1	6.188222000	-4.597220000	-2.618077000
6	4.312320000	-1.726418000	3.046400000
1	4.548088000	-0.717665000	2.647237000
6	5.342164000	-2.031238000	4.155159000
1	6.377703000	-2.051457000	3.757656000
1	5.149714000	-3.012339000	4.637772000
1	5.295993000	-1.257745000	4.949690000
6	2.875173000	-1.665587000	3.608260000
1	2.145232000	-1.392023000	2.817374000
1	2.804574000	-0.909064000	4.417538000
1	2.562445000	-2.641868000	4.035133000
6	3.839685000	2.410814000	-0.577660000
6	3.462550000	3.290960000	0.471284000
6	2.846815000	4.505707000	0.105387000
1	2.543617000	5.213857000	0.892628000
6	2.619515000	4.828122000	-1.239744000
1	2.142347000	5.785519000	-1.502242000
6	3.006161000	3.939683000	-2.252929000
1	2.826096000	4.207825000	-3.305796000
6	3.629432000	2.711153000	-1.949933000
6	3.710178000	2.974848000	1.947035000
1	4.165434000	1.964134000	2.005522000

	6	2.391216000	2.924105000	2.747043000
	1	1.682704000	2.187525000	2.315535000
	1	1.883987000	3.911523000	2.761619000
	1	2.588480000	2.636857000	3.800930000
	6	4.712197000	3.968012000	2.575328000
	1	4.926073000	3.692711000	3.629134000
	1	4.312673000	5.004042000	2.575736000
	1	5.675237000	3.982950000	2.024725000
	6	4.040495000	1.763911000	-3.078023000
	1	4.585241000	0.910914000	-2.621487000
	6	5.006394000	2.438076000	-4.075711000
	1	5.906182000	2.841025000	-3.567061000
	1	4.522071000	3.278124000	-4.616487000
	1	5.344711000	1.707490000	-4.839560000
	6	2.802442000	1.182962000	-3.795251000
	1	2.135352000	0.651155000	-3.084552000
	1	3.109237000	0.462866000	-4.582337000
	1	2.206390000	1.981301000	-4.285333000

## IV [Cu(OH)(IPr)]

	6	0.007088000	-0.000088000	-0.075555000
	7	1.095429000	-0.000118000	-0.926105000
	7	-1.076292000	-0.000250000	-0.932298000
	6	0.698501000	-0.000388000	-2.264321000
	6	-0.672241000	-0.000449000	-2.267863000
	6	2.474200000	0.000095000	-0.488622000
	6	-2.458140000	-0.000177000	-0.502630000
	1	1.421937000	-0.000464000	-3.085561000
	1	-1.391301000	-0.000583000	-3.092939000
	6	3.127147000	-1.245098000	-0.287674000
	6	4.475962000	-1.214219000	0.122665000
	6	5.145856000	0.000518000	0.324694000
	6	4.475394000	1.215037000	0.123279000
	6	3.126572000	1.245484000	-0.287093000
	6	2.409175000	-2.584224000	-0.456207000
1	5.009025000	-2.163039000	0.292992000	
1	6.199352000	0.000679000	0.647049000	
1	5.007996000	2.164030000	0.294098000	
6	2.408081000	2.584383000	-0.455205000	
6	-3.112123000	1.245040000	-0.305835000	
6	-4.467381000	1.214315000	0.082245000	
6	-5.141538000	-0.000026000	0.270554000	
6	-4.467352000	-1.214439000	0.082818000	
6	-3.112093000	-1.245318000	-0.305249000	
6	-2.389865000	2.584323000	-0.450968000	
1	-5.001174000	2.163336000	0.248861000	
1	-6.199832000	0.000033000	0.576593000	
1	-5.001123000	-2.163395000	0.249880000	
6	-2.389855000	-2.584669000	-0.449843000	
1	1.408035000	-2.375699000	-0.887623000	
6	2.181778000	-3.256908000	0.915678000	
6	3.143668000	-3.522778000	-1.435780000	
1	1.406748000	2.375531000	-0.886007000	
6	2.181259000	3.257123000	0.916732000	
6	3.141771000	3.523041000	-1.435303000	
1	-1.370913000	2.375822000	-0.838536000	
6	-3.085017000	3.515993000	-1.465496000	
6	-2.222602000	3.264436000	0.926310000	
1	-1.370793000	-2.376316000	-0.837197000	
6	-2.222969000	-3.264470000	0.927633000	

Zero-point correction= 0.565162 (Hartree/Particle)  
 Thermal correction to Energy= 0.600528  
 Thermal correction to Enthalpy= 0.601472  
 Thermal correction to Gibbs Free Energy= 0.494536  
 Sum of electronic and zero-point Energies= -1431.922688  
 Sum of electronic and thermal Energies= -1431.887321  
 Sum of electronic and thermal Enthalpies= -1431.886377  
 Sum of electronic and thermal Free Energies= -1431.993313

	6	-3.084821000	-3.516534000	-1.464323000
	1	1.611246000	-4.202207000	0.797509000
	1	3.145877000	-3.503917000	1.409306000
	1	1.609451000	-2.592216000	1.596460000
	1	2.565612000	-4.459397000	-1.581303000
	1	3.284219000	-3.049930000	-2.430005000
	1	4.146896000	-3.812079000	-1.057278000
	1	1.610345000	4.202218000	0.798781000
	1	1.609514000	2.592314000	1.597887000
	1	3.145528000	3.504535000	1.409826000
	1	2.563457000	4.459549000	-1.580519000
	1	4.145194000	3.812502000	-1.057444000
	1	3.281776000	3.050156000	-2.429588000
	1	-2.507474000	4.456369000	-1.587557000
	1	-3.177736000	3.039870000	-2.463803000
	1	-4.106306000	3.798415000	-1.132843000
	1	-1.640428000	4.205025000	0.828051000
	1	-3.206925000	3.523029000	1.371539000
	1	-1.691549000	2.601825000	1.641413000
	1	-1.640828000	-4.205115000	0.829721000
	1	-1.692033000	-2.601733000	1.642708000
	1	-3.207407000	-3.522915000	1.372691000
	1	-2.507329000	-4.456990000	-1.586006000
	1	-4.106223000	-3.798769000	-1.131857000
	1	-3.177245000	-3.040650000	-2.462772000
	29	-0.018107000	0.000060000	1.770653000
	1	0.689827000	0.000153000	3.983656000
	8	-0.187128000	0.000107000	3.553983000

## V [Au(PhCCPh)(IPr)]

	6	-0.000202000	-1.411872000	0.000160000
	7	-1.053044000	-2.239443000	-0.278790000
	7	1.052467000	-2.239600000	0.279316000
	6	-0.664001000	-3.572228000	-0.174731000
	6	0.663145000	-3.572328000	0.175582000
	6	-2.394380000	-1.803186000	-0.625150000
	6	2.393930000	-1.803520000	0.625423000
	1	-1.362662000	-4.394060000	-0.359750000
	1	1.361630000	-4.394266000	0.360794000
	6	-2.683262000	-1.520100000	-1.987159000
	6	-4.001352000	-1.119871000	-2.292407000
	6	-4.982177000	-1.024880000	-1.294619000
	6	-4.664786000	-1.319708000	0.039052000
	6	-3.362361000	-1.714021000	0.410830000
	6	-1.646813000	-1.645097000	-3.104891000
	1	-4.267083000	-0.893020000	-3.336814000
	1	-6.008140000	-0.725938000	-1.561662000
	1	-5.446328000	-1.246701000	0.811384000
	6	-3.050621000	-2.039782000	1.872339000
	6	2.683047000	-1.520144000	1.987322000
	6	4.001276000	-1.120175000	2.292306000
	6	4.982004000	-1.025678000	1.294372000
	6	4.664364000	-1.320721000	-0.039192000
	6	3.361793000	-1.714804000	-0.410704000
	6	1.646703000	-1.644575000	3.105216000
	1	4.267193000	-0.893117000	3.336621000
	1	6.008072000	-0.726919000	1.561219000
	1	5.445815000	-1.248082000	-0.811650000
	6	3.049768000	-2.040768000	-1.872104000
	1	-0.698155000	-2.001826000	-2.651329000
	6	-1.353129000	-0.277222000	-3.757737000
	6	-2.073158000	-2.693921000	-4.155422000
	1	-1.963215000	-2.251289000	1.949602000
	6	-3.344620000	-0.843480000	2.802232000
	6	-3.799692000	-3.309508000	2.334535000
	1	0.697820000	-2.000911000	2.651819000
	6	2.072741000	-2.693501000	4.155767000
	6	1.353734000	-0.276512000	3.757991000
	1	1.962284000	-2.251947000	-1.949180000
	6	3.344011000	-0.844731000	-2.802261000
	6	3.798382000	-3.310817000	-2.334140000
	1	-0.569547000	-0.377677000	-4.536956000

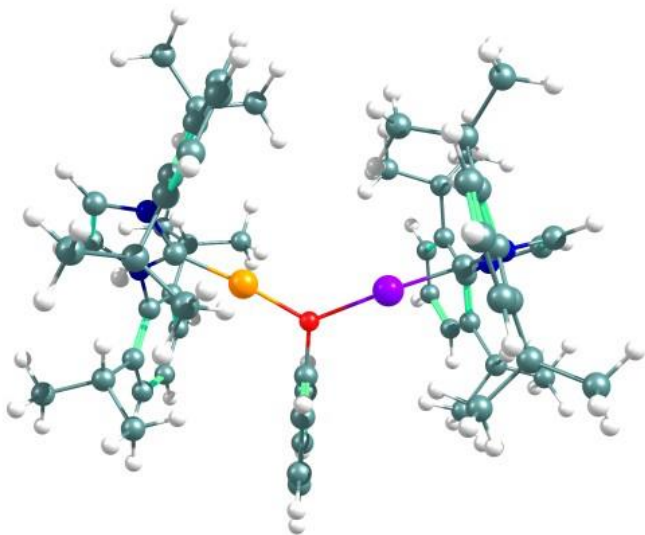
Zero-point correction=	0.740376 (Hartree/Particle)
Thermal correction to Energy=	0.786913
Thermal correction to Enthalpy=	0.787857
Thermal correction to Gibbs Free Energy=	0.652947
Sum of electronic and zero-point Energies=	-1833.283807
Sum of electronic and thermal Energies=	-1833.237270
Sum of electronic and thermal Enthalpies=	-1833.236326
Sum of electronic and thermal Free Energies=	-1833.371237

	1	-2.256336000	0.144807000	-4.246178000
	1	-0.996766000	0.460427000	-3.007851000
	1	-1.280636000	-2.819748000	-4.921948000
	1	-2.261931000	-3.684611000	-3.693240000
	1	-3.000075000	-2.389645000	-4.684887000
	1	-3.038193000	-1.079398000	3.842312000
	1	-2.799002000	0.067086000	2.479810000
	1	-4.426691000	-0.597534000	2.826988000
	1	-3.528447000	-3.562625000	3.380383000
	1	-4.899949000	-3.165627000	2.300388000
	1	-3.558951000	-4.185681000	1.697783000
	1	1.280320000	-2.818838000	4.922480000
	1	2.260908000	-3.684342000	3.693660000
	1	2.999929000	-2.389639000	4.684997000
	1	0.570176000	-0.376546000	4.537287000
	1	2.257188000	0.145115000	4.246321000
	1	0.997665000	0.461258000	3.008089000
	1	3.037367000	-1.080739000	-3.842257000
	1	2.798718000	0.066057000	-2.479919000
	1	4.426153000	-0.599122000	-2.827208000
	1	3.526923000	-3.564063000	-3.379902000
	1	4.898690000	-3.167274000	-2.300165000
	1	3.557449000	-4.186785000	-1.697177000
	79	0.000114000	0.614989000	-0.000007000
	6	-0.628135000	2.757328000	0.079098000
	6	0.628887000	2.757130000	-0.079354000
	6	-1.972470000	3.164156000	0.404480000
	6	-2.154880000	4.319982000	1.212189000
	6	-3.106855000	2.465254000	-0.083005000
	6	-3.448973000	4.764900000	1.512200000
	1	-1.275807000	4.859023000	1.596332000
	6	-4.395450000	2.920162000	0.229249000
	1	-2.968511000	1.571571000	-0.710988000
	6	-4.570209000	4.067958000	1.023663000
	1	-3.584173000	5.662802000	2.134944000
	1	-5.271142000	2.375855000	-0.155911000
	1	-5.584730000	4.422818000	1.263255000
	6	1.973248000	3.163819000	-0.404832000
	6	3.107624000	2.464221000	0.081645000
	6	2.155674000	4.320254000	-1.211679000
	6	4.396229000	2.919013000	-0.230768000
	1	2.969325000	1.570078000	0.708986000
	6	3.449769000	4.765043000	-1.511854000
	1	1.276605000	4.859856000	-1.595045000
	6	4.571006000	4.067383000	-1.024338000
	1	5.271911000	2.374142000	0.153616000
	1	3.584971000	5.663408000	-2.133930000
	1	5.585532000	4.422131000	-1.264073000

## VI [(IPr)Cu(OPh)Au(IPr)]

	79	-1.617821000	-0.226520000	-0.281334000
	8	0.326841000	-0.643382000	-0.962420000
	29	1.983774000	-0.065933000	-0.274810000
	6	-3.484131000	0.090839000	0.288715000
	7	-4.261244000	-0.734156000	1.061741000
	6	-5.542423000	-0.207258000	1.204395000
	1	-6.314589000	-0.718051000	1.787732000
	6	-5.567153000	0.972751000	0.505427000
	1	-6.365107000	1.705671000	0.351815000
	7	-4.300645000	1.139627000	-0.050017000
	6	-3.830446000	-1.992141000	1.643033000
	6	-4.010306000	-3.182560000	0.889638000
	6	-3.602903000	-4.391337000	1.491453000
	1	-3.728679000	-5.336361000	0.940403000
	6	-3.044795000	-4.412043000	2.777308000
	1	-2.736018000	-5.369224000	3.226281000
	6	-2.885970000	-3.219173000	3.496462000
	1	-2.453278000	-3.250168000	4.508928000
	6	-3.278326000	-1.979323000	2.950804000
	6	-4.644046000	-3.198117000	-0.502467000
	1	-4.771562000	-2.144694000	-0.829925000





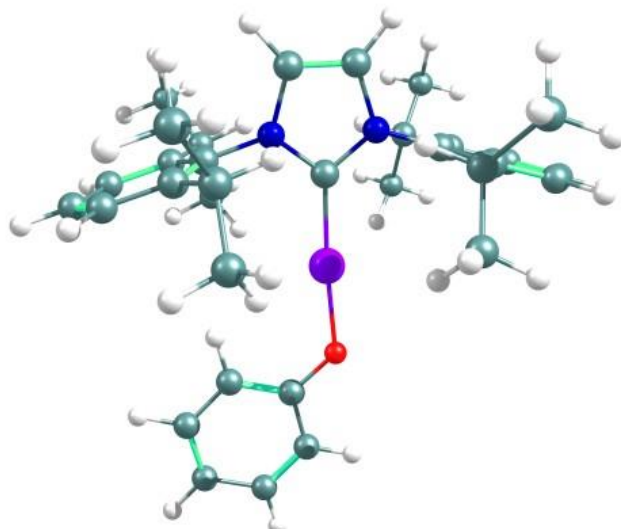
Zero-point correction= 1.200056  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.275065  
 Thermal correction to Enthalpy= 1.276009  
 Thermal correction to Gibbs Free Energy= 1.076457  
 Sum of electronic and zero-point Energies= -2957.157275  
 Sum of electronic and thermal Energies= -2957.082266  
 Sum of electronic and thermal Enthalpies= -2957.081322  
 Sum of electronic and thermal Free Energies= -  
 2957.280874

6	-3.741113000	-3.887879000	-1.546066000
1	-2.735732000	-3.421371000	-1.591465000
1	-4.197600000	-3.816811000	-2.555039000
1	-3.605247000	-4.967235000	-1.324656000
6	-6.048004000	-3.842533000	-0.461254000
1	-6.720009000	-3.323307000	0.252853000
1	-5.992938000	-4.907531000	-0.152201000
1	-6.523022000	-3.808375000	-1.463838000
6	-3.113414000	-0.698097000	3.769323000
1	-3.464859000	0.150925000	3.145915000
6	-3.987065000	-0.725529000	5.042528000
1	-3.900374000	0.233460000	5.594501000
1	-3.675314000	-1.536881000	5.733205000
1	-5.058223000	-0.885901000	4.802306000
6	-1.632412000	-0.427854000	4.108272000
1	-1.529971000	0.528959000	4.661455000
1	-1.014140000	-0.363876000	3.189143000
1	-1.207266000	-1.228794000	4.748825000
6	-3.921301000	2.269485000	-0.878050000
6	-3.415326000	3.432622000	-0.240493000
6	-3.063003000	4.518345000	-1.068284000
1	-2.663685000	5.437419000	-0.611826000
6	-3.214623000	4.448832000	-2.460391000
1	-2.934669000	5.310393000	-3.086919000
6	-3.729486000	3.289752000	-3.057400000
1	-3.850598000	3.251682000	-4.151289000
6	-4.101525000	2.171137000	-2.282872000
6	-3.224645000	3.524770000	1.273660000
1	-3.687497000	2.627630000	1.731088000
6	-1.724934000	3.501623000	1.639239000
1	-1.232500000	2.586277000	1.249427000
1	-1.591683000	3.524770000	2.741007000
1	-1.189485000	4.376747000	1.215201000
6	-3.934701000	4.757304000	1.876971000
1	-5.015297000	4.772068000	1.626328000
1	-3.493181000	5.709228000	1.514605000
1	-3.840721000	4.752744000	2.982870000
6	-4.662607000	0.922493000	-2.964283000
1	-4.970537000	0.210744000	-2.169312000
6	-3.582095000	0.217547000	-3.811947000
1	-3.986669000	-0.710639000	-4.266486000
1	-2.702153000	-0.059241000	-3.193864000
1	-3.226774000	0.868298000	-4.638627000
6	-5.921616000	1.240230000	-3.799173000
1	-6.352064000	0.307607000	-4.219213000
1	-5.692334000	1.910466000	-4.654164000
1	-6.705258000	1.733562000	-3.188069000
6	3.696641000	0.412216000	0.271413000
7	4.767710000	-0.439943000	0.408786000
6	5.920760000	0.254433000	0.763877000
1	6.877863000	-0.252253000	0.921368000
6	5.571623000	1.577882000	0.852853000
1	6.161765000	2.465649000	1.100258000
7	4.213643000	1.655273000	0.551712000
6	4.719756000	-1.875658000	0.209128000
6	5.045889000	-2.394027000	-1.072475000
6	5.022269000	-3.795824000	-1.225524000
1	5.270622000	-4.234845000	-2.204404000
6	4.691449000	-4.638519000	-0.155448000
1	4.682646000	-5.730477000	-0.299270000
6	4.377115000	-4.096174000	1.098527000
1	4.123424000	-4.769849000	1.932189000
6	4.387809000	-2.702699000	1.314834000
6	5.433628000	-1.502134000	-2.252531000
1	5.285841000	-0.446197000	-1.942009000
6	4.529077000	-1.742577000	-3.478881000
1	3.457348000	-1.596501000	-3.232394000
1	4.643175000	-2.771165000	-3.880409000
1	4.794602000	-1.039876000	-4.296069000
6	6.926802000	-1.672274000	-2.611371000
1	7.585913000	-1.457368000	-1.745047000
1	7.211177000	-0.984877000	-3.435208000
1	7.146386000	-2.707324000	-2.948080000
6	4.044597000	-2.141285000	2.695496000
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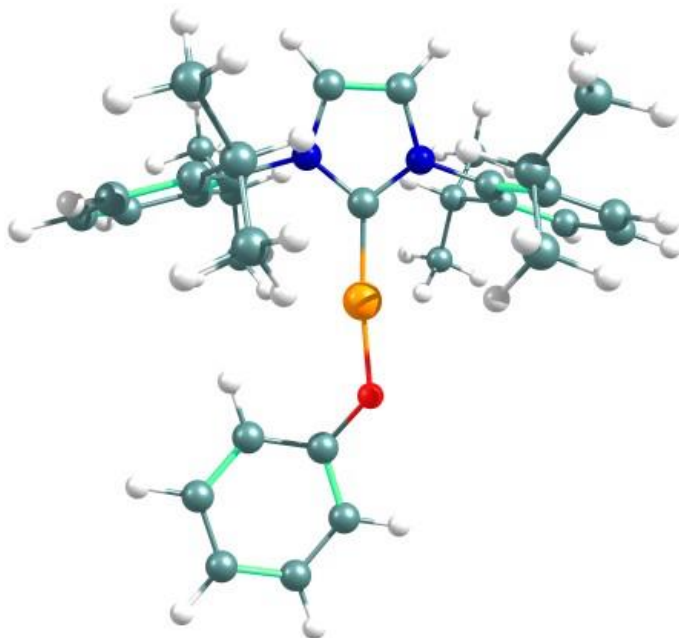
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	1	4.885049000	-3.779761000	3.918358000
	1	4.764653000	-2.210404000	4.766710000
	6	2.564337000	-2.400427000	3.049060000
	1	1.886342000	-1.961036000	2.287464000
	1	2.313654000	-1.951780000	4.032949000
	1	2.345339000	-3.487321000	3.110113000
	6	3.465780000	2.896412000	0.549599000
	6	2.980511000	3.393982000	1.788571000
	6	2.293207000	4.625394000	1.765570000
	1	1.905570000	5.045056000	2.707231000
	6	2.099535000	5.326586000	0.566954000
	1	1.565923000	6.290173000	0.574219000
	6	2.591987000	4.810048000	-0.639439000
	1	2.438210000	5.373793000	-1.573123000
	6	3.292635000	3.586431000	-0.679661000
	6	3.183442000	2.658489000	3.114716000
	1	3.731439000	1.717133000	2.900989000
	6	1.836322000	2.261472000	3.754539000
	1	1.231738000	1.633067000	3.068858000
	1	1.231478000	3.154273000	4.018178000
	1	2.005114000	1.686681000	4.688958000
	6	4.049326000	3.481406000	4.093497000
	1	4.235096000	2.908085000	5.025567000
	1	3.550729000	4.430856000	4.381048000
	1	5.033193000	3.742292000	3.652322000
	6	3.836419000	3.064464000	-2.009946000
	1	4.373930000	2.114339000	-1.808314000
	6	4.854715000	4.043738000	-2.632318000
	1	5.690930000	4.261530000	-1.936571000
	1	4.382086000	5.011434000	-2.902146000
	1	5.286291000	3.616085000	-3.561163000
	6	2.691662000	2.736591000	-2.992499000
	1	1.986789000	1.997963000	-2.555980000
	1	3.096639000	2.310901000	-3.934113000
	1	2.108546000	3.643470000	-3.258342000
	6	0.395188000	-1.627647000	-1.945025000
	6	0.391608000	-1.259876000	-3.306831000
	6	0.469396000	-2.989250000	-1.584239000
	6	0.461238000	-2.253550000	-4.299231000
	1	0.331346000	-0.193450000	-3.573642000
	6	0.539097000	-3.973957000	-2.584927000
	1	0.471189000	-3.260614000	-0.517136000
	6	0.534396000	-3.612870000	-3.944716000
	1	0.456702000	-1.959735000	-5.361086000
	1	0.598011000	-5.035511000	-2.296196000
	1	0.586712000	-4.387622000	-4.725086000

## VII [Au(OPh)(IPr)]

	6	-0.726063000	-0.795295000	0.004052000
	7	-2.090818000	-0.980186000	0.000273000
	7	-0.205422000	-2.069081000	0.002982000
	6	-2.409348000	-2.338242000	-0.003529000
	6	-1.222247000	-3.023482000	-0.001159000
	6	-3.073073000	0.084622000	-0.000737000
	6	1.207752000	-2.389389000	0.007472000
	1	-3.446014000	-2.688537000	-0.006740000
	1	-1.005985000	-4.096070000	-0.002003000
	6	-3.541245000	0.576437000	-1.247381000
	6	-4.517350000	1.593912000	-1.216613000
	6	-5.003295000	2.097753000	-0.002511000
	6	-4.518071000	1.595453000	1.212907000
	6	-3.542585000	0.577697000	1.245429000
	6	-3.016887000	0.065746000	-2.589916000
	1	-4.897940000	2.003412000	-2.165691000
	1	-5.763600000	2.894869000	-0.003227000
	1	-4.899687000	2.006961000	2.160570000
	6	-3.001026000	0.079166000	2.585470000
	6	1.867641000	-2.534892000	1.256178000
	6	3.236243000	-2.873859000	1.228853000
	6	3.915039000	-3.057653000	0.016355000
	6	3.237080000	-2.902437000	-1.200803000

 <p>           Zero-point correction= 0.644273 (Hartree/Particle)            Thermal correction to Energy= 0.684309            Thermal correction to Enthalpy= 0.685253            Thermal correction to Gibbs Free Energy= 0.566096            Sum of electronic and zero-point Energies= -1601.151247            Sum of electronic and thermal Energies= -1601.111211            Sum of electronic and thermal Enthalpies= -1601.110267            Sum of electronic and thermal Free Energies= -1601.229424         </p>	6	1.868099000	-2.566248000	-1.237088000
	6	1.161281000	-2.319855000	2.594927000
	1	3.781299000	-2.990232000	2.178761000
	1	4.984973000	-3.319669000	0.019821000
	1	3.783008000	-3.039756000	-2.147280000
	6	1.163782000	-2.370043000	-2.579864000
	1	-2.277964000	-0.735800000	-2.382107000
	6	-2.271631000	1.180832000	-3.354748000
	6	-4.142452000	-0.557620000	-3.443224000
	1	-2.345416000	-0.793181000	2.380342000
	6	-2.123035000	1.160773000	3.253015000
	6	-4.122745000	-0.405558000	3.526755000
	1	0.097545000	-2.084781000	2.381078000
	6	1.182822000	-3.594491000	3.465685000
	6	1.752665000	-1.108332000	3.347763000
	1	0.082339000	-2.223372000	-2.375355000
	6	1.671835000	-1.092532000	-3.284143000
	6	1.289494000	-3.609333000	-3.490861000
	1	-1.854929000	0.788350000	-4.306038000
	1	-2.949566000	2.023224000	-3.607802000
	1	-1.433451000	1.587438000	-2.751952000
	1	-3.731222000	-0.969588000	-4.388665000
	1	-4.656461000	-1.382033000	-2.906413000
	1	-4.912560000	0.194184000	-3.716820000
	1	-1.685686000	0.779576000	4.199709000
	1	-1.290621000	1.467421000	2.585459000
	1	-2.715261000	2.068467000	3.495283000
	1	-3.690325000	-0.828210000	4.457725000
	1	-4.797066000	0.424061000	3.826705000
	1	-4.746974000	-1.190832000	3.051922000
	1	0.615202000	-3.431567000	4.405857000
	1	0.730268000	-4.460244000	2.938844000
	1	2.218111000	-3.879061000	3.749802000
	1	1.193009000	-0.924315000	4.288843000
	1	2.816157000	-1.277609000	3.618939000
1	1.702833000	-0.187578000	2.730735000	
1	1.123968000	-0.927397000	-4.235693000	
1	1.529403000	-0.197609000	-2.643092000	
1	2.753059000	-1.167240000	-3.526341000	
1	0.708623000	-3.461903000	-4.425340000	
1	2.342874000	-3.799528000	-3.786527000	
1	0.910053000	-4.526052000	-2.993375000	
79	0.258892000	0.915452000	0.007418000	
6	2.454208000	2.984128000	-0.010646000	
6	3.453930000	1.971572000	-0.039812000	
6	2.889071000	4.340925000	-0.003737000	
6	4.818180000	2.303053000	-0.060120000	
1	3.129082000	0.916258000	-0.046671000	
6	4.254124000	4.658918000	-0.024361000	
1	2.120434000	5.129452000	0.018263000	
6	5.234469000	3.647249000	-0.052595000	
1	5.568406000	1.494537000	-0.082319000	
1	4.559738000	5.718910000	-0.018351000	
1	6.305512000	3.903475000	-0.068699000	
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## VIII [Cu(OPh)(IPr)]

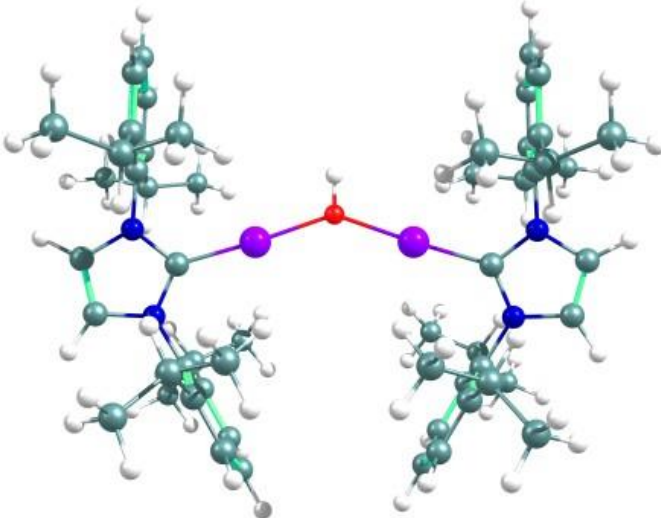


Zero-point correction= 0.644114 (Hartree/Particle)  
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 Thermal correction to Enthalpy= 0.685037  
 Thermal correction to Gibbs Free Energy= 0.565784  
 Sum of electronic and zero-point Energies= -1662.734983  
 Sum of electronic and thermal Energies= -1662.695004  
 Sum of electronic and thermal Enthalpies= -1662.694060  
 Sum of electronic and thermal Free Energies= -1662.813313

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8	0.832584000	-2.704418000	0.032510000
6	-0.576229000	0.671090000	0.007980000
7	0.026835000	1.910870000	0.015358000
6	-0.918350000	2.936095000	0.013400000
1	-0.628386000	3.991337000	0.019272000
6	-2.151184000	2.335335000	0.003882000
1	-3.160761000	2.757676000	-0.000646000
7	-1.925080000	0.959539000	0.000570000
6	1.457769000	2.129284000	0.023611000
6	2.124711000	2.228462000	1.273494000
6	3.514345000	2.467896000	1.250233000
1	4.063726000	2.543597000	2.201689000
6	4.207910000	2.603187000	0.039747000
1	5.293763000	2.788498000	0.046186000
6	3.524011000	2.495158000	-1.179021000
1	4.080927000	2.592314000	-2.124119000
6	2.134655000	2.256050000	-1.218547000
6	1.403428000	2.043642000	2.608654000
1	0.316444000	1.965803000	2.396752000
6	1.832536000	0.721121000	3.281993000
1	1.652813000	-0.147785000	2.614929000
1	1.264108000	0.558424000	4.221814000
1	2.912968000	0.730064000	3.538864000
6	1.599653000	3.249788000	3.550927000
1	1.274416000	4.199177000	3.076947000
1	2.662195000	3.370666000	3.850502000
1	1.010129000	3.112926000	4.481630000
6	1.423840000	2.098691000	-2.562901000
1	0.334775000	2.021819000	-2.361665000
6	1.633024000	3.320184000	-3.482210000
1	1.051625000	3.201722000	-4.420530000
1	2.698676000	3.442112000	-3.770031000
1	1.307037000	4.262508000	-2.994851000
6	1.852670000	0.786445000	-3.256269000
1	1.290694000	0.642851000	-4.203049000
1	1.664332000	-0.093244000	-2.606102000
1	2.935060000	0.795366000	-3.504826000
6	-2.973601000	-0.038278000	-0.013149000
6	-3.465020000	-0.492874000	-1.265634000
6	-4.504434000	-1.445726000	-1.248443000
1	-4.905680000	-1.821517000	-2.202985000
6	-5.028789000	-1.926859000	-0.041034000
1	-5.839365000	-2.672724000	-0.051892000
6	-4.518188000	-1.466327000	1.180257000
1	-4.930691000	-1.858643000	2.123277000
6	-3.479147000	-0.513886000	1.225785000
6	-2.897768000	-0.010136000	-2.600956000
1	-2.111970000	0.742321000	-2.381631000
6	-2.218866000	-1.167494000	-3.365260000
1	-1.420943000	-1.639000000	-2.755250000
1	-1.760910000	-0.796990000	-4.306350000
1	-2.949386000	-1.958568000	-3.636780000
6	-3.974104000	0.685678000	-3.461506000
1	-4.436768000	1.541304000	-2.926955000
1	-4.789637000	-0.014478000	-3.741113000
1	-3.530575000	1.070676000	-4.403745000
6	-2.927262000	-0.053430000	2.575280000
1	-2.140503000	0.703993000	2.377293000
6	-2.253858000	-1.222391000	3.326682000
1	-1.807032000	-0.867070000	4.278914000
1	-1.448110000	-1.681389000	2.717327000
1	-2.985155000	-2.019784000	3.576780000
6	-4.014039000	0.625469000	3.436177000
1	-3.581146000	0.995060000	4.389455000
1	-4.830810000	-0.081045000	3.695208000
1	-4.472920000	1.489177000	2.911467000
6	2.073671000	-3.188693000	-0.001136000
6	2.269838000	-4.600046000	0.050607000
6	3.237478000	-2.370231000	-0.088765000
6	3.557669000	-5.153278000	0.016893000
1	1.376578000	-5.241391000	0.118037000
6	4.521817000	-2.935107000	-0.121919000
1	3.104333000	-1.274923000	-0.130477000
6	4.698341000	-4.330760000	-0.069459000

	1	3.674190000	-6.249627000	0.058835000
	1	5.400927000	-2.271731000	-0.190166000
	1	5.707816000	-4.770528000	-0.095777000

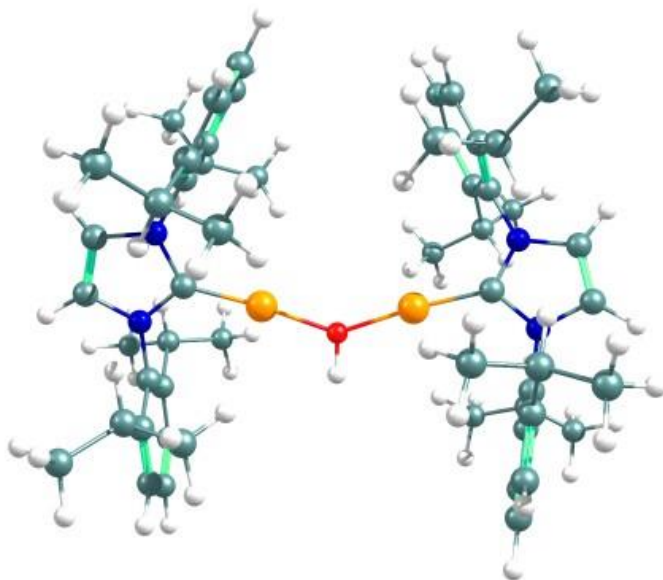
## IX [(IPr)Au(OH)Au(IPr)]

		79	-1.953001000	-0.449410000	-0.182734000
		8	-0.010430000	-1.137335000	-0.476214000
		1	-0.008880000	-2.112746000	-0.501234000
		79	1.933851000	-0.448827000	-0.194115000
		6	-3.834507000	0.106240000	0.043845000
		7	-4.912162000	-0.732511000	0.179229000
		6	-6.090845000	-0.000010000	0.300993000
		1	-7.063522000	-0.487718000	0.417197000
		6	-5.742811000	1.324854000	0.241405000
		1	-6.348206000	2.234752000	0.296546000
		7	-4.358629000	1.372968000	0.082927000
		6	-4.851084000	-2.182694000	0.186520000
		6	-4.973883000	-2.870493000	-1.049651000
		6	-4.924578000	-4.279541000	-1.010036000
		1	-5.016804000	-4.848378000	-1.948665000
		6	-4.764952000	-4.967051000	0.201164000
		1	-4.732823000	-6.067978000	0.207398000
		6	-4.652179000	-4.257964000	1.405376000
		1	-4.530881000	-4.810619000	2.350094000
		6	-4.694544000	-2.848509000	1.430875000
		6	-5.142774000	-2.150496000	-2.388157000
		1	-5.198739000	-1.060322000	-2.184497000
		6	-3.918908000	-2.378646000	-3.302027000
		1	-2.982412000	-2.039064000	-2.811701000
		1	-4.032573000	-1.816828000	-4.252498000
		1	-3.798905000	-3.451850000	-3.560415000
		6	-6.457389000	-2.550946000	-3.091986000
		1	-7.341207000	-2.365479000	-2.447437000
		1	-6.464107000	-3.626342000	-3.367540000
		1	-6.588714000	-1.969238000	-4.027974000
		6	-4.551658000	-2.103063000	2.758551000
		1	-4.711940000	-1.022245000	2.559960000
		6	-5.616542000	-2.540178000	3.786630000
		1	-5.527844000	-1.938087000	4.714687000
		1	-5.499039000	-3.606052000	4.073893000
		1	-6.645570000	-2.411114000	3.392563000
		6	-3.122215000	-2.254143000	3.324116000
		1	-3.010789000	-1.673619000	4.263685000
		1	-2.364612000	-1.887887000	2.599600000
		1	-2.888335000	-3.314870000	3.555049000
		6	-3.603207000	2.606629000	-0.019973000
		6	-3.133891000	3.211644000	1.175466000
		6	-2.435968000	4.430281000	1.049185000
		1	-2.058018000	4.930405000	1.954575000
		6	-2.223294000	5.018167000	-0.205451000
		1	-1.682444000	5.974734000	-0.279047000
		6	-2.702683000	4.396708000	-1.366947000
		1	-2.531487000	4.871155000	-2.346070000
		6	-3.406084000	3.175851000	-1.305638000
		6	-3.355998000	2.597804000	2.558655000
		1	-3.955778000	1.672874000	2.427587000
		6	-2.017809000	2.181644000	3.206009000
		1	-1.466959000	1.462727000	2.564728000
		1	-2.194683000	1.701509000	4.190981000
		1	-1.359290000	3.059277000	3.374604000
		6	-4.162355000	3.538570000	3.479760000
		1	-5.137718000	3.816796000	3.030157000
		1	-3.610992000	4.479026000	3.690167000
		1	-4.363666000	3.048084000	4.454821000
		6	-3.905078000	2.515343000	-2.591356000
		1	-4.487831000	1.614025000	-2.307143000
		6	-2.722657000	2.032970000	-3.459470000
		1	-3.093280000	1.510227000	-4.365809000
		1	-2.072702000	1.330674000	-2.896793000
		1	-2.093669000	2.883361000	-3.797194000
		6	-4.852929000	3.439652000	-3.384928000
		1	-5.245461000	2.914461000	-4.280272000

Zero-point correction= 1.121813  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.192101  
 Thermal correction to Enthalpy= 1.193045  
 Thermal correction to Gibbs Free Energy= 1.003533  
 Sum of electronic and zero-point Energies= -2664.779405  
 Sum of electronic and thermal Energies= -2664.709117  
 Sum of electronic and thermal Enthalpies= -2664.708173  
 Sum of electronic and thermal Free Energies= -2664.897685

	1	-4.333661000	4.354115000	-3.740550000
	1	-5.718993000	3.763797000	-2.771836000
	6	3.819652000	0.092735000	0.026224000
	7	4.896044000	-0.758480000	0.056990000
	6	6.081607000	-0.044618000	0.213752000
	1	7.054089000	-0.544162000	0.259876000
	6	5.739896000	1.281243000	0.283886000
	1	6.352723000	2.180096000	0.402491000
	7	4.352092000	1.348871000	0.167683000
	6	4.825941000	-2.204322000	-0.051322000
	6	4.926746000	-2.793095000	-1.339585000
	6	4.872066000	-4.200630000	-1.409803000
	1	4.947511000	-4.694760000	-2.391170000
	6	4.726477000	-4.981144000	-0.254372000
	1	4.689312000	-6.078994000	-0.334630000
	6	4.633300000	-4.368711000	1.003356000
	1	4.521881000	-4.993612000	1.903426000
	6	4.682844000	-2.965887000	1.139060000
	6	5.084590000	-1.970661000	-2.619320000
	1	5.114390000	-0.898318000	-2.332629000
	6	3.872994000	-2.153852000	-3.559079000
	1	2.924857000	-1.876186000	-3.053263000
	1	3.779463000	-3.204690000	-3.905259000
	1	3.981619000	-1.515445000	-4.460487000
	6	6.412167000	-2.289702000	-3.340532000
	1	7.288340000	-2.130087000	-2.678815000
	1	6.534602000	-1.640606000	-4.232396000
	1	6.444639000	-3.342955000	-3.690083000
	6	4.584424000	-2.329902000	2.526179000
	1	4.644542000	-1.228278000	2.400125000
	6	5.763297000	-2.752508000	3.429621000
	1	6.742210000	-2.503615000	2.970512000
	1	5.755549000	-3.844816000	3.628115000
	1	5.705649000	-2.236862000	4.410824000
	6	3.224233000	-2.635007000	3.189866000
	1	2.381912000	-2.292385000	2.553492000
	1	3.146558000	-2.121189000	4.170615000
	1	3.092989000	-3.722271000	3.372726000
	6	3.603080000	2.590021000	0.214630000
	6	3.200480000	3.086130000	1.482684000
	6	2.511465000	4.316465000	1.502441000
	1	2.185979000	4.736507000	2.467042000
	6	2.242221000	5.016950000	0.318579000
	1	1.709120000	5.979784000	0.359997000
	6	2.656959000	4.501358000	-0.917219000
	1	2.442268000	5.063512000	-1.839269000
	6	3.351269000	3.276856000	-1.002149000
	6	3.506507000	2.360560000	2.793919000
	1	3.992491000	1.394540000	2.542651000
	6	2.220275000	2.027438000	3.578371000
	1	1.516443000	1.427745000	2.965666000
	1	1.690269000	2.946781000	3.904747000
	1	2.463589000	1.445953000	4.491904000
	6	4.501871000	3.164592000	3.659487000
	1	4.760154000	2.602564000	4.581148000
	1	4.072613000	4.139795000	3.972095000
	1	5.444485000	3.375459000	3.113559000
	6	3.781512000	2.731633000	-2.364116000
	1	4.427072000	1.845834000	-2.185644000
	6	4.621072000	3.749825000	-3.163666000
	1	5.508333000	4.090116000	-2.591108000
	1	4.031736000	4.650267000	-3.436593000
	1	4.979299000	3.294669000	-4.110250000
	6	2.557418000	2.245824000	-3.171125000
	1	1.985157000	1.478926000	-2.607612000
	1	2.877634000	1.798918000	-4.135443000
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**X [(IPr)Cu(OH)Cu(IPr)]**



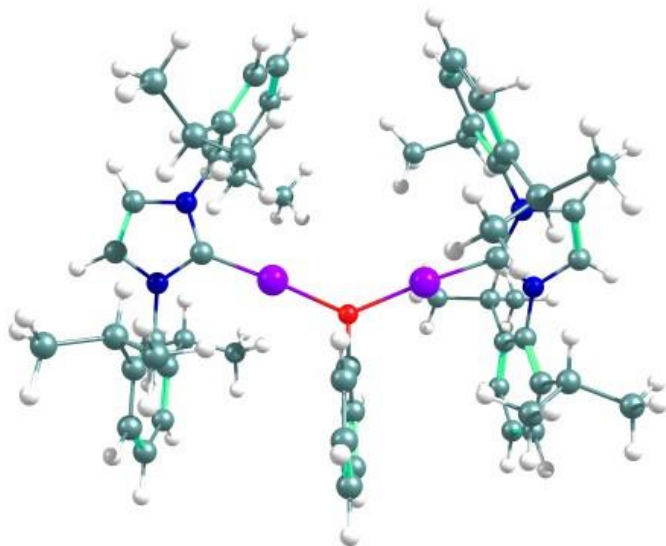
Zero-point correction= 1.121235  
 (Hartree/Particle)  
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 Thermal correction to Enthalpy= 1.192429  
 Thermal correction to Gibbs Free Energy= 1.003817  
 Sum of electronic and zero-point Energies= -2787.950520  
 Sum of electronic and thermal Energies= -2787.880271  
 Sum of electronic and thermal Enthalpies= -2787.879326  
 Sum of electronic and thermal Free Energies= -2788.067938

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8	-0.015617000	-1.032063000	-0.242764000
1	-0.027933000	-2.006083000	-0.313261000
29	1.755181000	-0.451347000	-0.137009000
6	-3.560847000	0.057980000	0.033683000
7	-4.621216000	-0.777299000	-0.231538000
6	-5.836130000	-0.122873000	-0.044302000
1	-6.796348000	-0.622823000	-0.204997000
6	-5.536423000	1.156893000	0.348700000
1	-6.181453000	2.004648000	0.599937000
7	-4.146423000	1.248326000	0.391813000
6	-4.494633000	-2.161282000	-0.645126000
6	-4.434547000	-2.454213000	-2.033853000
6	-4.330527000	-3.811428000	-2.403872000
1	-4.282449000	-4.077010000	-3.471717000
6	-4.290310000	-4.827219000	-1.438612000
1	-4.212604000	-5.880202000	-1.752212000
6	-4.354304000	-4.506534000	-0.075293000
1	-4.325168000	-5.313968000	0.673180000
6	-4.462472000	-3.168215000	0.356663000
6	-4.470310000	-1.370795000	-3.112641000
1	-4.566337000	-0.389091000	-2.603102000
6	-3.152657000	-1.338229000	-3.916859000
1	-2.277033000	-1.183043000	-3.252360000
1	-3.170550000	-0.513533000	-4.659521000
1	-2.991481000	-2.284769000	-4.474513000
6	-5.694749000	-1.528485000	-4.039900000
1	-6.645598000	-1.522100000	-3.468385000
1	-5.655515000	-2.478642000	-4.612891000
1	-5.733319000	-0.698968000	-4.776255000
6	-4.525844000	-2.852855000	1.851949000
1	-4.696817000	-1.761397000	1.962281000
6	-5.703050000	-3.571576000	2.544737000
1	-5.767173000	-3.270023000	3.610896000
1	-5.584230000	-4.675126000	2.521453000
1	-6.672257000	-3.328953000	2.062595000
6	-3.182261000	-3.173145000	2.542729000
1	-3.222330000	-2.905870000	3.619318000
1	-2.347740000	-2.605158000	2.079862000
1	-2.937606000	-4.254104000	2.474159000
6	-3.429156000	2.449585000	0.770021000
6	-3.140460000	2.664148000	2.143996000
6	-2.470568000	3.858221000	2.483625000
1	-2.233320000	4.062216000	3.539641000
6	-2.107516000	4.791677000	1.502695000
1	-1.592232000	5.720787000	1.793394000
6	-2.405448000	4.550210000	0.154234000
1	-2.116939000	5.292578000	-0.606379000
6	-3.077483000	3.377016000	-0.246545000
6	-3.523909000	1.665101000	3.236705000
1	-4.047910000	0.816156000	2.749507000
6	-2.273481000	1.086451000	3.933188000
1	-1.593109000	0.598693000	3.204542000
1	-2.566178000	0.329300000	4.690285000
1	-1.697021000	1.876592000	4.458521000
6	-4.503240000	2.283406000	4.257846000
1	-5.418209000	2.672004000	3.765299000
1	-4.038881000	3.125285000	4.812962000
1	-4.814146000	1.524729000	5.005807000
6	-3.387387000	3.139816000	-1.724995000
1	-4.006321000	2.220967000	-1.797593000
6	-2.093401000	2.880134000	-2.526568000
1	-2.329818000	2.659972000	-3.588537000
1	-1.529247000	2.017824000	-2.113592000
1	-1.419151000	3.762049000	-2.507506000
6	-4.210948000	4.292629000	-2.336972000
1	-4.482457000	4.058762000	-3.387375000
1	-3.641750000	5.245768000	-2.349205000
1	-5.149886000	4.470050000	-1.773330000
6	3.561212000	-0.033250000	-0.033150000
7	4.558256000	-0.910452000	0.326652000
6	5.806483000	-0.294140000	0.294570000
1	6.726254000	-0.829829000	0.549219000
6	5.593398000	1.003813000	-0.095257000
1	6.289075000	1.834007000	-0.252294000

	7	4.220595000	1.144409000	-0.291041000
	6	4.336686000	-2.298643000	0.681572000
	6	4.412145000	-3.280098000	-0.342984000
	6	4.193441000	-4.622509000	0.030726000
	1	4.243701000	-5.410855000	-0.736942000
	6	3.916724000	-4.970668000	1.360325000
	1	3.752275000	-6.026133000	1.628870000
	6	3.856071000	-3.979789000	2.350339000
	1	3.643565000	-4.267443000	3.391964000
	6	4.067026000	-2.620409000	2.038533000
	6	4.710775000	-2.933313000	-1.802207000
	1	4.862164000	-1.835332000	-1.866149000
	6	3.516593000	-3.279260000	-2.717534000
	1	2.594438000	-2.753639000	-2.392109000
	1	3.304615000	-4.369207000	-2.719226000
	1	3.728904000	-2.979968000	-3.765034000
	6	6.012088000	-3.603954000	-2.293004000
	1	6.878165000	-3.332792000	-1.654861000
	1	6.242347000	-3.290713000	-3.332547000
	1	5.929070000	-4.711097000	-2.290941000
	6	3.991606000	-1.563545000	3.141053000
	1	4.237359000	-0.581247000	2.685790000
	6	5.026699000	-1.823005000	4.256255000
	1	6.058556000	-1.877825000	3.852511000
	1	4.825523000	-2.774717000	4.791445000
	1	4.997206000	-1.008179000	5.009205000
	6	2.560431000	-1.452732000	3.710075000
	1	1.827203000	-1.217467000	2.910005000
	1	2.505827000	-0.649376000	4.474128000
	1	2.240327000	-2.398467000	4.196120000
	6	3.593307000	2.381672000	-0.711723000
	6	3.212287000	3.320457000	0.283431000
	6	2.644933000	4.534242000	-0.157221000
	1	2.341658000	5.288221000	0.586167000
	6	2.466978000	4.799707000	-1.522054000
	1	2.029495000	5.758333000	-1.842885000
	6	2.851429000	3.851756000	-2.480813000
	1	2.708688000	4.073815000	-3.550000000
	6	3.426568000	2.620826000	-2.101988000
	6	3.391373000	3.061531000	1.779989000
	1	3.865844000	2.064893000	1.898067000
	6	2.028490000	3.003262000	2.502754000
	1	1.367564000	2.230314000	2.058912000
	1	1.494562000	3.974687000	2.443393000
	1	2.167957000	2.763166000	3.577479000
	6	4.332819000	4.097704000	2.430747000
	1	4.493936000	3.858095000	3.502463000
	1	3.911047000	5.123513000	2.380036000
	1	5.324397000	4.119793000	1.933683000
	6	3.825103000	1.601361000	-3.170191000
	1	4.356821000	0.769595000	-2.661937000
	6	4.797632000	2.197365000	-4.209722000
	1	5.703136000	2.621423000	-3.729217000
	1	4.322072000	3.005995000	-4.803174000
	1	5.125046000	1.414749000	-4.925126000
	6	2.575501000	0.997150000	-3.847727000
	1	1.903899000	0.519144000	-3.103772000
	1	2.868675000	0.227376000	-4.591839000
	1	1.989809000	1.774838000	-4.381622000

**XI [(IPr)Au(OPh)Au(IPr)]**



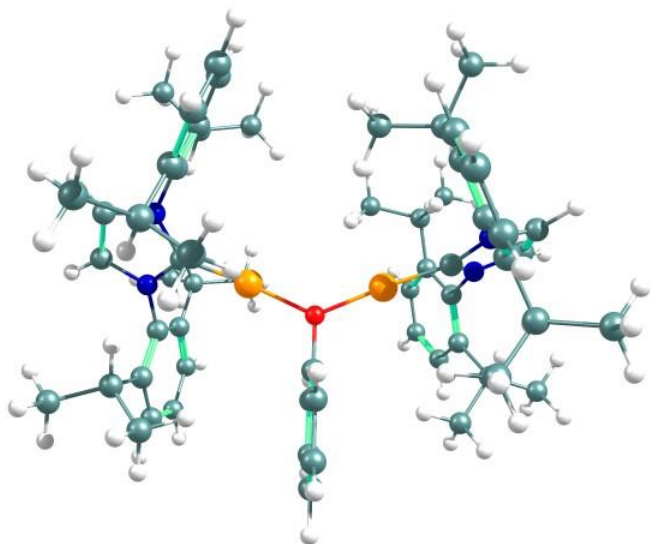


Zero-point correction= 1.200026  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.275126  
 Thermal correction to Enthalpy= 1.276070  
 Thermal correction to Gibbs Free Energy= 1.074768  
 Sum of electronic and zero-point Energies= -2895.571595  
 Sum of electronic and thermal Energies= -2895.496495  
 Sum of electronic and thermal Enthalpies= -2895.495551  
 Sum of electronic and thermal Free Energies= -2895.696853

79	-1.900095000	-0.300499000	-0.129265000
8	0.015168000	-1.084911000	-0.488658000
79	1.904564000	-0.251124000	-0.120302000
6	-3.758095000	0.311727000	0.149213000
7	-4.780311000	-0.434042000	0.680303000
6	-5.968696000	0.291765000	0.675923000
1	-6.902540000	-0.128848000	1.061179000
6	-5.684217000	1.516689000	0.128966000
1	-6.318037000	2.387825000	-0.063167000
7	-4.327086000	1.512682000	-0.188521000
6	-4.663663000	-1.796029000	1.169946000
6	-4.895149000	-2.864207000	0.263464000
6	-4.800254000	-4.174362000	0.777350000
1	-4.971481000	-5.029612000	0.105181000
6	-4.492596000	-4.406684000	2.124882000
1	-4.427539000	-5.439167000	2.502912000
6	-4.270464000	-3.329240000	2.993885000
1	-4.030750000	-3.525638000	4.050693000
6	-4.352260000	-1.996380000	2.540723000
6	-5.234732000	-2.646861000	-1.211468000
1	-5.237387000	-1.553154000	-1.403321000
6	-4.162123000	-3.265622000	-2.132784000
1	-3.151298000	-2.869936000	-1.902316000
1	-4.388305000	-3.040148000	-3.195769000
1	-4.122098000	-4.370054000	-2.029544000
6	-6.646180000	-3.173828000	-1.551009000
1	-7.425235000	-2.703607000	-0.916076000
1	-6.716689000	-4.272411000	-1.406935000
1	-6.895791000	-2.961447000	-2.611431000
6	-4.092133000	-0.843390000	3.511227000
1	-4.287396000	0.107433000	2.971791000
6	-5.045143000	-0.883629000	4.725132000
1	-4.878216000	-0.001390000	5.377419000
1	-4.880512000	-1.788711000	5.346350000
1	-6.109533000	-0.881214000	4.412185000
6	-2.612878000	-0.817252000	3.955073000
1	-2.422458000	0.047378000	4.624776000
1	-1.932995000	-0.734679000	3.081240000
1	-2.340379000	-1.738615000	4.511755000
6	-3.645397000	2.633670000	-0.807298000
6	-3.122935000	3.651920000	0.032859000
6	-2.502671000	4.750378000	-0.596630000
1	-2.086164000	5.560789000	0.021481000
6	-2.411649000	4.830510000	-1.993497000
1	-1.929203000	5.702166000	-2.463215000
6	-2.940538000	3.809520000	-2.794812000
1	-2.868075000	3.887606000	-3.890960000
6	-3.575238000	2.686564000	-2.224121000
6	-3.179521000	3.568950000	1.558605000
1	-3.864572000	2.737455000	1.827903000
6	-1.788121000	3.216454000	2.129154000
1	-1.404288000	2.268590000	1.696973000
1	-1.834261000	3.101827000	3.232403000
1	-1.048037000	4.011058000	1.898305000
6	-3.747440000	4.850002000	2.202476000
1	-4.747741000	5.105870000	1.796746000
1	-3.084394000	5.725330000	2.039504000
1	-3.847900000	4.717139000	3.299637000
6	-4.148880000	1.595283000	-3.128650000
1	-4.639814000	0.838173000	-2.481858000
6	-3.027932000	0.869847000	-3.904172000
1	-3.448651000	0.044807000	-4.515796000
1	-2.277717000	0.435875000	-3.210329000
1	-2.497240000	1.560642000	-4.592601000
6	-5.229933000	2.150461000	-4.080926000
1	-5.674291000	1.330240000	-4.682101000
1	-4.809732000	2.891517000	-4.792986000
1	-6.050279000	2.648759000	-3.524445000
6	3.733100000	0.429122000	0.197495000
7	4.871052000	-0.336371000	0.257689000
6	5.990973000	0.465252000	0.462898000
1	6.996943000	0.041618000	0.539854000
6	5.545354000	1.759503000	0.534339000
1	6.080826000	2.701674000	0.685760000
7	4.161532000	1.721295000	0.369735000

6	4.927222000	-1.781496000	0.133622000
6	5.127321000	-2.342776000	-1.155065000
6	5.210407000	-3.748007000	-1.238103000
1	5.362979000	-4.222084000	-2.220338000
6	5.102706000	-4.551282000	-0.094545000
1	5.170970000	-5.646735000	-0.185271000
6	4.910609000	-3.965128000	1.164237000
1	4.830548000	-4.608385000	2.054606000
6	4.820417000	-2.565707000	1.312887000
6	5.256900000	-1.494774000	-2.420906000
1	5.135519000	-0.429965000	-2.130746000
6	4.137638000	-1.818321000	-3.433289000
1	3.133645000	-1.700981000	-2.975686000
1	4.215036000	-2.859930000	-3.809311000
1	4.202534000	-1.142655000	-4.311601000
6	6.655647000	-1.639753000	-3.058970000
1	7.462908000	-1.371189000	-2.346735000
1	6.748772000	-0.978908000	-3.945912000
1	6.842411000	-2.680263000	-3.398189000
6	4.622442000	-1.956301000	2.701566000
1	4.589196000	-0.852216000	2.586971000
6	5.806200000	-2.282558000	3.638114000
1	6.773059000	-1.946904000	3.209621000
1	5.886880000	-3.373035000	3.830172000
1	5.675385000	-1.781655000	4.619921000
6	3.275757000	-2.388852000	3.320372000
1	2.424137000	-2.113172000	2.664312000
1	3.125428000	-1.899812000	4.305550000
1	3.236776000	-3.486272000	3.484338000
6	3.329390000	2.909211000	0.410989000
6	2.888561000	3.376315000	1.677488000
6	2.135127000	4.568493000	1.696802000
1	1.780443000	4.966280000	2.660650000
6	1.840414000	5.260365000	0.513745000
1	1.260199000	6.195698000	0.555012000
6	2.289886000	4.771629000	-0.720894000
1	2.053667000	5.325909000	-1.642294000
6	3.050523000	3.587199000	-0.804945000
6	3.203481000	2.651397000	2.986858000
1	3.810485000	1.754551000	2.742452000
6	1.916744000	2.148372000	3.675492000
1	1.335715000	1.481315000	3.005997000
1	1.256689000	2.990270000	3.972941000
1	2.166160000	1.580444000	4.595975000
6	4.046569000	3.529962000	3.936411000
1	4.319338000	2.962719000	4.850547000
1	3.489197000	4.433528000	4.261281000
1	4.985644000	3.872206000	3.454854000
6	3.520864000	3.072464000	-2.165526000
1	4.227160000	2.234971000	-1.983997000
6	4.286519000	4.145715000	-2.966895000
1	5.147273000	4.549203000	-2.394969000
1	3.634814000	5.001147000	-3.242354000
1	4.676500000	3.714857000	-3.912252000
6	2.333829000	2.500651000	-2.972093000
1	1.821639000	1.691445000	-2.409304000
1	2.683964000	2.081924000	-3.938691000
1	1.581550000	3.286249000	-3.195498000
6	0.008209000	-2.337613000	-1.100399000
6	0.107156000	-2.437201000	-2.503128000
6	-0.108112000	-3.501579000	-0.314850000
6	0.092460000	-3.703323000	-3.114295000
1	0.187654000	-1.516433000	-3.101590000
6	-0.120732000	-4.762303000	-0.936262000
1	-0.190158000	-3.402022000	0.778261000
6	-0.019662000	-4.869403000	-2.335366000
1	0.168470000	-3.777120000	-4.210917000
1	-0.210629000	-5.669852000	-0.318243000
1	-0.029943000	-5.858929000	-2.817878000

## XII [(IPr)Cu(OPh)Cu(IPr)]

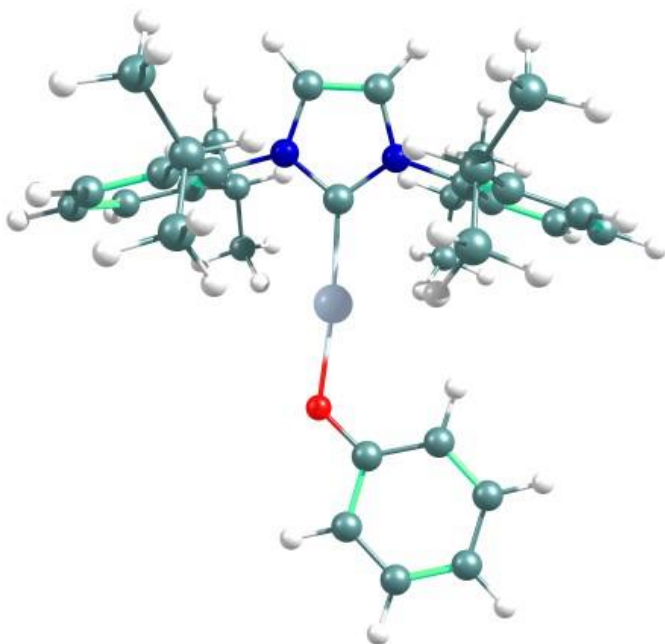


Zero-point correction= 1.200141  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.274937  
 Thermal correction to Enthalpy= 1.275881  
 Thermal correction to Gibbs Free Energy= 1.077794  
 Sum of electronic and zero-point Energies= -3018.742286  
 Sum of electronic and thermal Energies= -3018.667491  
 Sum of electronic and thermal Enthalpies= -3018.666546  
 Sum of electronic and thermal Free Energies= -3018.864634

29	-1.732354000	-0.213161000	-0.245804000
8	-0.001306000	-0.627037000	-0.874796000
29	1.704449000	-0.099517000	-0.266921000
6	-3.483112000	0.108331000	0.297895000
7	-4.274552000	-0.696992000	1.083050000
6	-5.544094000	-0.149106000	1.244957000
1	-6.318386000	-0.643843000	1.839396000
6	-5.556538000	1.030782000	0.544523000
1	-6.343674000	1.777724000	0.402130000
7	-4.294154000	1.170003000	-0.026532000
6	-3.859707000	-1.963794000	1.653582000
6	-4.090580000	-3.151437000	0.908897000
6	-3.695666000	-4.369948000	1.499693000
1	-3.860726000	-5.311605000	0.953184000
6	-3.101664000	-4.404497000	2.769010000
1	-2.803988000	-5.368886000	3.210035000
6	-2.893649000	-3.215507000	3.481918000
1	-2.433883000	-3.256673000	4.482060000
6	-3.270692000	-1.966670000	2.945802000
6	-4.762135000	-3.152874000	-0.465474000
1	-4.884181000	-2.096249000	-0.784215000
6	-3.894590000	-3.849550000	-1.534203000
1	-2.882478000	-3.399974000	-1.599837000
1	-4.372222000	-3.765040000	-2.532311000
1	-3.770598000	-4.932317000	-1.321975000
6	-6.172502000	-3.779468000	-0.390921000
1	-6.818444000	-3.255658000	0.343495000
1	-6.123828000	-4.847070000	-0.089729000
1	-6.673250000	-3.732883000	-1.380416000
6	-3.055264000	-0.690339000	3.760351000
1	-3.385529000	0.168396000	3.139045000
6	-3.914507000	-0.689898000	5.043553000
1	-3.789239000	0.264436000	5.596343000
1	-3.622982000	-1.513448000	5.728693000
1	-4.993055000	-0.812842000	4.814873000
6	-1.563075000	-0.466092000	4.082449000
1	-1.423671000	0.489721000	4.629168000
1	-0.952534000	-0.426800000	3.156568000
1	-1.155293000	-1.276447000	4.722439000
6	-3.903384000	2.286773000	-0.864547000
6	-3.328721000	3.428555000	-0.245999000
6	-2.965727000	4.502808000	-1.084111000
1	-2.513214000	5.403792000	-0.641501000
6	-3.175519000	4.445373000	-2.469331000
1	-2.888190000	5.298439000	-3.104121000
6	-3.758934000	3.309863000	-3.048180000
1	-3.927062000	3.282780000	-4.136306000
6	-4.141621000	2.202666000	-2.262147000
6	-3.079003000	3.508355000	1.260350000
1	-3.583971000	2.639603000	1.732691000
6	-1.572234000	3.383867000	1.572250000
1	-1.153691000	2.439698000	1.163738000
1	-1.396323000	3.392373000	2.668179000
1	-0.994579000	4.222505000	1.130309000
6	-3.682972000	4.780841000	1.889659000
1	-4.767374000	4.870166000	1.673695000
1	-3.189111000	5.702430000	1.516556000
1	-3.554688000	4.764185000	2.991936000
6	-4.804689000	0.991552000	-2.919140000
1	-4.978565000	0.230388000	-2.129730000
6	-3.891726000	0.341784000	-3.979952000
1	-4.378093000	-0.558225000	-4.410245000
1	-2.920812000	0.027492000	-3.544476000
1	-3.680266000	1.036337000	-4.820032000
6	-6.182566000	1.361342000	-3.511579000
1	-6.681122000	0.461419000	-3.928095000
1	-6.087361000	2.100312000	-4.334720000
1	-6.854784000	1.800224000	-2.745787000
6	3.454667000	0.323545000	0.201795000
7	4.501091000	-0.567326000	0.266684000
6	5.694904000	0.079268000	0.573281000
1	6.640696000	-0.462583000	0.670457000
6	5.397700000	1.411440000	0.706030000
1	6.031480000	2.273183000	0.936571000
7	4.029256000	1.542197000	0.478791000

6	4.392549000	-1.997069000	0.046651000
6	4.632176000	-2.503887000	-1.258549000
6	4.554838000	-3.901493000	-1.431327000
1	4.735342000	-4.331280000	-2.428788000
6	4.255510000	-4.751395000	-0.357622000
1	4.204590000	-5.840040000	-0.517040000
6	4.025378000	-4.220496000	0.919237000
1	3.794481000	-4.899436000	1.755189000
6	4.092853000	-2.831876000	1.155752000
6	4.989466000	-1.604189000	-2.442283000
1	4.850923000	-0.550686000	-2.119341000
6	4.055589000	-1.832694000	-3.648389000
1	2.989468000	-1.696631000	-3.373795000
1	4.166313000	-2.853965000	-4.069027000
1	4.296917000	-1.116661000	-4.461443000
6	6.473173000	-1.774526000	-2.839571000
1	7.154758000	-1.563836000	-1.989747000
1	6.737636000	-1.084552000	-3.667881000
1	6.681809000	-2.809066000	-3.184796000
6	3.838200000	-2.283092000	2.560355000
1	4.026463000	-1.189186000	2.536191000
6	4.803820000	-2.888690000	3.600973000
1	5.864130000	-2.730702000	3.315512000
1	4.648640000	-3.981348000	3.721123000
1	4.644618000	-2.422131000	4.595428000
6	2.363617000	-2.480372000	2.972957000
1	1.675754000	-1.995960000	2.248184000
1	2.175164000	-2.039800000	3.974266000
1	2.096852000	-3.557056000	3.023780000
6	3.333019000	2.811849000	0.534632000
6	2.930132000	3.305668000	1.804588000
6	2.303293000	4.568744000	1.837206000
1	1.982660000	4.987901000	2.803843000
6	2.088336000	5.303334000	0.662347000
1	1.604790000	6.291735000	0.713535000
6	2.498378000	4.789417000	-0.575585000
1	2.330716000	5.380041000	-1.489931000
6	3.135902000	3.534709000	-0.671869000
6	3.179730000	2.542546000	3.106938000
1	3.586003000	1.543891000	2.842058000
6	1.876642000	2.303922000	3.897169000
1	1.123714000	1.766290000	3.285390000
1	1.420831000	3.257410000	4.236992000
1	2.080308000	1.696062000	4.803185000
6	4.238546000	3.255705000	3.977445000
1	4.448211000	2.669925000	4.896657000
1	3.891863000	4.262225000	4.293042000
1	5.196309000	3.389817000	3.433784000
6	3.592832000	3.015686000	-2.035513000
1	4.103584000	2.043456000	-1.874578000
6	4.616013000	3.966162000	-2.693785000
1	5.492518000	4.142411000	-2.036908000
1	4.168156000	4.954685000	-2.928074000
1	4.985626000	3.536644000	-3.648106000
6	2.389307000	2.747253000	-2.964379000
1	1.683440000	2.022008000	-2.507593000
1	2.731184000	2.330093000	-3.934412000
1	1.824258000	3.678501000	-3.179790000
6	0.024703000	-1.563417000	-1.903214000
6	-0.053491000	-1.139215000	-3.247714000
6	0.130199000	-2.939886000	-1.608503000
6	-0.033426000	-2.089160000	-4.284211000
1	-0.127096000	-0.062345000	-3.465354000
6	0.151164000	-3.880110000	-2.653197000
1	0.195497000	-3.257184000	-0.556208000
6	0.067119000	-3.461923000	-3.993741000
1	-0.096509000	-1.750121000	-5.330631000
1	0.233810000	-4.952312000	-2.413980000
1	0.081647000	-4.201926000	-4.808617000

### XIII [Ag(IPr)(OPh)]

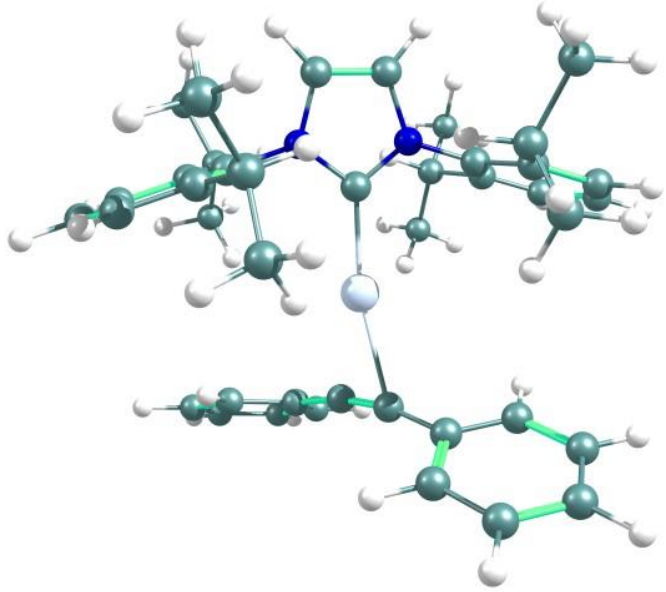


Zero-point correction= 0.643576 (Hartree/Particle)  
 Thermal correction to Energy= 0.683959  
 Thermal correction to Enthalpy= 0.684903  
 Thermal correction to Gibbs Free Energy= 0.563424  
 Sum of electronic and zero-point Energies= -1612.333909  
 Sum of electronic and thermal Energies= -1612.293526  
 Sum of electronic and thermal Enthalpies= -1612.292582  
 Sum of electronic and thermal Free Energies= -1612.414061

47	-0.343901000	1.035248000	0.000028000
8	-1.242782000	2.858838000	0.000086000
6	0.713241000	-0.704190000	-0.000068000
7	0.230884000	-1.990734000	-0.000157000
6	1.269359000	-2.921643000	-0.000265000
1	1.081748000	-3.999746000	-0.000352000
6	2.438559000	-2.204999000	-0.000246000
1	3.484124000	-2.528212000	-0.000316000
7	2.079601000	-0.857262000	-0.000113000
6	-1.173956000	-2.348523000	-0.000103000
6	-1.830487000	-2.526006000	1.246564000
6	-3.188886000	-2.903355000	1.214647000
1	-3.730942000	-3.044383000	2.162976000
6	-3.862010000	-3.093602000	-0.000022000
1	-4.923953000	-3.386143000	0.000012000
6	-3.188972000	-2.903320000	-1.214733000
1	-3.731093000	-3.044302000	-2.163032000
6	-1.830578000	-2.525962000	-1.246727000
6	-1.132807000	-2.303992000	2.588916000
1	-0.076446000	-2.034536000	2.380065000
6	-1.762123000	-1.119329000	3.353821000
1	-1.740656000	-0.189242000	2.749021000
1	-1.210733000	-0.929129000	4.298518000
1	-2.820716000	-1.323339000	3.619940000
6	-1.117537000	-3.587863000	3.446104000
1	-0.638553000	-4.433851000	2.910629000
1	-2.144385000	-3.906246000	3.724887000
1	-0.556546000	-3.418421000	4.389068000
6	-1.133001000	-2.303805000	-2.589108000
1	-0.076590000	-2.034501000	-2.380313000
6	-1.117942000	-3.587517000	-3.446538000
1	-0.556983000	-3.417966000	-4.389501000
1	-2.144844000	-3.905723000	-3.725330000
1	-0.639034000	-4.433667000	-2.911251000
6	-1.762270000	-1.118931000	-3.353731000
1	-1.210958000	-0.928614000	-4.298449000
1	-1.740650000	-0.188961000	-2.748757000
1	-2.820912000	-1.322787000	-3.619773000
6	3.031247000	0.235274000	-0.000041000
6	3.484072000	0.743304000	-1.246316000
6	4.429119000	1.789590000	-1.214432000
1	4.796193000	2.212336000	-2.162988000
6	4.900373000	2.306459000	0.000090000
1	5.636117000	3.126244000	0.000142000
6	4.429320000	1.789257000	1.214549000
1	4.796552000	2.211749000	2.163157000
6	3.484275000	0.742966000	1.246301000
6	2.976708000	0.217870000	-2.589755000
1	2.250221000	-0.595176000	-2.382609000
6	2.218200000	1.315597000	-3.366582000
1	1.370070000	1.715356000	-2.773094000
1	1.812969000	0.909934000	-4.317236000
1	2.883311000	2.167169000	-3.622747000
6	4.118763000	-0.390105000	-3.432333000
1	4.643370000	-1.202638000	-2.887815000
1	4.877463000	0.373872000	-3.704121000
1	3.721387000	-0.813997000	-4.378405000
6	2.977062000	0.217220000	2.589674000
1	2.250851000	-0.596047000	2.382427000
6	2.218160000	1.314651000	3.366542000
1	1.813051000	0.908816000	4.317175000
1	1.369903000	1.714143000	2.773053000
1	2.882980000	2.166444000	3.622729000
6	4.119247000	-0.390475000	3.432265000
1	3.721913000	-0.814666000	4.378221000
1	4.877649000	0.373712000	3.704293000
1	4.644199000	-1.202731000	2.887668000
6	-2.548143000	3.111773000	0.000176000
6	-2.992000000	4.469143000	0.000351000
6	-3.554575000	2.100555000	0.000100000
6	-4.357725000	4.784439000	0.000438000
1	-2.225378000	5.260333000	0.000411000

	6	-4.919405000	2.428320000	0.000190000
	1	-3.229729000	1.043996000	-0.000031000
	6	-5.338429000	3.772173000	0.000358000
	1	-4.665042000	5.844283000	0.000572000
	1	-5.668897000	1.618381000	0.000127000
	1	-6.409972000	4.027054000	0.000426000

## XIV [Ag(IPr)(PhCCPh)]

		6	-0.000343000	-1.328818000	-0.000174000
		7	-0.930442000	-2.163326000	-0.560793000
		7	0.929391000	-2.163911000	0.560184000
		6	-0.588597000	-3.497056000	-0.355228000
		6	0.586981000	-3.497428000	0.354173000
		6	-2.118721000	-1.727250000	-1.271036000
		6	2.117770000	-1.728553000	1.270698000
		1	-1.206441000	-4.319104000	-0.729953000
		1	1.204479000	-4.319863000	0.728617000
		6	-2.017428000	-1.463934000	-2.663146000
6	-3.192463000	-1.053669000	-3.327409000		
6	-4.407702000	-0.923158000	-2.640824000		
6	-4.475900000	-1.200337000	-1.268012000		
6	-3.335092000	-1.609105000	-0.546157000		
6	-0.713326000	-1.617873000	-3.447839000		
1	-3.154910000	-0.841001000	-4.407385000		
1	-5.313425000	-0.609325000	-3.183272000		
1	-5.438888000	-1.102622000	-0.742995000		
6	-3.449598000	-1.937684000	0.943907000		
6	2.016397000	-1.465626000	2.662885000		
6	3.191503000	-1.056028000	3.327426000		
6	4.406893000	-0.925808000	2.641042000		
6	4.475170000	-1.202624000	1.268166000		
6	3.334286000	-1.610695000	0.546030000		
6	0.712127000	-1.619290000	3.447353000		
1	3.153898000	-0.843664000	4.407460000		
1	5.312666000	-0.612494000	3.183708000		
1	5.438284000	-1.105181000	0.743322000		
6	3.448862000	-1.938656000	-0.944160000		
1	0.070157000	-1.968861000	-2.743304000		
6	-0.236695000	-0.266385000	-4.022014000		
6	-0.842359000	-2.684962000	-4.556965000		
1	-2.422851000	-2.090333000	1.339304000		
6	-4.076132000	-0.781495000	1.750668000		
6	-4.228494000	-3.255074000	1.159459000		
1	-0.071276000	-1.970241000	2.742707000		
6	0.840764000	-2.686272000	4.556627000		
6	0.235610000	-0.267656000	4.021280000		
1	2.422195000	-2.092036000	-1.339467000		
6	4.074287000	-0.781536000	-1.750469000		
6	4.228832000	-3.255277000	-1.160406000		
1	0.732509000	-0.386797000	-4.549007000		
1	-0.963975000	0.146366000	-4.752170000		
1	-0.098739000	0.489457000	-3.220061000		
1	0.129451000	-2.827142000	-5.073577000		
1	-1.158271000	-3.666086000	-4.146969000		
1	-1.586099000	-2.388016000	-5.325705000		
1	-4.073964000	-1.022945000	2.833762000		
1	-3.519167000	0.167474000	1.608906000		
1	-5.131797000	-0.599336000	1.459798000		
1	-4.268398000	-3.513928000	2.237923000		
1	-5.273748000	-3.168040000	0.795496000		
1	-3.759671000	-4.104977000	0.622209000		
1	-0.131205000	-2.828316000	5.072974000		
1	1.156708000	-3.667464000	4.146818000		
1	1.584295000	-2.389312000	5.325562000		
1	-0.733634000	-0.387864000	4.548246000		
1	0.962922000	0.145127000	4.751387000		
1	0.097775000	0.488067000	3.219186000		
1	4.072473000	-1.022583000	-2.833654000		
1	3.516352000	0.166824000	-1.608409000		
1	5.129722000	-0.598405000	-1.459378000		
1	4.268720000	-3.513639000	-2.238989000		
1	5.274106000	-3.167566000	-0.796660000		
1	3.760828000	-4.105792000	-0.623412000		

Zero-point correction= 0.739811 (Hartree/Particle)  
 Thermal correction to Energy= 0.786786  
 Thermal correction to Enthalpy= 0.787731  
 Thermal correction to Gibbs Free Energy= 0.649394  
 Sum of electronic and zero-point Energies= -1844.470395  
 Sum of electronic and thermal Energies= -1844.423419  
 Sum of electronic and thermal Enthalpies= -1844.422475  
 Sum of electronic and thermal Free Energies= -1844.560811

	47	0.000351000	0.749082000	0.000072000
	6	-0.574417000	2.965784000	0.250440000
	6	0.576058000	2.965648000	-0.249837000
	6	-1.841116000	3.252815000	0.872772000
	6	-1.877909000	3.741296000	2.206661000
	6	-3.054543000	3.095984000	0.151005000
	6	-3.105403000	4.075386000	2.794457000
	1	-0.937786000	3.866846000	2.764620000
	6	-4.274100000	3.437141000	0.751329000
	1	-3.026699000	2.716083000	-0.881547000
	6	-4.303357000	3.926027000	2.070715000
	1	-3.127512000	4.461471000	3.825321000
	1	-5.210561000	3.323715000	0.183722000
	1	-5.264116000	4.194588000	2.536867000
	6	1.842901000	3.252120000	-0.872111000
	6	3.056185000	3.095344000	-0.150087000
	6	1.880004000	3.740017000	-2.206207000
	6	4.275904000	3.435983000	-0.750373000
	1	3.028088000	2.715882000	0.882619000
	6	3.107656000	4.073586000	-2.793962000
	1	0.939988000	3.865546000	-2.764352000
	6	4.305466000	3.924290000	-2.069966000
	1	5.212257000	3.322608000	-0.182577000
	1	3.130007000	4.459226000	-3.824988000
	1	5.266355000	4.192447000	-2.536084000

## V+VII-XV TS

	6	-5.087539000	-0.280508000	0.351335000
	7	-5.619538000	-1.097932000	1.315929000
	7	-6.173809000	0.303450000	-0.250916000
	6	-7.011436000	-1.028705000	1.311941000
	6	-7.360783000	-0.145865000	0.322439000
	6	-4.863536000	-1.925694000	2.236034000
	6	-6.113993000	1.269635000	-1.331789000
	1	-7.620661000	-1.610004000	2.010845000
	1	-8.338660000	0.201561000	-0.024795000
	6	-4.416038000	-1.349890000	3.454550000
	6	-3.716399000	-2.190642000	4.344865000
	6	-3.482068000	-3.538677000	4.039479000
	6	-3.940032000	-4.077373000	2.829085000
	6	-4.642098000	-3.286250000	1.896196000
	6	-4.661614000	0.113979000	3.821968000
	1	-3.355222000	-1.780541000	5.301139000
	1	-2.940419000	-4.177527000	4.754948000
	1	-3.751556000	-5.138247000	2.601305000
	6	-5.133880000	-3.905038000	0.586864000
	6	-6.075972000	0.791968000	-2.668567000
	6	-6.037243000	1.756856000	-3.696625000
	6	-6.044766000	3.128609000	-3.406309000
	6	-6.090902000	3.567674000	-2.075615000
	6	-6.127547000	2.651312000	-1.003890000
	6	-6.075422000	-0.696831000	-3.017315000
	1	-6.005594000	1.424568000	-4.746169000
	1	-6.019909000	3.863289000	-4.226586000
	1	-6.101970000	4.647942000	-1.861597000
	6	-6.192961000	3.162996000	0.435993000
	1	-5.269688000	0.569856000	3.012857000
	6	-3.335855000	0.902401000	3.887481000
	6	-5.469143000	0.247919000	5.130944000
	1	-5.623516000	-3.103618000	-0.005379000
	6	-3.961184000	-4.439528000	-0.261824000
	6	-6.192815000	-4.999880000	0.842010000
	1	-6.142951000	-1.266621000	-2.066745000
	6	-7.302015000	-1.082340000	-3.872029000
	6	-4.754633000	-1.111024000	-3.700827000
	1	-6.170366000	2.281287000	1.110384000
	6	-4.968745000	4.033765000	0.788905000
	6	-7.515971000	3.913634000	0.704770000
	1	-3.530189000	1.972908000	4.107393000
	1	-2.669793000	0.511507000	4.685561000
	1	-2.787921000	0.842270000	2.923675000
	1	-5.689978000	1.314761000	5.343149000

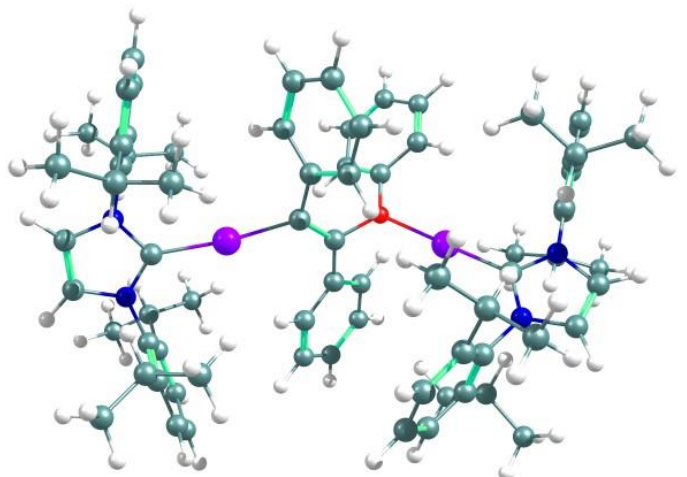
Zero-point correction=	1.386225 (Hartree/Particle)
Thermal correction to Energy=	1.472802
Thermal correction to Enthalpy=	1.473746
Thermal correction to Gibbs Free Energy=	1.249769
Sum of electronic and zero-point Energies=	-3434.437646
Sum of electronic and thermal Energies=	-3434.351069
Sum of electronic and thermal Enthalpies=	-3434.350125
Sum of electronic and thermal Free Energies=	-3434.574101

1	-6.434886000	-0.295422000	5.074874000
1	-4.909938000	-0.153324000	6.002202000
1	-4.332184000	-4.824987000	-1.234415000
1	-3.213115000	-3.646667000	-0.467578000
1	-3.435145000	-5.274831000	0.246272000
1	-6.574709000	-5.403418000	-0.118888000
1	-5.769074000	-5.850915000	1.415691000
1	-7.058266000	-4.609335000	1.416176000
1	-7.314941000	-2.175968000	-4.061034000
1	-8.253757000	-0.811186000	-3.370361000
1	-7.288180000	-0.576125000	-4.860097000
1	-4.743972000	-2.203546000	-3.896718000
1	-4.619940000	-0.595963000	-4.675343000
1	-3.880392000	-0.865608000	-3.062128000
1	-5.005071000	4.336610000	1.856159000
1	-4.018685000	3.488391000	0.614960000
1	-4.939044000	4.963588000	0.183192000
1	-7.572802000	4.235104000	1.765637000
1	-7.600668000	4.824387000	0.075483000
1	-8.400672000	3.278468000	0.492462000
79	-3.138656000	0.057639000	-0.113191000
6	-0.475065000	-0.437781000	-0.710049000
6	-1.179604000	0.649621000	-0.651396000
6	4.870121000	0.281035000	0.745191000
7	6.008465000	-0.471477000	0.587234000
7	5.176884000	1.181788000	1.735152000
6	7.004050000	-0.049205000	1.464955000
6	6.480437000	0.990299000	2.189284000
6	6.189865000	-1.538559000	-0.379610000
6	4.306736000	2.234194000	2.223184000
1	7.989765000	-0.523583000	1.490513000
1	6.912225000	1.610697000	2.980492000
6	6.629254000	-1.200121000	-1.687125000
6	6.833887000	-2.262323000	-2.592253000
6	6.618479000	-3.594114000	-2.211907000
6	6.189408000	-3.895064000	-0.911564000
6	5.964151000	-2.876772000	0.037659000
6	6.909098000	0.237912000	-2.125600000
1	7.174586000	-2.038247000	-3.615167000
1	6.790938000	-4.406687000	-2.935206000
1	6.027891000	-4.945517000	-0.623237000
6	5.518516000	-3.237565000	1.455018000
6	3.434206000	1.949711000	3.305897000
6	2.626901000	3.004862000	3.779223000
6	2.692985000	4.282705000	3.206609000
6	3.572149000	4.534018000	2.143699000
6	4.402838000	3.518793000	1.624815000
6	3.346219000	0.569152000	3.956319000
1	1.937451000	2.821704000	4.618247000
1	2.056476000	5.092731000	3.596077000
1	3.622072000	5.544569000	1.708361000
6	5.361967000	3.831108000	0.475026000
1	6.599222000	0.911215000	-1.299020000
6	6.080354000	0.633953000	-3.365356000
6	8.419902000	0.461060000	-2.359453000
1	5.291900000	-2.291206000	1.989897000
6	4.224441000	-4.077205000	1.454183000
6	6.649049000	-3.949978000	2.230632000
1	4.075041000	-0.093609000	3.444844000
6	3.735895000	0.615080000	5.449377000
6	1.948990000	-0.054167000	3.752624000
1	5.896800000	2.893929000	0.214068000
6	4.605711000	4.286064000	-0.791081000
6	6.429643000	4.864225000	0.897581000
1	6.247891000	1.702088000	-3.615427000
1	6.365029000	0.038947000	-4.258375000
1	4.994468000	0.485206000	-3.193552000
1	8.620849000	1.519417000	-2.627109000
1	9.016880000	0.217517000	-1.456261000
1	8.798628000	-0.170942000	-3.190133000
1	3.886867000	-4.264667000	2.495082000
1	3.406280000	-3.560749000	0.911919000
1	4.377185000	-5.067406000	0.975551000
1	6.334611000	-4.162581000	3.273830000
1	6.915214000	-4.918114000	1.756345000



	1	7.571902000	-3.335406000	2.271649000
	1	3.721993000	-0.404973000	5.887109000
	1	4.752904000	1.034058000	5.594541000
	1	3.030587000	1.238499000	6.038220000
	1	1.917097000	-1.082607000	4.169328000
	1	1.159060000	0.537956000	4.260813000
	1	1.692972000	-0.107147000	2.673833000
	1	5.315330000	4.443573000	-1.629727000
	1	3.858514000	3.531183000	-1.110947000
	1	4.072777000	5.246303000	-0.626793000
	1	7.149786000	5.039067000	0.071344000
	1	5.971964000	5.843384000	1.152070000
	1	7.003438000	4.524110000	1.784302000
	79	3.194538000	0.118771000	-0.297862000
	6	1.581580000	-0.353438000	-2.768237000
	6	0.799975000	0.296772000	-3.756912000
	6	2.430601000	-1.419696000	-3.157851000
	6	0.878718000	-0.108381000	-5.097963000
	1	0.148029000	1.128945000	-3.450658000
	6	2.508305000	-1.809480000	-4.506379000
	1	3.030426000	-1.930933000	-2.386858000
	6	1.732463000	-1.161133000	-5.483182000
	1	0.273371000	0.413844000	-5.856560000
	1	3.179994000	-2.634889000	-4.792295000
	1	1.793311000	-1.470182000	-6.538199000
	8	1.473806000	0.048650000	-1.472011000
	6	-0.937206000	2.088235000	-0.865470000
	6	-1.842680000	2.860551000	-1.634989000
	6	0.188724000	2.729974000	-0.294118000
	6	-1.610128000	4.228013000	-1.853280000
	1	-2.729413000	2.374304000	-2.071502000
	6	0.402926000	4.101762000	-0.498012000
	1	0.894349000	2.144727000	0.313457000
	6	-0.489227000	4.855521000	-1.282184000
	1	-2.316168000	4.807548000	-2.468528000
	1	1.281268000	4.582633000	-0.040208000
	1	-0.313199000	5.930625000	-1.444530000
	6	-0.255215000	-1.852989000	-0.603775000
	6	0.108232000	-2.436234000	0.641043000
	6	-0.389914000	-2.688947000	-1.746968000
	6	0.315593000	-3.817859000	0.738925000
	1	0.209597000	-1.790420000	1.525461000
	6	-0.173338000	-4.070453000	-1.637549000
	1	-0.672926000	-2.241159000	-2.710365000
	6	0.177737000	-4.637333000	-0.399203000
	1	0.580818000	-4.263131000	1.710354000
	1	-0.281812000	-4.710034000	-2.527200000
	1	0.341599000	-5.723614000	-0.317979000

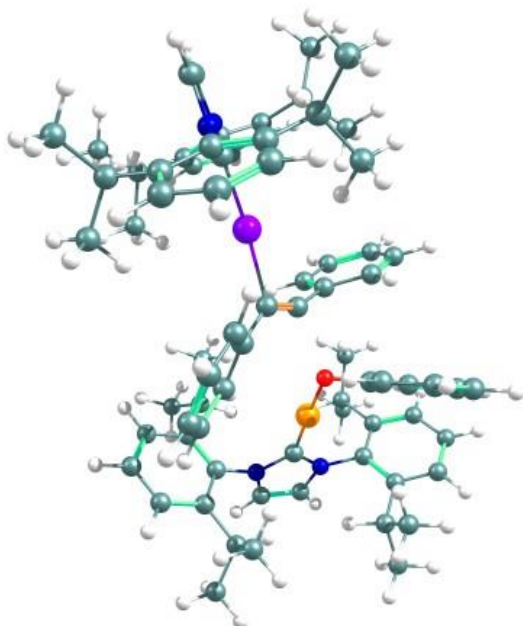
### XV [Au(IPr)(OPh)(PhCCPh)(IPr)(Au)]<sup>+</sup> min

	6	4.930464000	0.157710000	0.176442000
	7	5.650758000	1.318755000	0.029953000
	7	5.868694000	-0.779392000	0.539254000
	6	7.002979000	1.109258000	0.298329000
	6	7.139939000	-0.216197000	0.619481000
	6	5.119984000	2.609832000	-0.358788000
	6	5.600456000	-2.181561000	0.796098000
	1	7.737586000	1.917852000	0.234580000
	1	8.018963000	-0.807286000	0.894277000
	6	4.676693000	3.495806000	0.658448000
	6	4.225358000	4.769513000	0.253816000
	6	4.226850000	5.145706000	-1.097109000
	6	4.671272000	4.247852000	-2.078143000
	6	5.128557000	2.958296000	-1.735291000
	6	4.682077000	3.122709000	2.141673000
	1	3.877761000	5.485518000	1.015392000
	1	3.883765000	6.151602000	-1.387250000
	1	4.670122000	4.554540000	-3.135955000
	6	5.613299000	2.004465000	-2.827889000
	6	5.710844000	-3.098608000	-0.282629000
	6	5.483123000	-4.460858000	0.002969000
	6	5.168245000	-4.887851000	1.300947000

Zero-point correction=	1.388759 (Hartree/Particle)	6	5.067928000	-3.957411000	2.344490000
Thermal correction to Energy=	1.475710	6	5.282100000	-2.581620000	2.120414000
Thermal correction to Enthalpy=	1.476655	6	6.041651000	-2.661191000	-1.710455000
Thermal correction to Gibbs Free Energy=	1.252657	1	5.559674000	-5.202141000	-0.807971000
Sum of electronic and zero-point Energies=	-3434.453854	1	5.003016000	-5.958233000	1.501837000
Sum of electronic and thermal Energies=	-3434.366903	1	4.819307000	-4.305334000	3.359268000
Sum of electronic and thermal Enthalpies=	-3434.365958	6	5.164436000	-1.591372000	3.279196000
Sum of electronic and thermal Free Energies=	-3434.589956	1	5.107386000	2.101522000	2.232357000
		6	3.248961000	3.065840000	2.712299000
		6	5.583075000	4.068826000	2.964180000
		1	5.932224000	1.061761000	-2.335965000
		6	4.474859000	1.643244000	-3.805649000
		6	6.841906000	2.571141000	-3.572137000
		1	6.277585000	-1.576575000	-1.686965000
		6	7.285730000	-3.385625000	-2.266684000
		6	4.819539000	-2.837756000	-2.637839000
		1	5.388501000	-0.578864000	2.882770000
		6	3.725251000	-1.550230000	3.836517000
		6	6.195941000	-1.886832000	4.389330000
		1	3.267786000	2.751948000	3.776939000
		1	2.752034000	4.057865000	2.664644000
		1	2.622766000	2.340775000	2.152199000
		1	5.622218000	3.743163000	4.024581000
		1	6.621775000	4.087171000	2.574648000
		1	5.202963000	5.112038000	2.951926000
		1	4.827567000	0.901906000	-4.552772000
		1	3.605024000	1.210452000	-3.270548000
		1	4.118027000	2.533900000	-4.364305000
		1	7.212717000	1.841853000	-4.322298000
		1	6.595937000	3.508269000	-4.114616000
		1	7.675655000	2.797733000	-2.875917000
		1	7.542711000	-2.995309000	-3.273399000
		1	8.169419000	-3.245922000	-1.610454000
		1	7.115193000	-4.477685000	-2.371430000
		1	5.051715000	-2.479063000	-3.662497000
		1	4.521424000	-3.904809000	-2.714449000
		1	3.947170000	-2.264030000	-2.260060000
		1	3.641356000	-0.783289000	4.634932000
		1	2.992914000	-1.305427000	3.039547000
		1	3.429743000	-2.525078000	4.278020000
		1	6.133561000	-1.121283000	5.190697000
		1	6.017772000	-2.875770000	4.861705000
		1	7.233817000	-1.886529000	3.996777000
		79	2.924096000	-0.199121000	-0.034092000
		6	0.007433000	-0.239480000	-0.999778000
		6	0.947941000	-0.788440000	-0.180437000
		6	-4.697585000	0.639845000	0.531494000
		7	-5.958782000	0.117538000	0.404172000
		7	-4.850061000	1.785521000	1.268377000
		6	-6.888117000	0.928504000	1.049366000
		6	-6.190914000	1.977195000	1.592551000
		6	-6.300114000	-1.111615000	-0.289466000
		6	-3.785505000	2.688776000	1.667901000
		1	-7.954928000	0.685353000	1.061094000
		1	-6.524318000	2.840443000	2.176192000
		6	-6.360823000	-2.315116000	0.462601000
		6	-6.721754000	-3.488655000	-0.231863000
		6	-7.011539000	-3.461753000	-1.603412000
		6	-6.948149000	-2.255497000	-2.314448000
		6	-6.594382000	-1.048061000	-1.677076000
		6	-6.079419000	-2.374025000	1.965087000
		1	-6.781545000	-4.442074000	0.316059000
		1	-7.295337000	-4.390573000	-2.122815000
		1	-7.182377000	-2.248008000	-3.390428000
		6	-6.552958000	0.252284000	-2.480396000
		6	-3.453222000	3.765369000	0.803579000
		6	-2.434641000	4.640826000	1.233556000
		6	-1.790092000	4.456676000	2.464314000
		6	-2.151588000	3.390723000	3.300006000
		6	-3.160188000	2.479398000	2.926033000
		6	-4.190054000	4.026013000	-0.510898000
		1	-2.144303000	5.485961000	0.590890000
		1	-0.999696000	5.156002000	2.779163000
		1	-1.642044000	3.264153000	4.267410000
		6	-3.582588000	1.363292000	3.883661000

	1	-5.756332000	-1.363149000	2.292407000
	6	-4.927780000	-3.345956000	2.296622000
	6	-7.358207000	-2.726672000	2.757314000
	1	-6.226954000	1.066122000	-1.798901000
	6	-5.519970000	0.176599000	-3.624778000
	6	-7.953888000	0.632525000	-3.008664000
	1	-4.765384000	3.110083000	-0.763866000
	6	-5.205722000	5.180190000	-0.344606000
	6	-3.231705000	4.296526000	-1.686711000
	1	-4.175177000	0.624503000	3.302733000
	6	-2.383400000	0.606428000	4.487989000
	6	-4.497914000	1.921687000	4.998161000
	1	-4.712139000	-3.331117000	3.385277000
	1	-5.181826000	-4.392361000	2.026802000
	1	-3.995540000	-3.074178000	1.759895000
	1	-7.156457000	-2.715363000	3.848617000
	1	-8.179483000	-2.008824000	2.554325000
	1	-7.729563000	-3.739925000	2.496542000
	1	-5.456478000	1.149161000	-4.155609000
	1	-4.509687000	-0.073091000	-3.239430000
	1	-5.795684000	-0.594386000	-4.374383000
	1	-7.917845000	1.606493000	-3.539504000
	1	-8.337774000	-0.123056000	-3.725766000
	1	-8.694060000	0.718824000	-2.186689000
	1	-5.771003000	5.341415000	-1.286165000
	1	-5.939741000	4.975864000	0.461980000
	1	-4.690979000	6.131243000	-0.092624000
	1	-3.805233000	4.389887000	-2.632136000
	1	-2.671552000	5.245613000	-1.553841000
	1	-2.491787000	3.480958000	-1.813883000
	1	-2.739103000	-0.255871000	5.088842000
	1	-1.702154000	0.221400000	3.702731000
	1	-1.786297000	1.248806000	5.168346000
	1	-4.837980000	1.107305000	5.671398000
	1	-3.958442000	2.669521000	5.616676000
	1	-5.398722000	2.420289000	4.585308000
	79	-3.044917000	-0.111573000	-0.245638000
	6	-1.310984000	-2.158373000	-1.876504000
	6	-0.332888000	-2.440331000	-2.844134000
	6	-2.366438000	-3.048655000	-1.626911000
	6	-0.426229000	-3.639579000	-3.571400000
	1	0.492443000	-1.735906000	-3.020818000
	6	-2.446737000	-4.240851000	-2.366360000
	1	-3.114804000	-2.809748000	-0.853969000
	6	-1.478581000	-4.542395000	-3.339686000
	1	0.336825000	-3.863677000	-4.333216000
	1	-3.273120000	-4.940806000	-2.168394000
	1	-1.542264000	-5.479197000	-3.914003000
	8	-1.279079000	-0.946787000	-1.152632000
	6	0.613564000	-1.979635000	0.654057000
	6	-0.397972000	-1.913030000	1.645595000
	6	1.331628000	-3.194553000	0.523886000
	6	-0.686433000	-3.017528000	2.464512000
	1	-0.947291000	-0.966968000	1.785225000
	6	1.025703000	-4.306058000	1.325173000
	1	2.139831000	-3.259934000	-0.221250000
	6	0.017286000	-4.224379000	2.302153000
	1	-1.464561000	-2.932756000	3.240175000
	1	1.590986000	-5.241925000	1.191853000
	1	-0.211414000	-5.092194000	2.940730000
	6	0.037328000	0.976430000	-1.836999000
	6	-0.763821000	1.082201000	-3.005109000
	6	0.871094000	2.074584000	-1.502512000
	6	-0.699315000	2.220190000	-3.825429000
	1	-1.429355000	0.253146000	-3.287282000
	6	0.930601000	3.210009000	-2.322909000
	1	1.476015000	2.024359000	-0.583355000
	6	0.151612000	3.288176000	-3.492749000
	1	-1.317360000	2.268017000	-4.736035000
	1	1.592020000	4.043215000	-2.038957000
	1	0.201459000	4.180477000	-4.136550000

# V+VIII-XVI TS



Zero-point correction= 1.386120 (Hartree/Particle)  
 Thermal correction to Energy= 1.473475  
 Thermal correction to Enthalpy= 1.474419  
 Thermal correction to Gibbs Free Energy= 1.246942  
 Sum of electronic and zero-point Energies= -3496.021522  
 Sum of electronic and thermal Energies= -3495.934167  
 Sum of electronic and thermal Enthalpies= -3495.933223  
 Sum of electronic and thermal Free Energies= -3496.160699

6	-4.812833000	-0.284764000	0.289064000
7	-5.363524000	-1.186151000	1.163982000
7	-5.884241000	0.385246000	-0.245610000
6	-6.753350000	-1.081963000	1.172924000
6	-7.081415000	-0.090995000	0.283697000
6	-4.626879000	-2.135734000	1.976652000
6	-5.803382000	1.457118000	-1.220396000
1	-7.376647000	-1.718576000	1.808406000
1	-8.050759000	0.315759000	-0.020437000
6	-4.155997000	-1.718947000	3.249695000
6	-3.471670000	-2.676054000	4.027381000
6	-3.276298000	-3.984491000	3.563178000
6	-3.759885000	-4.366055000	2.304034000
6	-4.448284000	-3.453194000	1.478399000
6	-4.353827000	-0.299763000	3.783667000
1	-3.091841000	-2.390698000	5.020941000
1	-2.746326000	-4.716744000	4.192741000
1	-3.603551000	-5.397984000	1.952557000
6	-4.970721000	-3.901627000	0.113303000
6	-5.780642000	1.120343000	-2.599828000
6	-5.728713000	2.186529000	-3.521829000
6	-5.712263000	3.520498000	-3.090553000
6	-5.740879000	3.819423000	-1.720985000
6	-5.784801000	2.797123000	-0.750268000
6	-5.794807000	-0.323864000	-3.102646000
1	-5.707478000	1.965497000	-4.600391000
1	-5.680866000	4.335942000	-3.830350000
1	-5.729814000	4.870959000	-1.394210000
6	-5.825875000	3.155019000	0.736017000
1	-4.998939000	0.246585000	3.063984000
6	-3.010155000	0.458278000	3.850333000
6	-5.081017000	-0.289720000	5.145018000
1	-5.457072000	-3.027455000	-0.367879000
6	-3.819402000	-4.346045000	-0.813297000
6	-6.042136000	-5.005210000	0.251445000
1	-5.948515000	-0.987440000	-2.225644000
6	-6.960767000	-0.585551000	-4.079541000
6	-4.434513000	-0.704937000	-3.726933000
1	-5.761776000	2.208842000	1.313434000
6	-4.617481000	4.020670000	1.150100000
6	-7.161750000	3.833676000	1.112377000
1	-3.167033000	1.500952000	4.197483000
1	-2.305064000	-0.029358000	4.556419000
1	-2.524708000	0.496162000	2.851794000
1	-5.277383000	0.752851000	5.470915000
1	-6.054077000	-0.820326000	5.094644000
1	-4.476168000	-0.774011000	5.940182000
1	-4.210768000	-4.607834000	-1.818499000
1	-3.062992000	-3.543810000	-0.934038000
1	-3.299503000	-5.242745000	-0.415781000
1	-6.449516000	-5.278840000	-0.744069000
1	-5.621106000	-5.927889000	0.703423000
1	-6.889810000	-4.678904000	0.888695000
1	-6.989892000	-1.656923000	-4.367618000
1	-7.940554000	-0.326377000	-3.628175000
1	-6.856207000	0.002962000	-5.015071000
1	-4.436207000	-1.767836000	-4.046909000
1	-4.210324000	-0.085372000	-4.620858000
1	-3.606885000	-0.564628000	-2.999334000
1	-4.627285000	4.197666000	2.245776000
1	-3.657923000	3.530995000	0.885923000
1	-4.636093000	5.015086000	0.656711000
1	-7.199325000	4.043016000	2.201838000
1	-7.289166000	4.800848000	0.581845000
1	-8.033864000	3.196685000	0.857525000
79	-2.855502000	0.068956000	-0.125563000
6	-0.180869000	-0.399725000	-0.636415000
6	-0.881943000	0.689521000	-0.586158000
6	4.978691000	0.260577000	0.693777000
7	6.115374000	-0.494801000	0.508622000
7	5.321280000	1.139277000	1.696828000
6	7.131909000	-0.099266000	1.373855000

	6	6.630333000	0.931828000	2.125847000
	6	6.271690000	-1.538136000	-0.486118000
	6	4.473779000	2.195221000	2.212432000
	1	8.114316000	-0.581401000	1.374079000
	1	7.082802000	1.534418000	2.919458000
	6	6.704054000	-1.172143000	-1.789079000
	6	6.877247000	-2.211481000	-2.726778000
	6	6.638547000	-3.549109000	-2.382342000
	6	6.221631000	-3.879252000	-1.085016000
	6	6.029988000	-2.884389000	-0.103925000
	6	7.018241000	0.271377000	-2.184229000
	1	7.211743000	-1.964999000	-3.746582000
	1	6.785439000	-4.343699000	-3.130878000
	1	6.046345000	-4.934730000	-0.824181000
	6	5.613697000	-3.277093000	1.313968000
	6	3.609304000	1.908863000	3.301600000
	6	2.822800000	2.968395000	3.800183000
	6	2.902805000	4.254252000	3.247664000
	6	3.774827000	4.508960000	2.179554000
	6	4.582649000	3.488872000	1.634616000
	6	3.513540000	0.521220000	3.935624000
	1	2.140129000	2.782892000	4.644274000
	1	2.283662000	5.067726000	3.657422000
	1	3.837580000	5.526018000	1.761080000
	6	5.535062000	3.804224000	0.479967000
	1	6.712824000	0.926575000	-1.341588000
	6	6.216284000	0.723717000	-3.421891000
	6	8.536767000	0.466504000	-2.393334000
	1	5.405627000	-2.342132000	1.875657000
	6	4.316309000	-4.110546000	1.326614000
	6	6.759938000	-4.012088000	2.044270000
	1	4.231806000	-0.141270000	3.409344000
	6	3.916210000	0.544837000	5.425708000
	6	2.109118000	-0.086993000	3.737208000
	1	6.057929000	2.864333000	0.205744000
	6	4.773119000	4.278564000	-0.775513000
	6	6.616162000	4.822935000	0.902648000
	1	6.412083000	1.794779000	-3.636725000
	1	6.499764000	0.150353000	-4.329336000
	1	5.125112000	0.593759000	-3.271284000
	1	8.764750000	1.526778000	-2.630047000
	1	9.116333000	0.185549000	-1.489737000
	1	8.911376000	-0.152171000	-3.235915000
	1	4.006336000	-4.324448000	2.370985000
	1	3.485105000	-3.576738000	0.822392000
	1	4.449244000	-5.088407000	0.817562000
	1	6.471588000	-4.246549000	3.090351000
	1	7.009023000	-4.970295000	1.541405000
	1	7.686453000	-3.402523000	2.074835000
	1	3.900434000	-0.480918000	5.849848000
	1	4.937043000	0.955676000	5.566756000
	1	3.220089000	1.164388000	6.029413000
	1	2.069526000	-1.118426000	4.145867000
	1	1.328107000	0.509053000	4.254581000
	1	1.843352000	-0.130078000	2.660282000
	1	5.477223000	4.437758000	-1.618485000
	1	4.015905000	3.534607000	-1.097659000
	1	4.250192000	5.241926000	-0.597686000
	1	7.331904000	4.996942000	0.072427000
	1	6.170910000	5.804877000	1.168318000
	1	7.192915000	4.469375000	1.782063000
	29	3.380525000	0.124990000	-0.256587000
	6	1.952796000	-0.249452000	-2.622231000
	6	1.241176000	0.495926000	-3.598166000
	6	2.755264000	-1.339567000	-3.049177000
	6	1.343980000	0.162223000	-4.956923000
	1	0.621676000	1.342819000	-3.265992000
	6	2.857942000	-1.658079000	-4.414685000
	1	3.299787000	-1.926249000	-2.290935000
	6	2.151848000	-0.914033000	-5.376022000
	1	0.792495000	0.757469000	-5.702826000
	1	3.493510000	-2.502612000	-4.726148000
	1	2.230382000	-1.167273000	-6.444674000
	8	1.835447000	0.074458000	-1.308648000
	6	-0.644513000	2.133055000	-0.759326000

	6	-1.558212000	2.922971000	-1.501154000
	6	0.483219000	2.763537000	-0.179045000
	6	-1.333317000	4.296706000	-1.683332000
	1	-2.445678000	2.443975000	-1.944123000
	6	0.689858000	4.141474000	-0.346068000
	1	1.194443000	2.164101000	0.407204000
	6	-0.211026000	4.912819000	-1.102592000
	1	-2.046580000	4.889730000	-2.276907000
	1	1.568199000	4.613252000	0.120650000
	1	-0.040803000	5.992910000	-1.235316000
	6	0.023331000	-1.818782000	-0.561755000
	6	0.289990000	-2.446513000	0.685883000
	6	-0.050036000	-2.617175000	-1.737212000
	6	0.465339000	-3.834258000	0.754103000
	1	0.338751000	-1.830294000	1.595837000
	6	0.136048000	-4.005146000	-1.656793000
	1	-0.263500000	-2.135036000	-2.701908000
	6	0.392554000	-4.615968000	-0.416176000
	1	0.654099000	-4.313853000	1.727024000
	1	0.075769000	-4.615564000	-2.571226000
	1	0.531217000	-5.707222000	-0.358181000

## XVI [Cu(IPr)(OPh)(PhCCPh)(IPr)(Au)]<sup>+</sup> min

	6	4.613761000	0.072358000	0.164471000
	7	5.371580000	1.208582000	0.015137000
	7	5.520570000	-0.895283000	0.525675000
	6	6.716539000	0.954259000	0.280965000
	6	6.810086000	-0.374869000	0.602901000
	6	4.881982000	2.515772000	-0.373677000
	6	5.202904000	-2.286175000	0.786486000
	1	7.477503000	1.737979000	0.215884000
	1	7.669580000	-0.994352000	0.876962000
	6	4.453834000	3.409945000	0.642783000
	6	4.041874000	4.697163000	0.239016000
	6	4.067895000	5.078505000	-1.110188000
	6	4.498040000	4.172680000	-2.090371000
	6	4.914907000	2.869220000	-1.748552000
	6	4.443963000	3.035182000	2.125416000
	1	3.707048000	5.419489000	1.000396000
	1	3.755745000	6.094616000	-1.399619000
	1	4.516536000	4.483994000	-3.146660000
	6	5.387257000	1.907502000	-2.839806000
	6	5.277494000	-3.209928000	-0.289439000
6	5.001718000	-4.562321000	0.000936000	
6	4.672776000	-4.973432000	1.300485000	
6	4.607071000	-4.036451000	2.341035000	
6	4.871291000	-2.670207000	2.112325000	
6	5.623933000	-2.790101000	-1.718762000	
1	5.051158000	-5.308438000	-0.807747000	
1	4.469035000	-6.036440000	1.505111000	
1	4.346677000	-4.371889000	3.357088000	
6	4.791469000	-1.672499000	3.267911000	
1	4.813664000	1.992456000	2.213965000	
6	3.013755000	3.054872000	2.705099000	
6	5.399481000	3.931968000	2.942117000	
1	5.652865000	0.946667000	-2.351549000	
6	4.262588000	1.603872000	-3.852068000	
6	6.658110000	2.430803000	-3.543856000	
1	5.873818000	-1.708491000	-1.703566000	
6	6.862671000	-3.537454000	-2.256623000	
6	4.407596000	-2.958900000	-2.654968000	
1	5.049671000	-0.669720000	2.867628000	
6	3.356538000	-1.578267000	3.829771000	
6	5.815218000	-2.000473000	4.376236000	
1	3.022954000	2.736338000	3.768454000	
1	2.570515000	4.072408000	2.665643000	
1	2.345030000	2.367107000	2.147307000	
1	5.425184000	3.607634000	4.003366000	
1	6.435949000	3.891864000	2.548231000	
1	5.077385000	4.994518000	2.927063000	

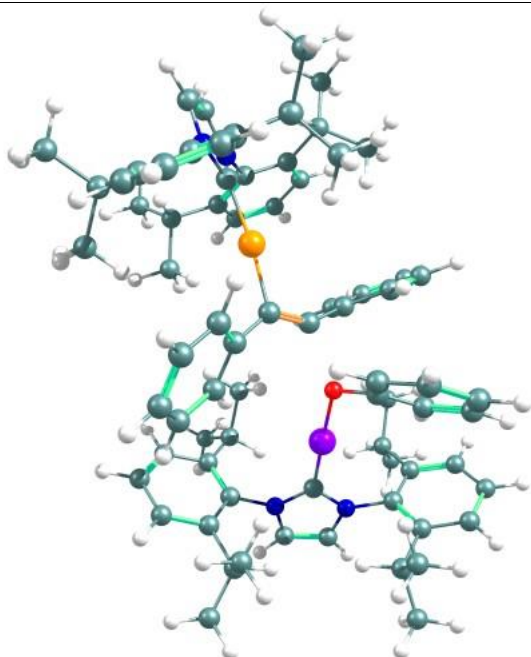
Zero-point correction= 1.388538 (Hartree/Particle)  
 Thermal correction to Energy= 1.475401  
 Thermal correction to Enthalpy= 1.476346  
 Thermal correction to Gibbs Free Energy= 1.252367  
 Sum of electronic and zero-point Energies= -3496.039637  
 Sum of electronic and thermal Energies= -3495.952773  
 Sum of electronic and thermal Enthalpies= -3495.951829  
 Sum of electronic and thermal Free Energies= -3496.175808

1	4.606696000	0.858846000	-4.599532000
1	3.363148000	1.198120000	-3.345848000
1	3.955066000	2.514134000	-4.408536000
1	7.018015000	1.695875000	-4.293812000
1	6.465933000	3.384334000	-4.079424000
1	7.481792000	2.613456000	-2.823139000
1	7.130643000	-3.166311000	-3.267739000
1	7.743921000	-3.398134000	-1.597022000
1	6.679258000	-4.628956000	-2.344197000
1	4.652515000	-2.609444000	-3.679833000
1	4.097306000	-4.022712000	-2.728163000
1	3.539189000	-2.372419000	-2.288111000
1	3.303380000	-0.806437000	4.626110000
1	2.630634000	-1.309058000	3.034664000
1	3.027880000	-2.540450000	4.275614000
1	5.779193000	-1.232856000	5.177208000
1	5.606124000	-2.982962000	4.849392000
1	6.851781000	-2.033885000	3.981633000
79	2.596063000	-0.219387000	-0.041737000
6	-0.310507000	-0.178500000	-1.034690000
6	0.601556000	-0.740961000	-0.192443000
6	-4.695093000	0.644869000	0.508083000
7	-5.967177000	0.142827000	0.362426000
7	-4.857288000	1.768728000	1.283315000
6	-6.898881000	0.937243000	1.023101000
6	-6.198143000	1.963733000	1.603467000
6	-6.310194000	-1.058031000	-0.374728000
6	-3.793901000	2.656221000	1.716175000
1	-7.967972000	0.703763000	1.018358000
1	-6.531881000	2.812176000	2.208349000
6	-6.411410000	-2.283644000	0.337915000
6	-6.771342000	-3.430816000	-0.400263000
6	-7.021145000	-3.359875000	-1.778288000
6	-6.919000000	-2.134413000	-2.451000000
6	-6.567361000	-0.951655000	-1.767733000
6	-6.185185000	-2.387290000	1.847272000
1	-6.862974000	-4.398097000	0.118119000
1	-7.305812000	-4.268202000	-2.332443000
1	-7.123361000	-2.091352000	-3.532255000
6	-6.494266000	0.372800000	-2.528628000
6	-3.438565000	3.745465000	0.876551000
6	-2.421803000	4.607500000	1.337669000
6	-1.800243000	4.400393000	2.576327000
6	-2.183950000	3.324306000	3.388976000
6	-3.192324000	2.426091000	2.983394000
6	-4.152948000	4.036104000	-0.444162000
1	-2.115439000	5.461386000	0.714203000
1	-1.011167000	5.089514000	2.916045000
1	-1.692687000	3.180787000	4.363361000
6	-3.645937000	1.303064000	3.919065000
1	-5.806245000	-1.405567000	2.202030000
6	-5.116725000	-3.441152000	2.203852000
6	-7.514430000	-2.665644000	2.585037000
1	-6.192789000	1.163177000	-1.809526000
6	-5.419359000	0.332852000	-3.635212000
6	-7.874087000	0.772426000	-3.096202000
1	-4.727145000	3.127557000	-0.724993000
6	-5.167272000	5.190096000	-0.269196000
6	-3.174763000	4.328857000	-1.597962000
1	-4.197465000	0.556709000	3.307694000
6	-2.472181000	0.564570000	4.591949000
6	-4.624068000	1.849494000	4.985890000
1	-4.936439000	-3.449998000	3.298973000
1	-5.434449000	-4.465534000	1.917707000
1	-4.150166000	-3.233383000	1.700751000
1	-7.353935000	-2.692111000	3.682941000
1	-8.276659000	-1.888578000	2.370241000
1	-7.943094000	-3.644782000	2.284602000
1	-5.345160000	1.318224000	-4.140368000
1	-4.420610000	0.084472000	-3.219242000
1	-5.656976000	-0.423602000	-4.412304000
1	-7.817570000	1.763596000	-3.592310000
1	-8.231761000	0.042167000	-3.852076000
1	-8.643725000	0.832703000	-2.299446000
1	-5.715403000	5.375227000	-1.216519000

	1	-5.915986000	4.969266000	0.519229000
	1	-4.653630000	6.133005000	0.013934000
	1	-3.731408000	4.442412000	-2.551154000
	1	-2.615383000	5.273936000	-1.436381000
	1	-2.433483000	3.515150000	-1.730050000
	1	-2.849324000	-0.305125000	5.168669000
	1	-1.735828000	0.192814000	3.851291000
	1	-1.930260000	1.214385000	5.310227000
	1	-4.986377000	1.030793000	5.642075000
	1	-4.123962000	2.603954000	5.629017000
	1	-5.510182000	2.336237000	4.529994000
	29	-3.154257000	-0.061191000	0.268275000
	6	-1.709192000	-2.038880000	-1.908843000
	6	-0.696274000	-2.428677000	-2.799549000
	6	-2.867864000	-2.813496000	-1.740872000
	6	-0.859833000	-3.617767000	-3.531626000
	1	0.208092000	-1.813915000	-2.913552000
	6	-3.015302000	-3.998324000	-2.481060000
	1	-3.648821000	-2.491309000	-1.030947000
	6	-2.013166000	-4.406472000	-3.378307000
	1	-0.069263000	-3.925941000	-4.233681000
	1	-3.923155000	-4.605584000	-2.344560000
	1	-2.129656000	-5.336830000	-3.954743000
	8	-1.622173000	-0.835199000	-1.180012000
	6	0.209934000	-1.902892000	0.658110000
	6	-0.790466000	-1.769561000	1.653932000
	6	0.857805000	-3.157373000	0.537369000
	6	-1.132391000	-2.845719000	2.490175000
	1	-1.282351000	-0.790919000	1.788668000
	6	0.497962000	-4.240005000	1.355689000
	1	1.654566000	-3.277302000	-0.213213000
	6	-0.496036000	-4.090758000	2.339364000
	1	-1.896905000	-2.707447000	3.271420000
	1	1.009732000	-5.207280000	1.230491000
	1	-0.765403000	-4.936011000	2.992073000
	6	-0.219780000	1.012986000	-1.903490000
	6	-0.980018000	1.109961000	-3.099230000
	6	0.634690000	2.095197000	-1.569794000
	6	-0.857491000	2.224250000	-3.945047000
	1	-1.656996000	0.291247000	-3.384931000
	6	0.751822000	3.207398000	-2.415899000
	1	1.207230000	2.051674000	-0.630000000
	6	0.012159000	3.276814000	-3.611378000
	1	-1.445091000	2.265869000	-4.875846000
	1	1.426681000	4.029612000	-2.131531000
	1	0.106606000	4.151093000	-4.274563000

## II+VII-XVII TS





Zero-point correction= 1.386474 (Hartree/Particle)  
 Thermal correction to Energy= 1.473712  
 Thermal correction to Enthalpy= 1.474657  
 Thermal correction to Gibbs Free Energy= 1.248368  
 Sum of electronic and zero-point Energies= -3496.010523  
 Sum of electronic and thermal Energies= -3495.923285  
 Sum of electronic and thermal Enthalpies= -3495.922341  
 Sum of electronic and thermal Free Energies= -3496.148630

6	-5.016897000	-0.313901000	0.356244000
7	-5.512434000	-1.227581000	1.256641000
7	-6.131870000	0.359912000	-0.084553000
6	-6.897152000	-1.124189000	1.372147000
6	-7.288971000	-0.121547000	0.522154000
6	-4.716107000	-2.183728000	1.999340000
6	-6.116059000	1.444123000	-1.046577000
1	-7.473561000	-1.766251000	2.045313000
1	-8.278035000	0.288922000	0.296339000
6	-4.099922000	-1.763241000	3.207760000
6	-3.351297000	-2.724203000	3.918951000
6	-3.233161000	-4.041907000	3.455137000
6	-3.862714000	-4.429137000	2.264052000
6	-4.619378000	-3.512015000	1.505652000
6	-4.224435000	-0.338134000	3.748224000
1	-2.861320000	-2.435078000	4.862034000
1	-2.651533000	-4.777571000	4.033062000
1	-3.768465000	-5.468779000	1.913492000
6	-5.318720000	-3.970789000	0.224922000
6	-6.155555000	1.127074000	-2.430689000
6	-6.162873000	2.206058000	-3.339543000
6	-6.142383000	3.534461000	-2.891036000
6	-6.106698000	3.814549000	-1.517729000
6	-6.091282000	2.778728000	-0.560798000
6	-6.191094000	-0.310338000	-2.951844000
1	-6.193951000	2.000289000	-4.421061000
1	-6.158152000	4.360022000	-3.620084000
1	-6.090041000	4.861730000	-1.177084000
6	-6.050965000	3.116335000	0.930430000
1	-4.927176000	0.212897000	3.088813000
6	-2.870721000	0.401555000	3.685954000
6	-4.819121000	-0.311593000	5.172260000
1	-5.755362000	-3.073362000	-0.261451000
6	-4.333814000	-4.596419000	-0.783546000
6	-6.483015000	-4.935960000	0.542809000
1	-6.218622000	-0.987931000	-2.072952000
6	-7.462704000	-0.585659000	-3.782750000
6	-4.910768000	-0.649889000	-3.745252000
1	-6.008040000	2.159694000	1.492104000
6	-4.781640000	3.914566000	1.296790000
6	-7.331536000	3.854616000	1.377865000
1	-2.981199000	1.449834000	4.033980000
1	-2.112013000	-0.089688000	4.331567000
1	-2.471522000	0.424895000	2.649486000
1	-4.967158000	0.735203000	5.510262000
1	-5.800782000	-0.826473000	5.215335000
1	-4.149761000	-0.803911000	5.908693000
1	-4.860858000	-4.853314000	-1.726038000
1	-3.504332000	-3.902790000	-1.029368000
1	-3.884757000	-5.533717000	-0.393252000
1	-7.017237000	-5.223226000	-0.386819000
1	-6.116115000	-5.868990000	1.020398000
1	-7.222272000	-4.478618000	1.232323000
1	-7.497876000	-1.649737000	-4.096549000
1	-8.384668000	-0.369554000	-3.204668000
1	-7.493187000	0.031820000	-4.704855000
1	-4.928204000	-1.708397000	-4.078886000
1	-4.812080000	-0.015424000	-4.651109000
1	-4.001296000	-0.500086000	-3.125606000
1	-4.740205000	4.093023000	2.391677000
1	-3.860454000	3.374058000	0.996853000
1	-4.764450000	4.906604000	0.798794000
1	-7.310204000	4.043168000	2.471549000
1	-7.432424000	4.838319000	0.872730000
1	-8.245720000	3.268071000	1.151007000
29	-3.225001000	0.035327000	-0.174218000
6	-0.698472000	-0.367481000	-0.872585000
6	-1.471566000	0.671020000	-0.729633000
6	4.458033000	0.261573000	0.765573000
7	5.598414000	-0.480116000	0.576297000
7	4.755624000	1.110465000	1.802254000
6	6.587271000	-0.101144000	1.480688000
6	6.057048000	0.899452000	2.253429000
6	5.786673000	-1.499017000	-0.440149000
6	3.877473000	2.131746000	2.339236000

	1	7.573357000	-0.575412000	1.489248000
	1	6.482764000	1.480874000	3.076914000
	6	6.247709000	-1.098473000	-1.722447000
	6	6.454076000	-2.115672000	-2.677485000
	6	6.218173000	-3.462632000	-2.368738000
	6	5.768803000	-3.825031000	-1.091169000
	6	5.543043000	-2.853991000	-0.093703000
	6	6.551338000	0.356945000	-2.079969000
	1	6.811793000	-1.844431000	-3.683010000
	1	6.391060000	-4.239005000	-3.130664000
	1	5.591805000	-4.887054000	-0.859672000
	6	5.077132000	-3.281285000	1.298267000
	6	3.033575000	1.796430000	3.430367000
	6	2.205279000	2.816883000	3.941398000
	6	2.228185000	4.109950000	3.399485000
	6	3.085735000	4.413006000	2.332568000
	6	3.935029000	3.433727000	1.775581000
	6	2.984661000	0.391953000	4.032762000
	1	1.533693000	2.595050000	4.785455000
	1	1.575576000	4.892040000	3.818362000
	1	3.104149000	5.436023000	1.924689000
	6	4.869682000	3.798745000	0.621397000
	1	6.214771000	0.991482000	-1.233132000
	6	5.773015000	0.822465000	-3.327941000
	6	8.071510000	0.577329000	-2.248378000
	1	4.871993000	-2.360723000	1.884356000
	6	3.760364000	-4.082501000	1.239945000
	6	6.181618000	-4.065659000	2.040968000
	1	3.813773000	-0.196861000	3.587003000
	6	3.204316000	0.401993000	5.559883000
	6	1.668667000	-0.320638000	3.652678000
	1	5.451936000	2.891523000	0.355540000
	6	4.079987000	4.213174000	-0.638206000
	6	5.884795000	4.885493000	1.037805000
	1	5.957811000	1.900371000	-3.516383000
	1	6.087337000	0.271895000	-4.239253000
	1	4.680421000	0.675343000	-3.205266000
	1	8.290092000	1.645290000	-2.457444000
	1	8.634183000	0.284615000	-1.337826000
	1	8.473640000	-0.018386000	-3.094797000
	1	3.410794000	-4.324207000	2.265575000
	1	2.960437000	-3.510345000	0.727193000
	1	3.888234000	-5.044753000	0.700962000
	1	5.852607000	-4.325281000	3.068879000
	1	6.425273000	-5.014199000	1.517753000
	1	7.120569000	-3.479985000	2.121437000
	1	3.241254000	-0.635735000	5.951588000
	1	4.154989000	0.903622000	5.834346000
	1	2.383017000	0.925006000	6.093181000
	1	1.654810000	-1.356197000	4.052734000
	1	0.787225000	0.214735000	4.064224000
	1	1.550470000	-0.372277000	2.549853000
	1	4.773001000	4.411190000	-1.482101000
	1	3.372646000	3.418283000	-0.952840000
	1	3.494835000	5.141081000	-0.466648000
	1	6.591252000	5.094804000	0.207811000
	1	5.380372000	5.841401000	1.291957000
	1	6.479220000	4.576413000	1.922320000
	79	2.793600000	0.153563000	-0.303460000
	6	1.255377000	-0.162686000	-2.855914000
	6	0.500617000	0.556162000	-3.812752000
	6	2.149216000	-1.169269000	-3.290488000
	6	0.649834000	0.271978000	-5.179518000
	1	-0.186276000	1.342978000	-3.466234000
	6	2.296798000	-1.437556000	-4.662711000
	1	2.726216000	-1.732226000	-2.538700000
	6	1.547422000	-0.722894000	-5.613512000
	1	0.065128000	0.844763000	-5.917301000
	1	3.001294000	-2.219767000	-4.987713000
	1	1.662424000	-0.936855000	-6.687405000
	8	1.088952000	0.121360000	-1.523881000
	6	-1.287477000	2.125751000	-0.879122000
	6	-2.176683000	2.882385000	-1.683320000
	6	-0.240144000	2.804371000	-0.207547000
	6	-1.999402000	4.266756000	-1.840715000

	1	-3.007980000	2.372013000	-2.195390000
	6	-0.084880000	4.192123000	-0.347416000
	1	0.451837000	2.231426000	0.427663000
	6	-0.956462000	4.929168000	-1.169847000
	1	-2.689998000	4.832239000	-2.485875000
	1	0.732285000	4.699124000	0.189163000
	1	-0.825737000	6.016838000	-1.284001000
	6	-0.549512000	-1.808811000	-0.790975000
	6	-0.253879000	-2.432848000	0.449097000
	6	-0.672926000	-2.614676000	-1.954279000
	6	-0.101271000	-3.824732000	0.524365000
	1	-0.158470000	-1.810992000	1.351575000
	6	-0.509549000	-4.006095000	-1.870693000
	1	-0.902143000	-2.137486000	-2.918149000
	6	-0.224016000	-4.614083000	-0.634943000
	1	0.110868000	-4.298466000	1.495297000
	1	-0.609101000	-4.620930000	-2.778894000
	1	-0.101029000	-5.707028000	-0.573733000

## XVII [Au(IPr)(OPh)(PhCCPh)(IPr)(Cu)]<sup>+</sup> min

	6	4.979817000	0.166561000	0.197447000
	7	5.680652000	1.351720000	0.201107000
	7	5.943686000	-0.783490000	0.453752000
	6	7.035574000	1.143839000	0.454765000
	6	7.201685000	-0.207583000	0.612623000
	6	5.120010000	2.664510000	-0.040645000
	6	5.708994000	-2.210988000	0.540733000
	1	7.751219000	1.970537000	0.500932000
	1	8.093724000	-0.806978000	0.819306000
	6	4.528560000	3.365539000	1.044250000
	6	4.028092000	4.657988000	0.782141000
	6	4.131911000	5.233121000	-0.492660000
	6	4.732674000	4.520871000	-1.540409000
	6	5.238801000	3.218937000	-1.343162000
	6	4.415315000	2.767507000	2.447509000
	1	3.561541000	5.231347000	1.598397000
	1	3.747704000	6.250399000	-0.669035000
	1	4.814986000	4.985487000	-2.535831000
	6	5.889664000	2.468489000	-2.506588000
	6	5.746992000	-2.979092000	-0.653883000
	6	5.557185000	-4.371614000	-0.532884000
	6	5.356295000	-4.971288000	0.718575000
	6	5.329587000	-4.186837000	1.879725000
	6	5.503176000	-2.788426000	1.821466000
	6	5.973680000	-2.355594000	-2.032003000
	1	5.577295000	-4.999471000	-1.437500000
	1	5.222854000	-6.062461000	0.789183000
	1	5.169373000	-4.669547000	2.856476000
	6	5.473670000	-1.961586000	3.107534000
	1	5.032002000	1.844495000	2.469873000
	6	2.961008000	2.348540000	2.755152000
	6	4.971604000	3.712534000	3.532859000
	1	6.196509000	1.469028000	-2.134244000
	6	4.891660000	2.232778000	-3.660093000
	6	7.164125000	3.186561000	-3.001397000
	1	6.203485000	-1.279783000	-1.882837000
	6	7.180286000	-2.984173000	-2.760338000
	6	4.692015000	-2.428786000	-2.890292000
	1	5.569728000	-0.892786000	2.823105000
	6	4.129869000	-2.114390000	3.850931000
	6	6.668547000	-2.304122000	4.024126000
	1	2.892841000	1.885938000	3.761980000
	1	2.275996000	3.222592000	2.735239000
	1	2.588416000	1.607538000	2.014232000
	1	4.959941000	3.210496000	4.522573000
	1	6.016469000	4.016368000	3.316823000

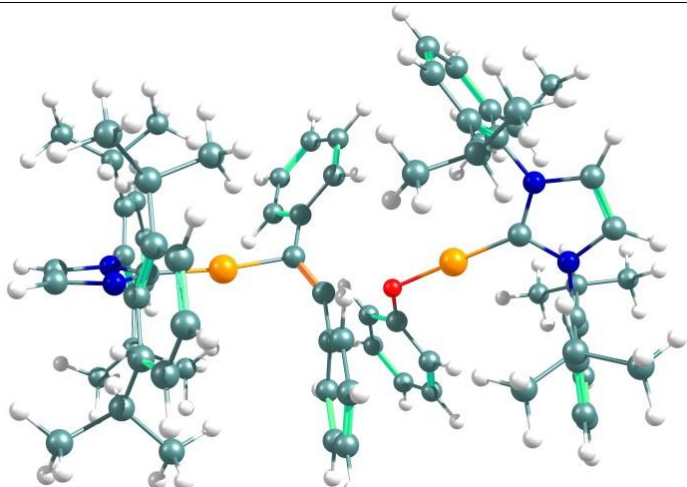
  

Zero-point correction=	1.388242
(Hartree/Particle)	
Thermal correction to Energy=	1.475152
Thermal correction to Enthalpy=	1.476096
Thermal correction to Gibbs Free Energy=	1.251334
Sum of electronic and zero-point Energies=	-3496.021815
Sum of electronic and thermal Energies=	-3495.934905
Sum of electronic and thermal Enthalpies=	-3495.933961
Sum of electronic and thermal Free Energies=	-3496.158723

	1	4.365249000	4.637672000	3.628915000
	1	5.364637000	1.630189000	-4.463430000
	1	3.987177000	1.694956000	-3.310052000
	1	4.559208000	3.188751000	-4.116631000
	1	7.655360000	2.598577000	-3.804523000
	1	6.931325000	4.188914000	-3.418921000
	1	7.901058000	3.328979000	-2.184209000
	1	7.366881000	-2.462565000	-3.722199000
	1	8.105546000	-2.918782000	-2.151625000
	1	7.008631000	-4.055538000	-2.995691000
	1	4.849497000	-1.934449000	-3.871715000
	1	4.396347000	-3.481223000	-3.086338000
	1	3.842156000	-1.924870000	-2.382520000
	1	4.101198000	-1.447236000	4.737841000
	1	3.271843000	-1.860936000	3.195533000
	1	3.977811000	-3.152520000	4.213675000
	1	6.663647000	-1.661120000	4.929070000
	1	6.628682000	-3.360086000	4.365361000
	1	7.639509000	-2.157654000	3.507325000
	29	3.113486000	-0.175494000	-0.025014000
	6	0.339684000	-0.274702000	-0.986125000
	6	1.289247000	-0.769451000	-0.149138000
	6	-4.417737000	0.614323000	0.462033000
	7	-5.645896000	0.007237000	0.396493000
	7	-4.640349000	1.819031000	1.077246000
	6	-6.623053000	0.823524000	0.959012000
	6	-5.990595000	1.962262000	1.387501000
	6	-5.913117000	-1.305596000	-0.163205000
	6	-3.642310000	2.833347000	1.367461000
	1	-7.673743000	0.520743000	0.999691000
	1	-6.375210000	2.860257000	1.880161000
	6	-5.951446000	-2.417786000	0.719865000
	6	-6.251132000	-3.675381000	0.156195000
	6	-6.498981000	-3.816079000	-1.216744000
	6	-6.453102000	-2.697713000	-2.060561000
	6	-6.162508000	-1.412580000	-1.557235000
	6	-5.711343000	-2.292767000	2.225409000
	1	-6.294775000	-4.561324000	0.808592000
	1	-6.735423000	-4.808024000	-1.632898000
	1	-6.652531000	-2.822331000	-3.136338000
	6	-6.146656000	-0.208784000	-2.499860000
	6	-3.427342000	3.858190000	0.409163000
	6	-2.483808000	4.854165000	0.736339000
	6	-1.799447000	4.832332000	1.958991000
	6	-2.043913000	3.811513000	2.888679000
	6	-2.973779000	2.786157000	2.620123000
	6	-4.202362000	3.941795000	-0.906659000
	1	-2.286704000	5.665266000	0.018473000
	1	-1.070664000	5.624107000	2.193549000
	1	-1.506362000	3.813416000	3.849347000
	6	-3.278699000	1.723513000	3.677153000
	1	-5.377935000	-1.253621000	2.431691000
	6	-4.589099000	-3.231928000	2.714194000
	6	-7.018728000	-2.522629000	3.016822000
	1	-5.827036000	0.677604000	-1.912432000
	6	-5.122783000	-0.389002000	-3.639968000
	6	-7.559262000	0.088597000	-3.050167000
	1	-4.773641000	2.997236000	-1.027769000
	6	-5.228383000	5.097374000	-0.864986000
	6	-3.269989000	4.063560000	-2.128023000
	1	-3.838301000	0.903886000	3.178304000
	6	-2.005709000	1.099908000	4.282682000
	6	-4.190462000	2.302902000	4.783398000
	1	-4.398370000	-3.071735000	3.795754000
	1	-4.859005000	-4.300928000	2.585120000
	1	-3.639699000	-3.053823000	2.168913000
	1	-6.847455000	-2.379479000	4.104057000
	1	-7.819862000	-1.822146000	2.702906000
	1	-7.403204000	-3.553993000	2.871035000
	1	-5.076215000	0.526084000	-4.266024000
	1	-4.106191000	-0.587389000	-3.241385000
	1	-5.394342000	-1.233203000	-4.307455000
	1	-7.543141000	0.990880000	-3.696320000
	1	-7.941959000	-0.754229000	-3.663244000
	1	-8.289728000	0.265842000	-2.234022000

1	-5.820712000	5.127632000	-1.803247000
1	-5.937542000	4.992308000	-0.017883000
1	-4.722924000	6.079881000	-0.755103000
1	-3.863197000	4.047490000	-3.065912000
1	-2.699295000	5.015513000	-2.119359000
1	-2.537756000	3.232063000	-2.168432000
1	-2.275452000	0.277660000	4.977098000
1	-1.340341000	0.683750000	3.499424000
1	-1.419506000	1.838653000	4.867930000
1	-4.450708000	1.520378000	5.526404000
1	-3.683781000	3.128842000	5.325690000
1	-5.136734000	2.708467000	4.370182000
79	-2.732822000	-0.127024000	-0.255682000
6	-0.987053000	-2.238881000	-1.759092000
6	-0.025896000	-2.561987000	-2.731130000
6	-2.026875000	-3.126430000	-1.441059000
6	-0.119743000	-3.799288000	-3.391570000
1	0.786369000	-1.857843000	-2.961071000
6	-2.108281000	-4.357093000	-2.114188000
1	-2.760681000	-2.854838000	-0.664916000
6	-1.156676000	-4.699572000	-3.090348000
1	0.629621000	-4.055603000	-4.156811000
1	-2.922246000	-5.054118000	-1.861990000
1	-1.221085000	-5.666093000	-3.613083000
8	-0.954876000	-0.990942000	-1.104059000
6	0.984391000	-1.923873000	0.741255000
6	0.007975000	-1.816087000	1.765963000
6	1.693247000	-3.147437000	0.634955000
6	-0.251815000	-2.885271000	2.639429000
1	-0.540409000	-0.866544000	1.882686000
6	1.413373000	-4.224759000	1.491261000
1	2.469542000	-3.252463000	-0.139610000
6	0.442511000	-4.100741000	2.501144000
1	-1.002911000	-2.766902000	3.437293000
1	1.969733000	-5.167881000	1.372516000
1	0.234876000	-4.941548000	3.181611000
6	0.359934000	0.906391000	-1.870653000
6	-0.462042000	0.984224000	-3.025820000
6	1.211687000	2.004834000	-1.587386000
6	-0.403797000	2.097657000	-3.880259000
1	-1.140572000	0.153489000	-3.269836000
6	1.263463000	3.116662000	-2.439654000
1	1.830094000	1.976258000	-0.675185000
6	0.460469000	3.168355000	-3.594956000
1	-1.038592000	2.124150000	-4.780199000
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## II+VIII-XVIII TS

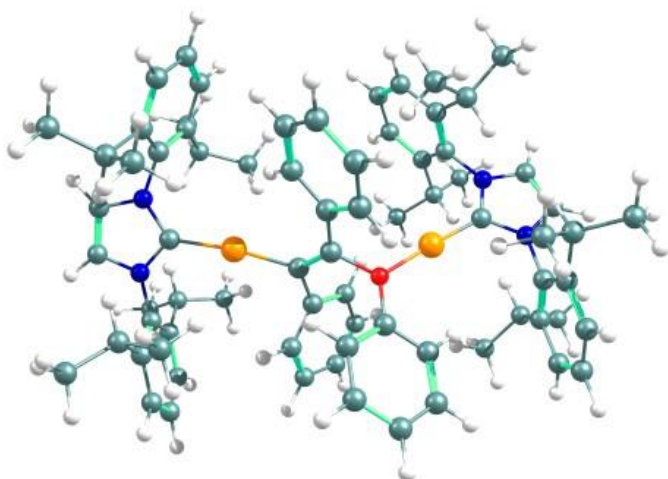
	6	-4.756672000	-0.281093000	0.284218000
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	6	-7.036438000	-0.108825000	0.278644000
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	6	-4.018440000	-1.485157000	3.295563000
	6	-3.311426000	-2.377108000	4.128651000
	6	-3.161815000	-3.728220000	3.785480000
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	6	-4.177653000	-0.019399000	3.701898000
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	1	-2.615039000	-4.408043000	4.458078000
	1	-3.596807000	-5.283765000	2.339557000
	6	-5.039567000	-3.941109000	0.435949000
	6	-5.715080000	0.906076000	-2.684560000
	6	-5.666658000	1.904134000	-3.680149000
	6	-5.690654000	3.265875000	-3.345956000
	6	-5.760424000	3.660722000	-2.002754000

Zero-point correction= 1.386041 (Hartree/Particle)

Thermal correction to Energy=	1.473336	6	-5.803718000	2.709393000	-0.962140000
Thermal correction to Enthalpy=	1.474280	6	-5.689605000	-0.571473000	-3.079153000
Thermal correction to Gibbs Free Energy=	1.247013	1	-5.618160000	1.607282000	-4.739515000
Sum of electronic and zero-point Energies=	-3557.595121	1	-5.661089000	4.026845000	-4.141778000
Sum of electronic and thermal Energies=	-3557.507827	1	-5.783049000	4.733085000	-1.753196000
Sum of electronic and thermal Enthalpies=	-3557.506883	6	-5.893722000	3.173993000	0.492409000
Sum of electronic and thermal Free Energies=	-3557.734150	1	-4.885320000	0.453114000	2.988673000
		6	-2.837319000	0.737398000	3.580247000
		6	-4.785354000	0.130995000	5.112281000
		1	-5.421076000	-3.086503000	-0.161241000
		6	-3.999152000	-4.671811000	-0.437141000
		6	-6.241648000	-4.857734000	0.756688000
		1	-5.877426000	-1.169199000	-2.162405000
		6	-6.803498000	-0.924731000	-4.086977000
		6	-4.297022000	-0.978142000	-3.608184000
		1	-5.848788000	2.272692000	1.139271000
		6	-4.700068000	4.071190000	0.881716000
		6	-7.240712000	3.876443000	0.773296000
		1	-2.967396000	1.810341000	3.833165000
		1	-2.073477000	0.316984000	4.268157000
		1	-2.432792000	0.676713000	2.546645000
		1	-4.960557000	1.202128000	5.344060000
		1	-5.755151000	-0.400522000	5.199170000
		1	-4.111458000	-0.268461000	5.899065000
		1	-4.461386000	-4.999600000	-1.391592000
		1	-3.135970000	-4.018910000	-0.678131000
		1	-3.605547000	-5.580801000	0.064241000
		1	-6.715277000	-5.223439000	-0.178207000
		1	-5.924914000	-5.746348000	1.342570000
		1	-7.018723000	-4.330360000	1.347561000
		1	-6.805787000	-2.015381000	-4.292335000
		1	-7.806727000	-0.647368000	-3.703123000
		1	-6.661403000	-0.408924000	-5.059559000
		1	-4.269102000	-2.062381000	-3.844179000
		1	-4.037173000	-0.424590000	-4.535112000
		1	-3.505755000	-0.768822000	-2.856601000
		1	-4.746098000	4.327672000	1.960725000
		1	-3.731253000	3.569060000	0.683627000
		1	-4.703460000	5.026342000	0.316117000
		1	-7.313191000	4.167931000	1.841888000
		1	-7.349243000	4.800179000	0.166802000
		1	-8.104703000	3.220709000	0.539239000
		29	-2.932073000	0.048592000	-0.139903000
		6	-0.398652000	-0.385882000	-0.747477000
		6	-1.149285000	0.667543000	-0.621445000
		6	4.551645000	0.265656000	0.682540000
		7	5.707922000	-0.449973000	0.465499000
		7	4.861892000	1.090807000	1.739584000
		6	6.706588000	-0.080557000	1.362254000
		6	6.172196000	0.891640000	2.168305000
		6	5.891409000	-1.440555000	-0.577359000
		6	3.982202000	2.089450000	2.311612000
		1	7.701032000	-0.536998000	1.344310000
		1	6.603596000	1.460526000	2.997678000
		6	6.322568000	-1.004817000	-1.859100000
		6	6.518834000	-1.995696000	-2.843647000
		6	6.302071000	-3.352237000	-2.564430000
		6	5.885948000	-3.751467000	-1.286461000
		6	5.673558000	-2.807795000	-0.260097000
		6	6.616674000	0.460876000	-2.181763000
		1	6.853356000	-1.696281000	-3.849100000
		1	6.466096000	-4.107398000	-3.349351000
		1	5.727679000	-4.821075000	-1.077289000
		6	5.261129000	-3.275222000	1.136263000
		6	3.132651000	1.716211000	3.386801000
		6	2.319798000	2.723285000	3.947459000
		6	2.357270000	4.039402000	3.464942000
		6	3.211203000	4.378086000	2.405893000
		6	4.046088000	3.414071000	1.802302000
		6	3.106582000	0.298950000	3.960178000
		1	1.649617000	2.473343000	4.784780000
		1	1.717994000	4.810270000	3.923410000
		1	3.238837000	5.417361000	2.041868000
		6	4.975705000	3.817706000	0.656887000
		1	6.266826000	1.072649000	-1.323696000

	6	5.851934000	0.952108000	-3.427933000
	6	8.137640000	0.693660000	-2.327613000
	1	5.041179000	-2.371843000	1.743161000
	6	3.974815000	-4.125203000	1.106235000
	6	6.416706000	-4.029553000	1.831207000
	1	3.696969000	-0.349842000	3.279875000
	6	3.779117000	0.250059000	5.350353000
	6	1.678449000	-0.280698000	4.008744000
	1	5.545789000	2.916118000	0.349788000
	6	4.180396000	4.290563000	-0.578387000
	6	6.004102000	4.877221000	1.108471000
	1	6.029256000	2.036415000	-3.584318000
	1	6.185302000	0.430396000	-4.349378000
	1	4.759246000	0.790509000	-3.328121000
	1	8.352532000	1.766651000	-2.513757000
	1	8.691003000	0.386996000	-1.415989000
	1	8.552483000	0.115416000	-3.180061000
	1	3.669896000	-4.398377000	2.138181000
	1	3.135093000	-3.576813000	0.632748000
	1	4.119628000	-5.072703000	0.545880000
	1	6.130601000	-4.318445000	2.864178000
	1	6.679002000	-4.958929000	1.283117000
	1	7.335099000	-3.410078000	1.892723000
	1	3.795930000	-0.788830000	5.741403000
	1	4.825464000	0.616529000	5.313173000
	1	3.232252000	0.877894000	6.085116000
	1	1.702203000	-1.338759000	4.342950000
	1	1.030430000	0.274067000	4.719302000
	1	1.194898000	-0.243082000	3.010938000
	1	4.868704000	4.516333000	-1.419200000
	1	3.462147000	3.517085000	-0.919744000
	1	3.604590000	5.215556000	-0.364926000
	1	6.705622000	5.113905000	0.281679000
	1	5.510798000	5.826459000	1.405996000
	1	6.602868000	4.526530000	1.974257000
	29	2.968960000	0.141067000	-0.293543000
	6	1.595998000	-0.200708000	-2.710412000
	6	0.887621000	0.560572000	-3.671931000
	6	2.445423000	-1.246035000	-3.148251000
	6	1.039303000	0.282450000	-5.039410000
	1	0.232595000	1.374648000	-3.326427000
	6	2.595837000	-1.509190000	-4.521158000
	1	2.986130000	-1.844114000	-2.396652000
	6	1.892759000	-0.750854000	-5.473520000
	1	0.490562000	0.888495000	-5.778411000
	1	3.265608000	-2.321650000	-4.845272000
	1	2.008874000	-0.960868000	-6.548097000
	8	1.438062000	0.070393000	-1.379110000
	6	-0.960123000	2.120897000	-0.766733000
	6	-1.747786000	2.854140000	-1.689911000
	6	-0.017599000	2.822501000	0.024797000
	6	-1.572796000	4.239352000	-1.840289000
	1	-2.498345000	2.325146000	-2.298429000
	6	0.135068000	4.211256000	-0.114189000
	1	0.592974000	2.271581000	0.756459000
	6	-0.634484000	4.925993000	-1.049906000
	1	-2.183993000	4.786180000	-2.575442000
	1	0.869388000	4.735985000	0.516553000
	1	-0.506465000	6.014388000	-1.159185000
	6	-0.268975000	-1.827771000	-0.671991000
	6	-0.010914000	-2.464881000	0.570288000
	6	-0.379561000	-2.624089000	-1.843418000
	6	0.120501000	-3.859115000	0.638641000
	1	0.070375000	-1.851925000	1.480453000
	6	-0.238557000	-4.018275000	-1.765853000
	1	-0.581811000	-2.136958000	-2.808191000
	6	0.012046000	-4.638795000	-0.528865000
	1	0.305310000	-4.342647000	1.610406000
	1	-0.327764000	-4.625480000	-2.680241000
	1	0.117986000	-5.733739000	-0.472749000

# XVIII [Cu(IPr)(OPh)(PhCCPh)(IPr)(Cu)]<sup>+</sup> min



Zero-point correction= 1.387764  
 (Hartree/Particle)  
 Thermal correction to Energy= 1.474701  
 Thermal correction to Enthalpy= 1.475645  
 Thermal correction to Gibbs Free Energy= 1.250251  
 Sum of electronic and zero-point Energies= -3557.607692  
 Sum of electronic and thermal Energies= -3557.520755  
 Sum of electronic and thermal Enthalpies= -3557.519811  
 Sum of electronic and thermal Free Energies= -3557.745205

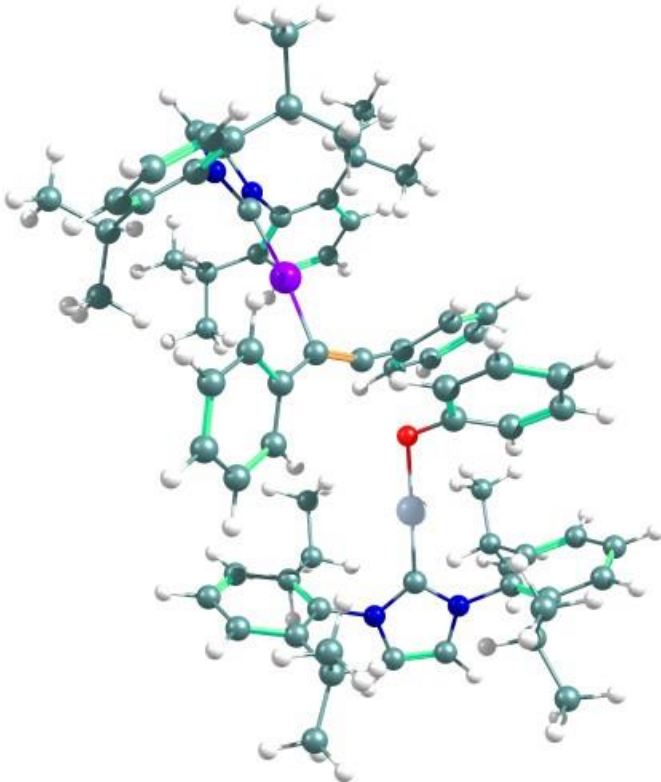
6	4.626924000	0.062074000	0.174570000
7	5.371325000	1.219781000	0.139162000
7	5.548409000	-0.909186000	0.497568000
6	6.711495000	0.975103000	0.434387000
6	6.823424000	-0.372501000	0.658950000
6	4.862192000	2.539177000	-0.170926000
6	5.256172000	-2.320180000	0.654753000
1	7.456410000	1.776485000	0.459337000
1	7.687557000	-0.993261000	0.915314000
6	4.262330000	3.300221000	0.867960000
6	3.805982000	4.593738000	0.539994000
6	3.959440000	5.112882000	-0.753643000
6	4.570339000	4.343240000	-1.753901000
6	5.034695000	3.037333000	-1.490068000
6	4.096127000	2.763358000	2.290489000
1	3.333340000	5.212038000	1.319040000
1	3.607557000	6.131507000	-0.981812000
1	4.695326000	4.764863000	-2.763739000
6	5.704491000	2.225660000	-2.600528000
6	5.293104000	-3.153819000	-0.494878000
6	5.046584000	-4.529398000	-0.303559000
6	4.788945000	-5.050568000	0.972548000
6	4.762265000	-4.202409000	2.088041000
6	4.994386000	-2.817311000	1.958878000
6	5.574671000	-2.614315000	-1.897978000
1	5.066740000	-5.207252000	-1.171322000
1	4.610570000	-6.130239000	1.098694000
1	4.556384000	-4.623404000	3.084711000
6	4.955334000	-1.919171000	3.195502000
1	4.691323000	1.829395000	2.367871000
6	2.624558000	2.388596000	2.570914000
6	4.642374000	3.739901000	3.352654000
1	5.967500000	1.232590000	-2.180427000
6	4.744632000	1.975395000	-3.782844000
6	7.017229000	2.889012000	-3.071518000
1	5.846126000	-1.542498000	-1.798808000
6	6.768195000	-3.328669000	-2.566143000
6	4.308432000	-2.680390000	-2.779628000
1	5.152557000	-0.878168000	2.864074000
6	3.558762000	-1.928017000	3.853113000
6	6.059838000	-2.296006000	4.206579000
1	2.514150000	1.976545000	3.595764000
1	1.958387000	3.273041000	2.485362000
1	2.259870000	1.620794000	1.853440000
1	4.593075000	3.278100000	4.360646000
1	5.698942000	4.013851000	3.154380000
1	4.053418000	4.680184000	3.395383000
1	5.230731000	1.332369000	-4.545937000
1	3.812658000	1.474726000	-3.450282000
1	4.456485000	2.922941000	-4.284756000
1	7.522190000	2.256441000	-3.831019000
1	6.829003000	3.879755000	-3.536379000
1	7.725590000	3.044269000	-2.231724000
1	6.997635000	-2.863148000	-3.547247000
1	7.682019000	-3.272402000	-1.939584000
1	6.555474000	-4.402076000	-2.753847000
1	4.506562000	-2.247356000	-3.782398000
1	3.972053000	-3.728818000	-2.925247000
1	3.470776000	-2.113913000	-2.319276000
1	3.530206000	-1.222628000	4.710022000
1	2.769171000	-1.633546000	3.131749000
1	3.296233000	-2.934148000	4.241839000
1	6.051751000	-1.598640000	5.070207000
1	5.914352000	-3.321458000	4.606867000
1	7.068988000	-2.257731000	3.746764000
29	2.753821000	-0.219189000	-0.080493000
6	-0.008039000	-0.268830000	-1.113237000
6	0.911469000	-0.744179000	-0.231520000
6	-4.353521000	0.660220000	0.470115000
7	-5.629299000	0.160465000	0.349469000
7	-4.508435000	1.822117000	1.189216000
6	-6.555837000	0.992272000	0.970042000



	6	-5.848287000	2.041442000	1.498752000
	6	-5.979169000	-1.073503000	-0.327325000
	6	-3.442072000	2.721963000	1.587870000
	1	-7.626486000	0.765966000	0.977327000
	1	-6.176515000	2.920648000	2.061117000
	6	-6.057900000	-2.267131000	0.440497000
	6	-6.428777000	-3.446694000	-0.238774000
	6	-6.709187000	-3.436553000	-1.612840000
	6	-6.626879000	-2.241695000	-2.340872000
	6	-6.265880000	-1.028800000	-1.717776000
	6	-5.802523000	-2.300110000	1.948326000
	1	-6.504199000	-4.390717000	0.323114000
	1	-7.001687000	-4.369235000	-2.120490000
	1	-6.854003000	-2.247478000	-3.418379000
	6	-6.216737000	0.261819000	-2.536421000
	6	-3.064886000	3.763000000	0.697793000
	6	-2.050922000	4.642963000	1.130206000
	6	-1.455171000	4.501426000	2.390677000
	6	-1.859655000	3.472189000	3.252594000
	6	-2.864189000	2.557114000	2.876227000
	6	-3.759309000	3.991294000	-0.645641000
	1	-1.729286000	5.460750000	0.467330000
	1	-0.671777000	5.207002000	2.709363000
	1	-1.388961000	3.379440000	4.243149000
	6	-3.338427000	1.485929000	3.861083000
	1	-5.386227000	-1.313530000	2.242801000
	6	-4.761239000	-3.366778000	2.343948000
	6	-7.125431000	-2.494648000	2.724035000
	1	-5.881276000	1.079784000	-1.864779000
	6	-5.191436000	0.167243000	-3.685870000
	6	-7.617654000	0.646424000	-3.061849000
	1	-4.332328000	3.071927000	-0.890658000
	6	-4.773632000	5.153832000	-0.537231000
	6	-2.766589000	4.228933000	-1.799661000
	1	-3.887972000	0.714254000	3.280318000
	6	-2.178066000	0.773344000	4.583210000
	6	-4.324175000	2.091077000	4.888279000
	1	-4.559850000	-3.319393000	3.434301000
	1	-5.117241000	-4.394839000	2.123800000
	1	-3.798306000	-3.219522000	1.813522000
	1	-6.944250000	-2.467073000	3.818733000
	1	-7.866431000	-1.705430000	2.481161000
	1	-7.591754000	-3.473622000	2.485065000
	1	-5.129225000	1.131801000	-4.231193000
	1	-4.178435000	-0.078026000	-3.304725000
	1	-5.471877000	-0.614332000	-4.422559000
	1	-7.577411000	1.614587000	-3.602956000
	1	-8.010861000	-0.114054000	-3.768729000
	1	-8.352379000	0.746849000	-2.236696000
	1	-5.311859000	5.293763000	-1.497928000
	1	-5.530767000	4.972562000	0.253326000
	1	-4.261360000	6.108779000	-0.294770000
	1	-3.312375000	4.302946000	-2.762864000
	1	-2.204660000	5.177965000	-1.673702000
	1	-2.028512000	3.406486000	-1.888758000
	1	-2.567552000	-0.065477000	5.196396000
	1	-1.435647000	0.361968000	3.870186000
	1	-1.640502000	1.453809000	5.276029000
	1	-4.702366000	1.307627000	5.577611000
	1	-3.824981000	2.870505000	5.501736000
	1	-5.200018000	2.563613000	4.398901000
	29	-2.827512000	-0.099682000	-0.284638000
	6	-1.434026000	-2.176857000	-1.845077000
	6	-0.433431000	-2.627027000	-2.721469000
	6	-2.593841000	-2.935222000	-1.617088000
	6	-0.607788000	-3.859990000	-3.374170000
	1	0.470080000	-2.022699000	-2.885146000
	6	-2.751635000	-4.165098000	-2.277289000
	1	-3.369548000	-2.564985000	-0.925111000
	6	-1.760641000	-4.634012000	-3.157081000
	1	0.173680000	-4.214506000	-4.064445000
	1	-3.659735000	-4.759277000	-2.092802000
	1	-1.886049000	-5.599233000	-3.670955000
	8	-1.329852000	-0.933912000	-1.192155000
	6	0.544465000	-1.834089000	0.714790000

6	-0.410536000	-1.615480000	1.741852000
6	1.167951000	-3.106390000	0.656582000
6	-0.731953000	-2.624924000	2.664830000
1	-0.884053000	-0.622047000	1.825363000
6	0.826024000	-4.123020000	1.563049000
1	1.928036000	-3.297063000	-0.117709000
6	-0.122245000	-3.889214000	2.575080000
1	-1.463133000	-2.420129000	3.463365000
1	1.316469000	-5.105964000	1.482711000
1	-0.377377000	-4.683047000	3.294578000
6	0.077649000	0.843318000	-2.081803000
6	-0.749563000	0.890451000	-3.235114000
6	1.002283000	1.901832000	-1.886967000
6	-0.632090000	1.934111000	-4.168010000
1	-1.478423000	0.087295000	-3.418173000
6	1.113694000	2.944051000	-2.818047000
1	1.631597000	1.900706000	-0.981455000
6	0.301014000	2.965137000	-3.967527000
1	-1.275171000	1.936283000	-5.062378000
1	1.838889000	3.752084000	-2.635263000
1	0.390027000	3.784926000	-4.697594000

## IV+XIII-XIX TS

	6	-5.011312000	-0.281854000	0.356435000
	7	-5.550044000	-1.231901000	1.185548000
	7	-6.084827000	0.449110000	-0.086044000
	6	-6.935332000	-1.097669000	1.256977000
	6	-7.272350000	-0.037748000	0.454506000
	6	-4.807131000	-2.254122000	1.897306000
	6	-6.012645000	1.580423000	-0.991736000
	1	-7.549302000	-1.765591000	1.868919000
	1	-8.242138000	0.411164000	0.218981000
	6	-4.294155000	-1.947515000	3.185376000
	6	-3.613937000	-2.976698000	3.868915000
	6	-3.458365000	-4.248206000	3.299163000
	6	-3.977115000	-4.518573000	2.025316000
	6	-4.664541000	-3.530069000	1.291172000
	6	-4.462948000	-0.576194000	3.840974000
	1	-3.204429000	-2.778055000	4.871966000
	1	-2.929844000	-5.038269000	3.855728000
	1	-3.848188000	-5.521384000	1.588702000
	6	-5.219172000	-3.857355000	-0.095942000
	6	-6.076701000	1.335992000	-2.389432000
	6	-6.032428000	2.459149000	-3.241594000
	6	-5.938066000	3.759579000	-2.725852000
	6	-5.881682000	3.967040000	-1.340400000
	6	-5.917179000	2.884414000	-0.437183000
	6	-6.196499000	-0.068059000	-2.982974000
	1	-6.079591000	2.311044000	-4.331924000
	1	-5.913194000	4.621080000	-3.411771000
	1	-5.811518000	4.993583000	-0.947883000
	6	-5.873215000	3.143872000	1.069396000
	1	-5.002658000	0.077638000	3.124161000
	6	-3.098705000	0.090278000	4.120017000
	6	-5.321882000	-0.663607000	5.121321000
	1	-5.704146000	-2.941436000	-0.493679000
	6	-4.090249000	-4.231937000	-1.079585000
	6	-6.299928000	-4.958250000	-0.029844000
	1	-6.218762000	-0.790995000	-2.140704000
	6	-7.514875000	-0.240455000	-3.768013000
	6	-4.968909000	-0.421057000	-3.849593000
	1	-5.826393000	2.159625000	1.581048000
	6	-4.610042000	3.929023000	1.481025000
	6	-7.159320000	3.850689000	1.552218000
	1	-3.243050000	1.105519000	4.544838000
	1	-2.501111000	-0.494208000	4.850987000
	1	-2.500382000	0.189259000	3.190465000
	1	-5.479734000	0.346377000	5.553897000
	1	-6.318251000	-1.106996000	4.917356000
	1	-4.832567000	-1.286161000	5.899696000
	1	-4.504225000	-4.409542000	-2.094064000
	1	-3.331943000	-3.425484000	-1.150730000

Zero-point correction= 1.385044 (Hartree/Particle)  
 Thermal correction to Energy= 1.473062  
 Thermal correction to Enthalpy= 1.474006  
 Thermal correction to Gibbs Free Energy= 1.241990  
 Sum of electronic and zero-point Energies= -3445.625104  
 Sum of electronic and thermal Energies= -3445.537086  
 Sum of electronic and thermal Enthalpies= -3445.536142  
 Sum of electronic and thermal Free Energies= -3445.768158

	1	-3.566663000	-5.159610000	-0.766890000
	1	-6.729792000	-5.142795000	-1.036364000
	1	-5.880321000	-5.919860000	0.333453000
	1	-7.131289000	-4.679239000	0.649920000
	1	-7.611613000	-1.281551000	-4.140355000
	1	-8.400084000	-0.019833000	-3.136521000
	1	-7.558060000	0.432263000	-4.650257000
	1	-5.046807000	-1.461599000	-4.227806000
	1	-4.884602000	0.247700000	-4.731806000
	1	-4.028341000	-0.335839000	-3.266730000
	1	-4.571304000	4.045252000	2.584197000
	1	-3.684826000	3.411572000	1.154398000
	1	-4.598842000	4.948746000	1.042119000
	1	-7.139757000	3.985948000	2.653784000
	1	-7.266182000	4.856476000	1.094148000
	1	-8.069542000	3.269850000	1.296355000
	79	-3.066751000	0.060039000	-0.114544000
	6	-0.434776000	-0.416296000	-0.662246000
	6	-1.106588000	0.686428000	-0.631297000
	6	5.157460000	0.306079000	0.684271000
	7	6.296401000	-0.440921000	0.516019000
	7	5.495537000	1.234028000	1.637270000
	6	7.321047000	0.009655000	1.345533000
	6	6.814681000	1.068048000	2.055800000
	6	6.439865000	-1.548468000	-0.409661000
	6	4.622856000	2.281800000	2.129300000
	1	8.309533000	-0.459932000	1.353832000
	1	7.268431000	1.713570000	2.814127000
	6	6.828149000	-1.270065000	-1.747352000
	6	6.984012000	-2.371051000	-2.615173000
	6	6.770656000	-3.683388000	-2.171364000
	6	6.394283000	-3.925531000	-0.842754000
	6	6.220626000	-2.866411000	0.072188000
	6	7.104305000	0.145255000	-2.257077000
	1	7.283957000	-2.193510000	-3.659727000
	1	6.903583000	-4.526879000	-2.867070000
	1	6.234421000	-4.961748000	-0.505427000
	6	5.819964000	-3.165061000	1.517829000
	6	3.795286000	2.009905000	3.250473000
	6	2.975047000	3.058405000	3.716808000
	6	2.987519000	4.318662000	3.103166000
	6	3.823479000	4.558800000	2.003333000
	6	4.661119000	3.548317000	1.486558000
	6	3.772308000	0.652371000	3.954137000
	1	2.318536000	2.884755000	4.583843000
	1	2.342718000	5.123801000	3.489108000
	1	3.832123000	5.556333000	1.536424000
	6	5.578303000	3.846216000	0.299509000
	1	6.838062000	0.855891000	-1.446732000
	6	6.228781000	0.499741000	-3.477029000
	6	8.606323000	0.340945000	-2.562149000
	1	5.715189000	-2.195798000	2.048975000
	6	4.449627000	-3.870754000	1.590950000
	6	6.911501000	-3.974484000	2.251447000
	1	4.495247000	-0.011001000	3.435384000
	6	4.228011000	0.766830000	5.424883000
	6	2.385884000	-0.016700000	3.842148000
	1	6.068805000	2.894878000	0.005196000
	6	4.791878000	4.345311000	-0.930577000
	6	6.694335000	4.839478000	0.693377000
	1	6.393077000	1.555767000	-3.776071000
	1	6.472205000	-0.132290000	-4.356611000
	1	5.149003000	0.366523000	-3.258757000
	1	8.806356000	1.384962000	-2.881783000
	1	9.237575000	0.128720000	-1.674496000
	1	8.944774000	-0.329270000	-3.380171000
	1	4.151013000	-4.027326000	2.648825000
	1	3.659039000	-3.273056000	1.092280000
	1	4.477021000	-4.867835000	1.103353000
	1	6.628401000	-4.139346000	3.312046000
	1	7.060152000	-4.972022000	1.787261000
	1	7.890055000	-3.451798000	2.237068000
	1	4.259528000	-0.235335000	5.901108000
	1	5.239405000	1.215369000	5.505780000
	1	3.534648000	1.396452000	6.021227000

	1	2.400979000	-1.021913000	4.313048000
	1	1.600593000	0.579702000	4.352550000
	1	2.084718000	-0.136849000	2.780487000
	1	5.475119000	4.485553000	-1.793765000
	1	4.004825000	3.624188000	-1.232086000
	1	4.303148000	5.323762000	-0.738883000
	1	7.384264000	5.008610000	-0.159415000
	1	6.274572000	5.825482000	0.984476000
	1	7.294525000	4.467300000	1.549114000
	47	3.392912000	0.114380000	-0.341273000
	6	1.694415000	-0.346895000	-2.754707000
	6	0.897584000	0.300738000	-3.739583000
	6	2.515446000	-1.433583000	-3.164082000
	6	0.937468000	-0.118921000	-5.077055000
	1	0.263132000	1.144425000	-3.427384000
	6	2.555012000	-1.838328000	-4.509688000
	1	3.124346000	-1.951930000	-2.403709000
	6	1.765664000	-1.188481000	-5.474707000
	1	0.320000000	0.403871000	-5.825814000
	1	3.206571000	-2.677472000	-4.803174000
	1	1.795503000	-1.508498000	-6.527770000
	8	1.632997000	0.060793000	-1.471395000
	6	-0.863366000	2.122931000	-0.837533000
	6	-1.800975000	2.919054000	-1.540901000
	6	0.304725000	2.739479000	-0.324993000
	6	-1.561534000	4.286179000	-1.752474000
	1	-2.718630000	2.451460000	-1.931292000
	6	0.527308000	4.110554000	-0.521997000
	1	1.034086000	2.133124000	0.230834000
	6	-0.398775000	4.888391000	-1.241017000
	1	-2.294230000	4.884825000	-2.315906000
	1	1.438380000	4.572533000	-0.110891000
	1	-0.216069000	5.963059000	-1.398862000
	6	-0.154692000	-1.813471000	-0.544982000
	6	0.211596000	-2.371252000	0.712393000
	6	-0.236736000	-2.664030000	-1.683626000
	6	0.477207000	-3.740895000	0.825281000
	1	0.266934000	-1.713840000	1.592933000
	6	0.036664000	-4.033730000	-1.556985000
	1	-0.521936000	-2.235583000	-2.654993000
	6	0.392611000	-4.574562000	-0.308457000
	1	0.745967000	-4.166848000	1.804414000
	1	-0.029712000	-4.684676000	-2.442501000
	1	0.601216000	-5.652143000	-0.214966000

### XIX [Ag(IPr)(OPh)(PhCCPh)(IPr)(Au)]<sup>+</sup> min

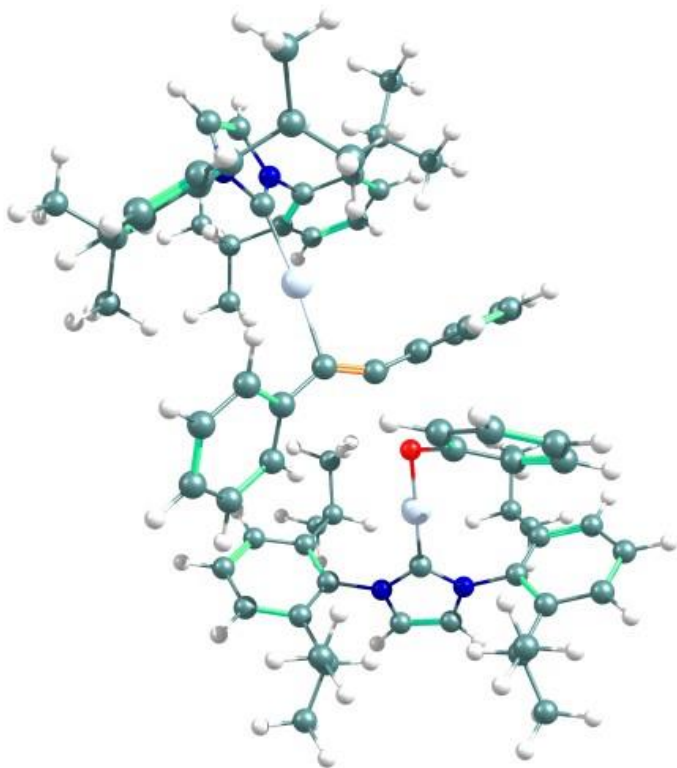
	6	4.836589000	0.177921000	0.227348000
	7	5.539301000	1.357176000	0.167228000
	7	5.784501000	-0.766654000	0.540749000
	6	6.891227000	1.151382000	0.439983000
	6	7.045649000	-0.190434000	0.674328000
	6	4.982219000	2.660218000	-0.135229000
	6	5.530849000	-2.184726000	0.710287000
	1	7.613087000	1.973868000	0.442824000
	1	7.930873000	-0.784695000	0.920969000
	6	4.442917000	3.432094000	0.927976000
	6	3.942952000	4.711384000	0.607570000
	6	3.992671000	5.203579000	-0.704578000
	6	4.537911000	4.419603000	-1.731315000
	6	5.044598000	3.128369000	-1.474402000
	6	4.387067000	2.929601000	2.371163000
	1	3.517072000	5.338734000	1.406457000
	1	3.609276000	6.212019000	-0.927622000
	1	4.576160000	4.818204000	-2.757446000
	6	5.630391000	2.296854000	-2.616947000
	6	5.641883000	-3.032729000	-0.423395000
6	5.427975000	-4.411984000	-0.220625000	
6	5.124717000	-4.920976000	-1.050165000	
6	5.022760000	-4.057368000	2.149448000	
6	5.224547000	-2.668604000	2.009301000	

Zero-point correction= 1.387937 (Hartree/Particle)  
Thermal correction to Energy= 1.475244

Thermal correction to Enthalpy=	1.476189	6	5.960862000	-2.506806000	-1.823684000
Thermal correction to Gibbs Free Energy=	1.248832	1	5.506452000	-5.101656000	-1.075633000
Sum of electronic and zero-point Energies=	-3445.646698	1	4.969482000	-6.003106000	1.185395000
Sum of electronic and thermal Energies=	-3445.559391	1	4.782190000	-4.469125000	3.142139000
Sum of electronic and thermal Enthalpies=	-3445.558447	6	5.105313000	-1.753843000	3.228443000
Sum of electronic and thermal Free Energies=	-3445.785803	1	4.921445000	1.957719000	2.412060000
		6	2.930398000	2.663129000	2.807934000
		6	5.107688000	3.887145000	3.343729000
		1	5.985025000	1.336342000	-2.188516000
		6	4.556178000	1.951845000	-3.670371000
		6	6.850901000	2.991482000	-3.258640000
		1	6.175384000	-1.420949000	-1.737259000
		6	7.217203000	-3.174148000	-2.422204000
		6	4.740202000	-2.652708000	-2.758311000
		1	5.315255000	-0.715906000	2.894893000
		6	3.670626000	-1.765569000	3.798090000
		6	6.149347000	-2.105950000	4.310114000
		1	2.900239000	2.269170000	3.845319000
		1	2.323735000	3.593079000	2.781312000
		1	2.446666000	1.917322000	2.141959000
		1	5.120577000	3.459672000	4.367965000
		1	6.158233000	4.069180000	3.036768000
		1	4.600678000	4.873081000	3.405357000
		1	4.988854000	1.313010000	-4.468550000
		1	3.703542000	1.407899000	-3.215127000
		1	4.153254000	2.864845000	-4.157027000
		1	7.293994000	2.346907000	-4.046020000
		1	6.570601000	3.953539000	-3.736882000
		1	7.641108000	3.208639000	-2.510550000
		1	7.464797000	-2.720914000	-3.404662000
		1	8.099558000	-3.056483000	-1.759917000
		1	7.066794000	-4.261259000	-2.590472000
		1	4.961366000	-2.226062000	-3.759046000
		1	4.464841000	-3.719137000	-2.900689000
		1	3.856984000	-2.122925000	-2.343536000
		1	3.584146000	-1.052137000	4.644387000
		1	2.928247000	-1.480613000	3.024268000
		1	3.390953000	-2.770105000	4.179016000
		1	6.084775000	-1.393088000	5.158510000
		1	5.986683000	-3.124724000	4.720739000
		1	7.183799000	-2.068488000	3.910409000
		79	2.836011000	-0.184315000	-0.026611000
		6	-0.062673000	-0.234764000	-1.064926000
		6	0.863992000	-0.767472000	-0.218080000
		6	-4.900189000	0.591574000	0.483293000
		7	-6.116204000	-0.040788000	0.435476000
		7	-5.153838000	1.790344000	1.097810000
		6	-7.111336000	0.749489000	1.004929000
		6	-6.503144000	1.905514000	1.423916000
		6	-6.354711000	-1.356740000	-0.128304000
		6	-4.172402000	2.824239000	1.372295000
		1	-8.154265000	0.422021000	1.056564000
		1	-6.905912000	2.794473000	1.918912000
		6	-6.355847000	-2.476608000	0.746790000
		6	-6.619639000	-3.738906000	0.175625000
		6	-6.870753000	-3.877967000	-1.196968000
		6	-6.864187000	-2.752932000	-2.033002000
		6	-6.609679000	-1.463020000	-1.521863000
		6	-6.123468000	-2.352282000	2.253742000
		1	-6.633473000	-4.630356000	0.821680000
		1	-7.079817000	-4.873854000	-1.618396000
		1	-7.067898000	-2.875833000	-3.108229000
		6	-6.641304000	-0.252859000	-2.456172000
		6	-3.976471000	3.842048000	0.401517000
		6	-3.041947000	4.852396000	0.710101000
		6	-2.345334000	4.850695000	1.926053000
		6	-2.567856000	3.835543000	2.867134000
		6	-3.488827000	2.797100000	2.617787000
		6	-4.763378000	3.902157000	-0.908755000
		1	-2.860094000	5.658572000	-0.017300000
		1	-1.623421000	5.653002000	2.145448000
		1	-2.018638000	3.852053000	3.821100000
		6	-3.765443000	1.739084000	3.687459000
		1	-5.777533000	-1.317112000	2.459695000
		6	-5.022031000	-3.307208000	2.758203000

	6	-7.441868000	-2.562168000	3.033130000
	1	-6.346328000	0.639304000	-1.864965000
	6	-5.623731000	-0.391583000	-3.607954000
	6	-8.068051000	0.001230000	-2.991525000
	1	-5.306383000	2.940396000	-1.024847000
	6	-5.823792000	5.025921000	-0.858020000
	6	-3.846655000	4.054838000	-2.138953000
	1	-4.326134000	0.910608000	3.204701000
	6	-2.475250000	1.132687000	4.274766000
	6	-4.663635000	2.316864000	4.805392000
	1	-4.834742000	-3.138709000	3.839090000
	1	-5.311763000	-4.372371000	2.641025000
	1	-4.065917000	-3.155818000	2.216574000
	1	-7.279172000	-2.421595000	4.122049000
	1	-8.229754000	-1.850205000	2.711937000
	1	-7.839422000	-3.587827000	2.882079000
	1	-5.610529000	0.529273000	-4.227161000
	1	-4.596322000	-0.563859000	-3.224212000
	1	-5.875612000	-1.238323000	-4.279838000
	1	-8.089166000	0.909646000	-3.628835000
	1	-8.427193000	-0.848676000	-3.609032000
	1	-8.796288000	0.145600000	-2.167028000
	1	-6.422354000	5.041190000	-1.792688000
	1	-6.524194000	4.896329000	-0.007202000
	1	-5.347098000	6.022596000	-0.747286000
	1	-4.447513000	4.015204000	-3.071272000
	1	-3.311599000	5.027293000	-2.138134000
	1	-3.082819000	3.252131000	-2.186750000
	1	-2.723216000	0.310831000	4.977736000
	1	-1.817043000	0.720312000	3.483056000
	1	-1.887298000	1.880928000	4.845932000
	1	-4.902183000	1.537277000	5.558735000
	1	-4.157298000	3.152725000	5.332588000
	1	-5.621394000	2.708237000	4.405262000
	47	-3.137480000	-0.122517000	-0.290987000
	6	-1.374645000	-2.145495000	-1.931980000
	6	-0.394383000	-2.457585000	-2.889241000
	6	-2.449499000	-3.015252000	-1.686586000
	6	-0.506649000	-3.660393000	-3.608020000
	1	0.446390000	-1.770921000	-3.063931000
	6	-2.549342000	-4.211780000	-2.416175000
	1	-3.196784000	-2.760763000	-0.915749000
	6	-1.579083000	-4.540250000	-3.378951000
	1	0.257880000	-3.906489000	-4.361640000
	1	-3.390802000	-4.893517000	-2.218260000
	1	-1.656525000	-5.480063000	-3.946592000
	8	-1.341677000	-0.934662000	-1.220324000
	6	0.501139000	-1.942620000	0.628892000
	6	-0.485338000	-1.825873000	1.641064000
	6	1.163672000	-3.187837000	0.493659000
	6	-0.801833000	-2.910197000	2.476910000
	1	-0.987299000	-0.854564000	1.789304000
	6	0.829677000	-4.278517000	1.312659000
	1	1.951170000	-3.294065000	-0.268759000
	6	-0.152448000	-4.146698000	2.310758000
	1	-1.555763000	-2.785269000	3.270881000
	1	1.351896000	-5.238700000	1.175997000
	1	-0.401912000	-4.998364000	2.963091000
	6	-0.024755000	0.980793000	-1.904236000
	6	-0.835491000	1.092793000	-3.065263000
	6	0.810968000	2.077772000	-1.571070000
	6	-0.786067000	2.240070000	-3.874215000
	1	-1.495804000	0.260867000	-3.352107000
	6	0.856783000	3.221413000	-2.380582000
	1	1.427626000	2.019820000	-0.660057000
	6	0.061537000	3.309711000	-3.538858000
	1	-1.412252000	2.293242000	-4.779024000
	1	1.518859000	4.053904000	-2.095635000
	1	0.099101000	4.209377000	-4.173202000

# XIII+XIV-XXX TS



Zero-point correction= 1.385034 (Hartree/Particle)  
 Thermal correction to Energy= 1.472988  
 Thermal correction to Enthalpy= 1.473932  
 Thermal correction to Gibbs Free Energy= 1.244027  
 Sum of electronic and zero-point Energies= -3456.806664  
 Sum of electronic and thermal Energies= -3456.718710  
 Sum of electronic and thermal Enthalpies= -3456.717766  
 Sum of electronic and thermal Free Energies= -3456.947671

6	-5.114723000	-0.303839000	0.346786000
7	-5.647555000	-1.256143000	1.177452000
7	-6.201478000	0.408408000	-0.094831000
6	-7.034943000	-1.141786000	1.251637000
6	-7.385348000	-0.088650000	0.445646000
6	-4.891444000	-2.267154000	1.890459000
6	-6.140944000	1.536394000	-1.004717000
1	-7.640791000	-1.814840000	1.866267000
1	-8.361004000	0.347206000	0.209182000
6	-4.378707000	-1.951851000	3.176838000
6	-3.682657000	-2.970149000	3.860952000
6	-3.511321000	-4.240677000	3.293506000
6	-4.029230000	-4.520325000	2.021310000
6	-4.732377000	-3.542826000	1.287244000
6	-4.564078000	-0.581521000	3.830081000
1	-3.273702000	-2.764085000	4.862757000
1	-2.971091000	-5.022514000	3.850512000
1	-3.886816000	-5.521808000	1.585859000
6	-5.288998000	-3.882029000	-0.096207000
6	-6.202243000	1.286431000	-2.401857000
6	-6.164273000	2.406139000	-3.258985000
6	-6.077799000	3.709338000	-2.748882000
6	-6.023950000	3.922976000	-1.364300000
6	-6.053773000	2.843939000	-0.456551000
6	-6.318841000	-0.120710000	-2.989141000
1	-6.210325000	2.253366000	-4.348760000
1	-6.057305000	4.568005000	-3.438483000
1	-5.960036000	4.951577000	-0.976122000
6	-6.013954000	3.110007000	1.049065000
1	-5.121374000	0.060593000	3.116332000
6	-3.208181000	0.107697000	4.094446000
6	-5.408958000	-0.677938000	5.119010000
1	-5.780130000	-2.971180000	-0.497786000
6	-4.162093000	-4.258418000	-1.081361000
6	-6.363724000	-4.988237000	-0.018734000
1	-6.318672000	-0.840827000	-2.144234000
6	-7.650357000	-0.306086000	-3.748974000
6	-5.106234000	-0.467166000	-3.878946000
1	-5.959383000	2.128034000	1.564109000
6	-4.758270000	3.907643000	1.459294000
6	-7.306675000	3.807593000	1.527480000
1	-3.363974000	1.122513000	4.516216000
1	-2.594755000	-0.464625000	4.821921000
1	-2.617773000	0.211953000	3.160132000
1	-5.580503000	0.331149000	5.548473000
1	-6.399179000	-1.139530000	4.926069000
1	-4.901706000	-1.288089000	5.895722000
1	-4.579042000	-4.444813000	-2.093054000
1	-3.406064000	-3.450649000	-1.162088000
1	-3.633190000	-5.181757000	-0.764902000
1	-6.795497000	-5.182727000	-1.022581000
1	-5.937823000	-5.944729000	0.350845000
1	-7.194654000	-4.708429000	0.661201000
1	-7.745391000	-1.348433000	-4.118306000
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1	-8.211197000	3.217436000	1.272875000
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6	-1.153588000	0.732136000	-0.705721000
6	4.922148000	0.247222000	0.745713000
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	7	5.237104000	1.100249000	1.773357000
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	6	3.569582000	4.408849000	2.281188000
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## XX [Ag(IPr)(OPh)(PhCCPh)(IPr)(Ag)]<sup>+</sup> min

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	6	4.065725000	4.687193000	0.466447000
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	6	6.297787000	-2.015347000	4.346839000
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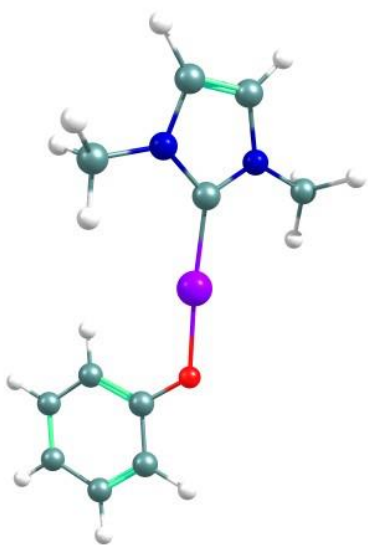
  

Zero-point correction=	1.386971
(Hartree/Particle)	
Thermal correction to Energy=	1.474554
Thermal correction to Enthalpy=	1.475498
Thermal correction to Gibbs Free Energy=	1.245395
Sum of electronic and zero-point Energies=	-3456.821278
Sum of electronic and thermal Energies=	-3456.733695
Sum of electronic and thermal Enthalpies=	-3456.732751
Sum of electronic and thermal Free Energies=	-3456.962854

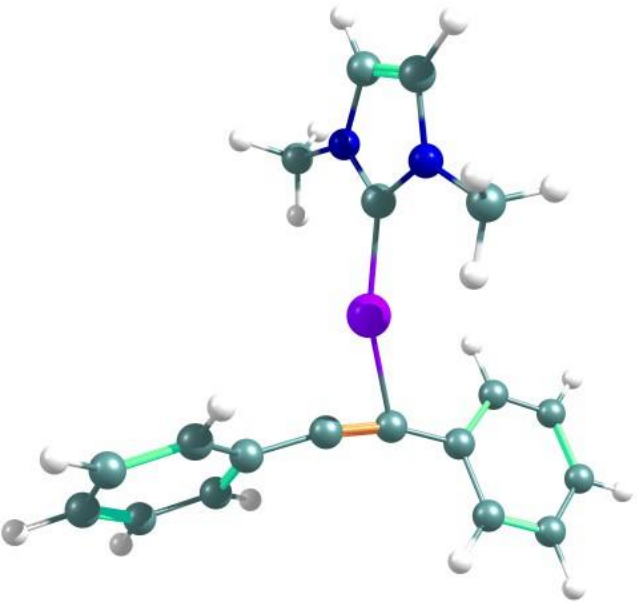
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	1	7.656688000	-2.828536000	-3.324333000
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	1	6.137352000	-3.024526000	4.781262000
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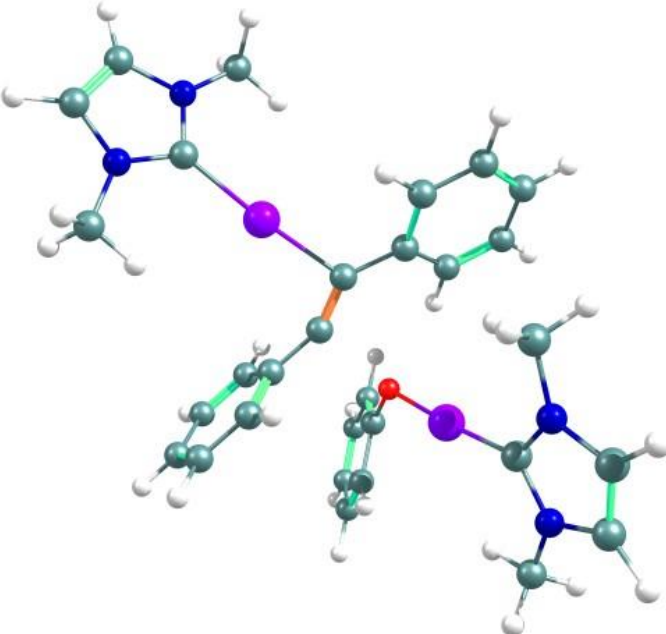
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1	3.717122000	-2.607769000	0.097418000	
1	2.300544000	3.060630000	1.490834000	
1	0.850372000	2.294957000	0.732516000	
1	1.916935000	3.371414000	-0.250313000	
Zero-point correction= 0.216312 (Hartree/Particle) Thermal correction to Energy= 0.231935 Thermal correction to Enthalpy= 0.232879 Thermal correction to Gibbs Free Energy= 0.169561 Sum of electronic and zero-point Energies= -746.982050 Sum of electronic and thermal Energies= -746.966428 Sum of electronic and thermal Enthalpies= -746.965484 Sum of electronic and thermal Free Energies= -747.028802				

## XXI [Au(IMe)(PhCCPh)]<sup>+</sup>

	6	-2.537548000	0.001089000	-0.000013000
	7	-3.366706000	-0.448164000	-0.991881000
	7	-3.366396000	0.450638000	0.991974000
	6	-4.693748000	-0.283589000	-0.624919000
	6	-4.693552000	0.286592000	0.625193000
	6	-2.932928000	-1.043744000	-2.257447000
	1	-5.524610000	-0.582936000	-1.272619000
	1	-5.524211000	0.586237000	1.273013000
	79	-0.511091000	0.000404000	-0.000064000
	6	1.627633000	0.627109000	-0.089632000
	6	1.626733000	-0.628577000	0.089383000
	6	2.022144000	2.013896000	-0.110950000
	6	3.113542000	2.427930000	0.700621000
	6	1.367517000	2.962381000	-0.939640000
	6	3.538753000	3.762489000	0.669115000
	1	3.618984000	1.695175000	1.347541000
	6	1.799760000	4.295270000	-0.956745000
	1	0.528224000	2.638925000	-1.574523000
	6	2.884233000	4.697290000	-0.155129000
	1	4.387711000	4.077265000	1.295553000
	1	1.291658000	5.025925000	-1.604762000
	1	3.222770000	5.744916000	-0.173653000
	6	2.019998000	-2.015741000	0.110874000
	6	1.364367000	-2.963541000	0.939554000
	6	3.111120000	-2.430858000	-0.700499000
6	1.795392000	-4.296820000	0.956876000	
1	0.525264000	-2.639243000	1.574259000	
6	3.535103000	-3.765805000	-0.668791000	
1	3.617321000	-1.698643000	-1.347437000	
6	2.879615000	-4.699918000	0.155459000	
Zero-point correction= 0.312416 (Hartree/Particle) Thermal correction to Energy= 0.334556				

Thermal correction to Enthalpy=	0.335500	1	1.286532000	-5.026944000	1.604897000
Thermal correction to Gibbs Free Energy=	0.255233	1	4.383854000	-4.081428000	-1.295083000
Sum of electronic and zero-point Energies=	-979.110519	1	3.217190000	-5.747851000	0.174146000
Sum of electronic and thermal Energies=	-979.088380	1	-3.405307000	-0.511497000	-3.105730000
Sum of electronic and thermal Enthalpies=	-979.087436	1	-3.211087000	-2.115651000	-2.292264000
Sum of electronic and thermal Free Energies=	-979.167702	1	-1.834093000	-0.949904000	-2.333381000
		6	-2.932192000	1.046421000	2.257296000
		1	-1.833664000	0.949856000	2.334296000
		1	-3.406679000	0.516221000	3.105672000
		1	-3.207631000	2.119078000	2.290812000

## XXI+XXII-XXIII TS

	6	-4.903116000	-0.381763000	-0.519470000
	7	-5.925782000	-0.934002000	0.204889000
	7	-5.496245000	0.117590000	-1.648182000
	6	-7.136710000	-0.781096000	-0.458859000
	6	-6.865836000	-0.117080000	-1.628630000
	6	-5.778909000	-1.586660000	1.505659000
	6	-4.796499000	0.804536000	-2.732579000
	1	-8.082413000	-1.151462000	-0.049626000
	1	-7.529301000	0.203838000	-2.438443000
	79	-2.934634000	-0.332885000	-0.006335000
	6	-0.461751000	0.751989000	0.277961000
	6	-0.921272000	-0.403011000	0.657056000
	6	3.996588000	-1.537833000	-1.069221000
	7	3.716975000	-2.835579000	-1.408867000
	7	5.277126000	-1.320167000	-1.506826000
6	4.803677000	-3.416927000	-2.051152000	
6	5.786910000	-2.462434000	-2.112164000	
6	2.455079000	-3.524058000	-1.140198000	
6	6.020323000	-0.070428000	-1.352686000	
1	4.790591000	-4.453094000	-2.404587000	
1	6.799094000	-2.504030000	-2.527494000	
79	2.813720000	-0.259626000	-0.122455000	
6	1.950232000	2.252388000	1.311205000	
6	1.509794000	2.787518000	2.548582000	
6	2.754388000	3.057982000	0.467068000	
6	1.891223000	4.080943000	2.937465000	
1	0.880091000	2.164174000	3.202477000	
6	3.132004000	4.350108000	0.866451000	
1	3.076549000	2.650489000	-0.505622000	
6	2.704927000	4.869222000	2.102319000	
1	1.553892000	4.475980000	3.909213000	
1	3.764881000	4.960011000	0.201827000	
1	3.004743000	5.881759000	2.413351000	
8	1.573144000	0.990085000	0.974020000	
6	-0.457947000	-1.569622000	1.430627000	
6	-0.966896000	-2.861177000	1.137185000	
6	0.469502000	-1.435245000	2.495882000	
6	-0.552629000	-3.983441000	1.872484000	
1	-1.696776000	-2.972810000	0.318790000	
6	0.867420000	-2.558511000	3.237727000	
1	0.872666000	-0.439919000	2.725266000	
6	0.363292000	-3.835787000	2.929717000	
1	-0.958965000	-4.977656000	1.627234000	
1	1.579314000	-2.433006000	4.069037000	

Zero-point correction= 0.529350 (Hartree/Particle)  
 Thermal correction to Energy= 0.568418  
 Thermal correction to Enthalpy= 0.569362  
 Thermal correction to Gibbs Free Energy= 0.445954  
 Sum of electronic and zero-point Energies= -1726.101265  
 Sum of electronic and thermal Energies= -1726.062196  
 Sum of electronic and thermal Enthalpies= -1726.061252  
 Sum of electronic and thermal Free Energies= -1726.184661

	1	0.676616000	-4.712216000	3.518730000
	6	-0.533944000	2.003851000	-0.420614000
	6	-0.146897000	2.081895000	-1.787683000
	6	-0.954103000	3.185611000	0.247764000
	6	-0.208545000	3.303707000	-2.469081000
	1	0.196742000	1.169113000	-2.298236000
	6	-1.007220000	4.405031000	-0.443498000
	1	-1.248118000	3.129620000	1.305747000
	6	-0.638664000	4.466752000	-1.799050000
	1	0.084416000	3.354777000	-3.529565000
	1	-1.336276000	5.315094000	0.081369000
	1	-0.681144000	5.426740000	-2.337344000
	1	5.382535000	0.647736000	-0.804949000
	1	6.278060000	0.348692000	-2.345632000
	1	6.948750000	-0.247189000	-0.774584000
	1	1.821341000	-2.870958000	-0.511532000
	1	2.649131000	-4.469646000	-0.597465000
	1	1.926866000	-3.745096000	-2.089313000
	1	-4.705389000	-1.597124000	1.771469000
	1	-6.154166000	-2.627801000	1.455082000
	1	-6.341571000	-1.029414000	2.280772000
	1	-4.906095000	0.238963000	-3.679263000
	1	-3.725100000	0.872551000	-2.468471000
	1	-5.204927000	1.825910000	-2.864712000

### XXIII [Au(IMe)(OPh)(PhCCPh)(IMe)(Au)]<sup>+</sup> min

	6	4.970210000	-0.697123000	-0.333116000
	7	5.669481000	-1.466139000	0.560396000
	7	5.881038000	-0.381034000	-1.307500000
	6	6.988550000	-1.626387000	0.152944000
	6	7.121770000	-0.941280000	-1.028589000
	6	5.113357000	-2.024627000	1.791006000
	6	5.591027000	0.432856000	-2.486725000
	1	7.717349000	-2.206076000	0.728967000
	1	7.988629000	-0.809690000	-1.684505000
	79	3.006266000	-0.113003000	-0.228314000
	6	0.073648000	-0.010040000	0.557862000
	6	1.073183000	0.603871000	-0.134456000
	6	-4.535898000	-1.089196000	-0.895122000
	7	-5.848681000	-0.750404000	-0.711115000
	7	-4.548754000	-2.168770000	-1.735518000
	6	-6.672815000	-1.606855000	-1.430441000
	6	-5.854483000	-2.499148000	-2.075714000
	6	-6.334814000	0.348343000	0.124198000
	6	-3.366087000	-2.877781000	-2.226511000
	1	-7.763804000	-1.514600000	-1.421296000
1	-6.092615000	-3.335825000	-2.740632000	
79	-2.947220000	-0.211944000	-0.108457000	
6	-1.258535000	1.876200000	1.515595000	
6	-0.383808000	2.053585000	2.598249000	
6	-2.234485000	2.831813000	1.195436000	
6	-0.507238000	3.215282000	3.380359000	
1	0.386329000	1.300132000	2.818904000	
6	-2.349070000	3.983721000	1.992554000	
1	-2.878951000	2.679265000	0.314739000	
6	-1.487880000	4.179151000	3.086323000	
1	0.172867000	3.361799000	4.233956000	
1	-3.108962000	4.740518000	1.742914000	
1	-1.576362000	5.085048000	3.705016000	
8	-1.205996000	0.700436000	0.735127000	
6	0.836784000	1.891811000	-0.846980000	
6	-0.142471000	1.989414000	-1.868762000	
6	1.624988000	3.038087000	-0.573566000	
6	-0.329350000	3.185205000	-2.581639000	
1	-0.744668000	1.101330000	-2.122617000	
6	1.421439000	4.239764000	-1.270472000	
1	2.401916000	2.977054000	0.205391000	
6	0.445635000	4.319564000	-2.280431000	
1	-1.084237000	3.230173000	-3.383414000	
1	2.037516000	5.120483000	-1.028419000	

Zero-point correction= 0.531810 (Hartree/Particle)  
 Thermal correction to Energy= 0.570404  
 Thermal correction to Enthalpy= 0.571349  
 Thermal correction to Gibbs Free Energy= 0.450942  
 Sum of electronic and zero-point Energies= -1726.117504  
 Sum of electronic and thermal Energies= -1726.078909  
 Sum of electronic and thermal Enthalpies= -1726.077965  
 Sum of electronic and thermal Free Energies= -1726.198372

	1	0.296563000	5.258200000	-2.836873000
	6	0.008657000	-1.345929000	1.186979000
	6	-0.800546000	-1.581638000	2.330693000
	6	0.733138000	-2.442061000	0.648264000
	6	-0.855356000	-2.851574000	2.928168000
	1	-1.376351000	-0.753700000	2.772227000
	6	0.677435000	-3.708175000	1.250157000
	1	1.333228000	-2.286021000	-0.262357000
	6	-0.114356000	-3.920588000	2.394688000
	1	-1.478812000	-3.003602000	3.823442000
	1	1.245914000	-4.543686000	0.810885000
	1	-0.159653000	-4.916446000	2.862794000
	1	-5.464475000	0.846299000	0.589751000
	1	-6.999267000	-0.043198000	0.919330000
	1	-6.889578000	1.081185000	-0.494233000
	1	-2.477504000	-2.495801000	-1.691023000
	1	-3.240177000	-2.708632000	-3.314409000
	1	-3.469894000	-3.962451000	-2.029731000
	1	4.029271000	-1.805832000	1.811274000
	1	5.595538000	-1.565069000	2.677102000
	1	5.268012000	-3.121422000	1.817441000
	1	4.540144000	0.772034000	-2.422559000
	1	5.728423000	-0.163377000	-3.410896000
	1	6.259564000	1.316023000	-2.516820000

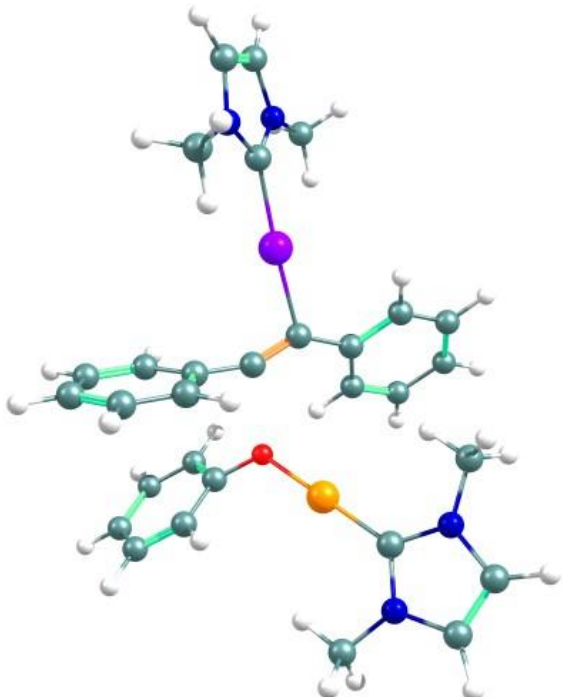
## XXIV [Cu(IMe)(OPh)]

	29	0.343120000	-0.458284000	-0.166935000
	8	-1.356909000	-1.057440000	-0.340989000
	6	2.128755000	0.024218000	-0.037543000
	7	2.683010000	1.271971000	-0.209025000
	6	4.059441000	1.243424000	-0.018913000
	1	4.686409000	2.136633000	-0.108682000
	6	4.388961000	-0.055205000	0.278906000
	1	5.359144000	-0.513528000	0.497305000
	7	3.203598000	-0.780589000	0.263967000
	6	1.917490000	2.468547000	-0.543460000
	6	3.105278000	-2.212818000	0.524810000
	6	-2.522629000	-0.454966000	-0.107066000
	6	-3.729600000	-1.085651000	-0.528565000
	6	-2.640330000	0.798635000	0.560890000
	6	-4.976537000	-0.486992000	-0.298930000
	1	-3.650533000	-2.056373000	-1.043408000
	6	-3.893381000	1.389130000	0.785661000
	1	-1.715220000	1.292581000	0.908089000
	6	-5.075342000	0.755349000	0.358136000
	1	-5.891331000	-1.000443000	-0.640510000
	1	-3.947525000	2.360003000	1.307105000
	1	-6.057643000	1.220580000	0.535952000
	1	0.857096000	2.175714000	-0.664654000
	1	2.282848000	2.910982000	-1.492146000
	1	1.995565000	3.221814000	0.266685000
	1	3.533963000	-2.456146000	1.517848000
	1	3.638685000	-2.791477000	-0.256644000
	1	2.034427000	-2.492266000	0.513939000

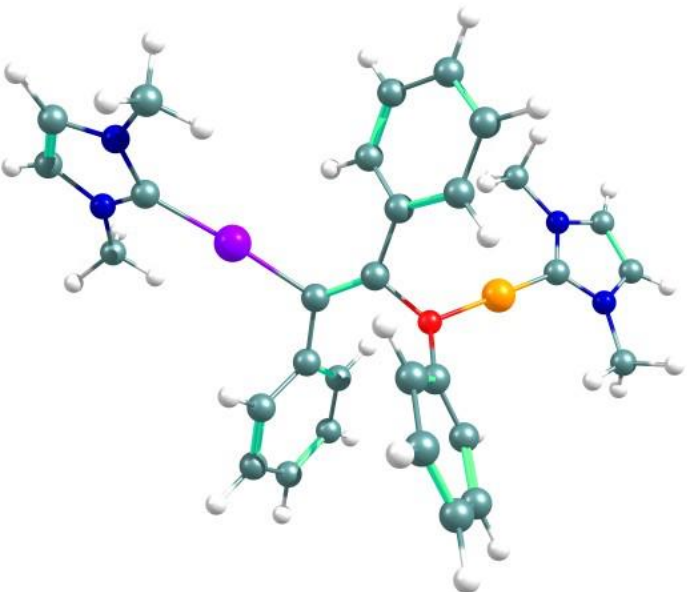
Zero-point correction=	0.216076 (Hartree/Particle)
Thermal correction to Energy=	0.231729
Thermal correction to Enthalpy=	0.232673
Thermal correction to Gibbs Free Energy=	0.168959
Sum of electronic and zero-point Energies=	-808.565019
Sum of electronic and thermal Energies=	-808.549366
Sum of electronic and thermal Enthalpies=	-808.548422
Sum of electronic and thermal Free Energies=	-808.612136

## XXIV+XXII-XXV TS

	6	-4.557671000	-0.254469000	-0.418803000
	7	-5.561396000	-0.784347000	0.347481000
	7	-5.190125000	0.303559000	-1.497418000
	6	-6.799587000	-0.559600000	-0.241200000
	6	-6.565482000	0.127388000	-1.405628000
	6	-5.371323000	-1.483378000	1.618289000
	6	-4.522935000	0.994021000	-2.600016000
	1	-7.736380000	-0.901478000	0.211048000
	1	-7.258440000	0.501125000	-2.166628000
	79	-2.564343000	-0.306330000	-0.015905000
	6	-0.053195000	0.667381000	0.208019000
	6	-0.522702000	-0.497327000	0.534564000
	6	4.258847000	-1.559678000	-1.035741000
	7	3.981182000	-2.838782000	-1.448530000
	7	5.563258000	-1.353317000	-1.413373000
	6	5.082530000	-3.413513000	-2.070208000
	6	6.083268000	-2.474497000	-2.047178000
	6	2.697171000	-3.510765000	-1.264696000
	6	6.314959000	-0.124769000	-1.168049000
	1	5.068658000	-4.432306000	-2.471356000
	1	7.111171000	-2.516900000	-2.422318000
	29	3.144009000	-0.361046000	-0.146957000
	6	2.496974000	2.042863000	1.195568000
	6	2.147691000	2.545123000	2.476665000
	6	3.275504000	2.861975000	0.336300000
	6	2.591891000	3.810297000	2.890504000
	1	1.537219000	1.914998000	3.142460000
	6	3.716029000	4.125894000	0.759996000
	1	3.521584000	2.486609000	-0.671237000
	6	3.379153000	4.607701000	2.038489000
1	2.323977000	4.177299000	3.894430000	
1	4.325876000	4.744219000	0.081580000	
1	3.727614000	5.598346000	2.368766000	
8	2.073842000	0.811420000	0.825196000	
6	-0.061694000	-1.728225000	1.200901000	
6	-0.642536000	-2.978042000	0.863753000	
6	0.941227000	-1.696819000	2.204744000	
6	-0.225754000	-4.160122000	1.496768000	
1	-1.429344000	-3.009351000	0.092591000	
6	1.342803000	-2.880638000	2.844153000	
1	1.395143000	-0.731870000	2.468371000	
6	0.766364000	-4.115613000	2.492970000	
1	-0.688539000	-5.120559000	1.219318000	
1	2.113207000	-2.836147000	3.630383000	
1	1.082581000	-5.039686000	3.002171000	
6	-0.088481000	1.969815000	-0.386634000	
6	0.264243000	2.140097000	-1.755076000	
6	-0.436944000	3.111873000	0.385269000	
6	0.240108000	3.413690000	-2.335652000	
1	0.551300000	1.257196000	-2.346753000	
6	-0.453821000	4.383462000	-0.206580000	
1	-0.705930000	2.983909000	1.443616000	
6	-0.119039000	4.536942000	-1.563489000	
1	0.506367000	3.536951000	-3.397194000	
1	-0.727090000	5.262111000	0.397764000	
1	-0.132243000	5.537725000	-2.023200000	
1	5.651918000	0.593004000	-0.649160000	
1	6.655159000	0.318754000	-2.125153000	
1	7.195133000	-0.330796000	-0.526763000	
1	2.042140000	-2.863827000	-0.651482000	
1	2.841578000	-4.473820000	-0.736953000	
1	2.212658000	-3.698739000	-2.244104000	
1	-4.286628000	-1.539758000	1.826752000	
1	-5.786278000	-2.508725000	1.556196000	
1	-5.872644000	-0.931987000	2.438336000	
1	-4.719515000	0.469439000	-3.556108000	
1	-3.435413000	0.998359000	-2.401623000	
1	-4.884759000	2.038723000	-2.672191000	

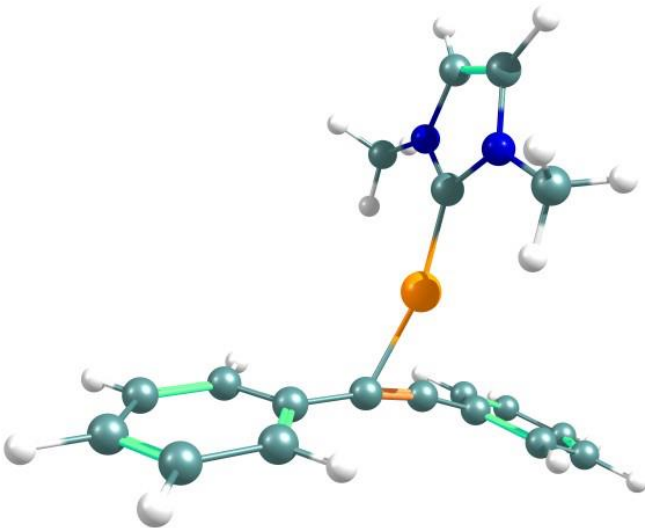
## XXV [Cu(Ime)(OPh)(PhCCPh)(Ime)(Au)]<sup>+</sup> min



	6	4.533795000	-0.724952000	-0.205667000
	7	5.193291000	-1.503357000	0.709546000
	7	5.479569000	-0.422603000	-1.150746000
	6	6.522072000	-1.683347000	0.343784000
	6	6.702490000	-1.000829000	-0.832906000
	6	4.591267000	-2.053955000	1.921870000
	6	5.239264000	0.395510000	-2.338327000
	1	7.223801000	-2.273163000	0.942700000
	1	7.591552000	-0.881926000	-1.460943000
	79	2.575818000	-0.110118000	-0.172900000
	6	-0.414085000	-0.006150000	0.383647000
	6	0.653898000	0.641129000	-0.159616000
	6	-4.728527000	-1.158991000	-0.834487000
	7	-6.026262000	-0.728051000	-0.935796000
	7	-4.744519000	-2.436227000	-1.332677000
	6	-6.833945000	-1.714130000	-1.486907000
	6	-6.023364000	-2.793120000	-1.738711000
	6	-6.507200000	0.586701000	-0.516107000
	6	-3.573209000	-3.305638000	-1.440910000
	1	-7.907578000	-1.573774000	-1.650477000
1	-6.253794000	-3.774247000	-2.166999000	
29	-3.251529000	-0.244297000	-0.163967000	
6	-1.812096000	1.834099000	1.331551000	
6	-1.089978000	1.923609000	2.531085000	
6	-2.709711000	2.837941000	0.936489000	
6	-1.289177000	3.045459000	3.355017000	
1	-0.377062000	1.133714000	2.809770000	
6	-2.902369000	3.949055000	1.775247000	
1	-3.224216000	2.756742000	-0.033925000	
6	-2.194909000	4.055817000	2.985598000	
1	-0.728844000	3.124631000	4.299697000	
1	-3.599323000	4.744619000	1.468841000	
1	-2.343369000	4.930266000	3.637188000	
8	-1.699442000	0.699029000	0.499315000	
6	0.499272000	1.989107000	-0.777278000	
6	-0.382944000	2.187461000	-1.870541000	
6	1.273456000	3.093040000	-0.340037000	
6	-0.488005000	3.440082000	-2.497161000	
1	-0.970576000	1.334679000	-2.248182000	
6	1.150494000	4.350312000	-0.952577000	
1	1.975043000	2.953229000	0.497979000	
6	0.272243000	4.530108000	-2.036536000	
1	-1.165493000	3.564862000	-3.357436000	
1	1.753449000	5.196130000	-0.585465000	
1	0.187713000	5.512918000	-2.526294000	
6	-0.553847000	-1.395157000	0.872561000	
6	-1.462499000	-1.720374000	1.917394000	
6	0.187804000	-2.454725000	0.285458000	
6	-1.600517000	-3.043135000	2.371780000	
1	-2.040314000	-0.921732000	2.409129000	
6	0.048857000	-3.773413000	0.744845000	
1	0.871397000	-2.224781000	-0.547321000	
6	-0.844540000	-4.076356000	1.790382000	
1	-2.297226000	-3.263650000	3.196018000	
1	0.635370000	-4.577191000	0.271478000	
1	-0.952235000	-5.112523000	2.147740000	
1	4.192518000	0.751713000	-2.306441000	
1	5.395463000	-0.203141000	-3.257939000	
1	5.922476000	1.267809000	-2.347525000	
1	3.514736000	-1.800467000	1.918952000	
1	5.067151000	-1.616839000	2.822550000	
1	4.710047000	-3.155432000	1.942932000	
1	-2.725961000	-2.832982000	-0.908802000	
1	-3.299221000	-3.456317000	-2.504380000	
1	-3.785478000	-4.286882000	-0.973817000	
1	-5.655943000	1.154810000	-0.096928000	
1	-7.288360000	0.481297000	0.262726000	
1	-6.923917000	1.140056000	-1.381164000	

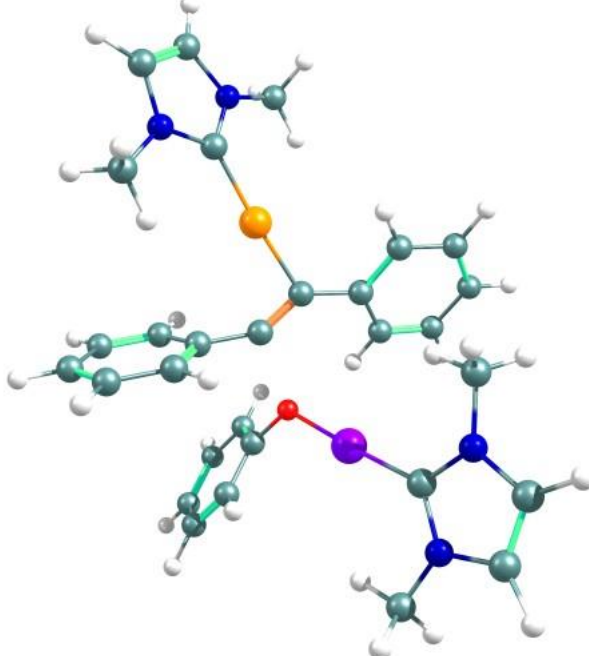
Zero-point correction= 0.531690 (Hartree/Particle)  
 Thermal correction to Energy= 0.570183  
 Thermal correction to Enthalpy= 0.571127  
 Thermal correction to Gibbs Free Energy= 0.451450  
 Sum of electronic and zero-point Energies= -1787.703411  
 Sum of electronic and thermal Energies= -1787.664918  
 Sum of electronic and thermal Enthalpies= -1787.663974  
 Sum of electronic and thermal Free Energies= -1787.783651

## XXVI [Cu(Ime)(PhCCPh)]

	6	0.036525000	2.347450000	-0.000062000
	7	0.051838000	3.184387000	-1.085156000
	7	0.051237000	3.184238000	1.085144000
	6	0.075589000	4.512682000	-0.686808000
	6	0.075211000	4.512590000	0.686998000
	6	0.044623000	2.747411000	-2.480941000
	6	0.043094000	2.746966000	2.480842000
	1	0.090808000	5.343582000	-1.400202000
	1	0.089984000	5.343379000	1.400531000
	29	0.004348000	0.446694000	-0.000373000
	6	0.604739000	-1.519976000	0.000009000
	6	-0.653806000	-1.501177000	-0.000177000
	6	2.020021000	-1.787632000	0.000212000
	6	2.721210000	-1.930589000	1.228222000
	6	2.721172000	-1.931601000	-1.227738000
	6	4.092436000	-2.217733000	1.220032000
	1	2.177323000	-1.828247000	2.179630000
	6	4.092378000	-2.218738000	-1.219388000
	1	2.177195000	-1.830019000	-2.179174000
	6	4.780417000	-2.360486000	0.000375000
1	4.629343000	-2.336325000	2.173820000	
1	4.629263000	-2.338115000	-2.173090000	
1	5.857806000	-2.587491000	0.000443000	
6	-2.076227000	-1.728471000	-0.000116000	
6	-2.781194000	-1.851195000	1.227904000	
6	-2.781266000	-1.851911000	-1.228037000	
6	-4.160139000	-2.098816000	1.219746000	
1	-2.234602000	-1.764617000	2.179326000	
6	-4.160205000	-2.099535000	-1.219652000	
1	-2.234719000	-1.765853000	-2.179534000	
6	-4.852006000	-2.221476000	0.000106000	
1	-4.700189000	-2.201996000	2.173551000	
1	-4.700328000	-2.203270000	-2.173355000	
1	-5.935516000	-2.417189000	0.000189000	
1	0.023285000	1.641498000	2.502034000	
1	-0.854173000	3.136323000	3.001148000	
1	0.953514000	3.103960000	3.001501000	
1	0.955311000	3.104669000	-3.000948000	
1	-0.852401000	3.136711000	-3.001711000	
1	0.025042000	1.641942000	-2.502399000	

Zero-point correction= 0.312378 (Hartree/Particle)  
 Thermal correction to Energy= 0.334474  
 Thermal correction to Enthalpy= 0.335418  
 Thermal correction to Gibbs Free Energy= 0.255278  
 Sum of electronic and zero-point Energies= -1040.690636  
 Sum of electronic and thermal Energies= -1040.668540  
 Sum of electronic and thermal Enthalpies= -1040.667595  
 Sum of electronic and thermal Free Energies= -1040.747736

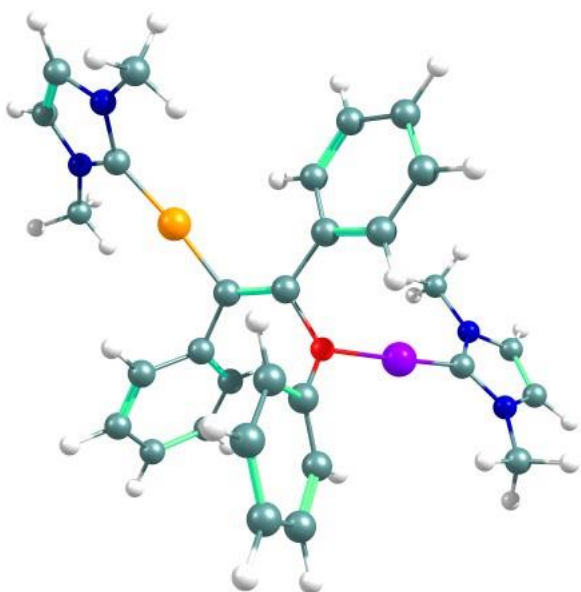
## XXI+XXVI-XXVII TS

	6	-4.849025000	-0.780211000	-0.520571000
	7	-5.867279000	-1.472556000	0.084969000
	7	-5.427387000	-0.228649000	-1.635532000
	6	-7.049875000	-1.356453000	-0.634216000
	6	-6.771187000	-0.569337000	-1.723830000
	6	-5.732375000	-2.225953000	1.330024000
	6	-4.723629000	0.598547000	-2.613085000
	1	-7.983661000	-1.832971000	-0.317612000
	1	-7.414949000	-0.228606000	-2.541591000
	29	-3.047053000	-0.633552000	0.066444000
	6	-0.885660000	0.597453000	0.388941000
	6	-1.227241000	-0.605062000	0.761179000
	6	3.602595000	-1.295110000	-1.103554000
	7	3.398774000	-2.594089000	-1.488560000
	7	4.887626000	-1.004872000	-1.479352000
	6	4.537953000	-3.105369000	-2.098514000
	6	5.476067000	-2.104610000	-2.091979000
	6	2.160803000	-3.348287000	-1.293812000
	6	5.563601000	0.273614000	-1.261509000
	1	4.589237000	-4.130494000	-2.479570000
1	6.505397000	-2.086855000	-2.464721000	
79	2.317031000	-0.106062000	-0.177430000	
6	1.230347000	2.355008000	1.248943000	
6	0.730138000	2.842036000	2.479352000	
6	1.991769000	3.212869000	0.422684000	
6	1.013214000	4.157103000	2.881475000	
1	0.134306000	2.171315000	3.117683000	
6	2.275623000	4.524455000	0.838065000	
1	2.357427000	2.833109000	-0.545689000	
6	1.789182000	5.003265000	2.067695000	

Zero-point correction= 0.529566 (Hartree/Particle)

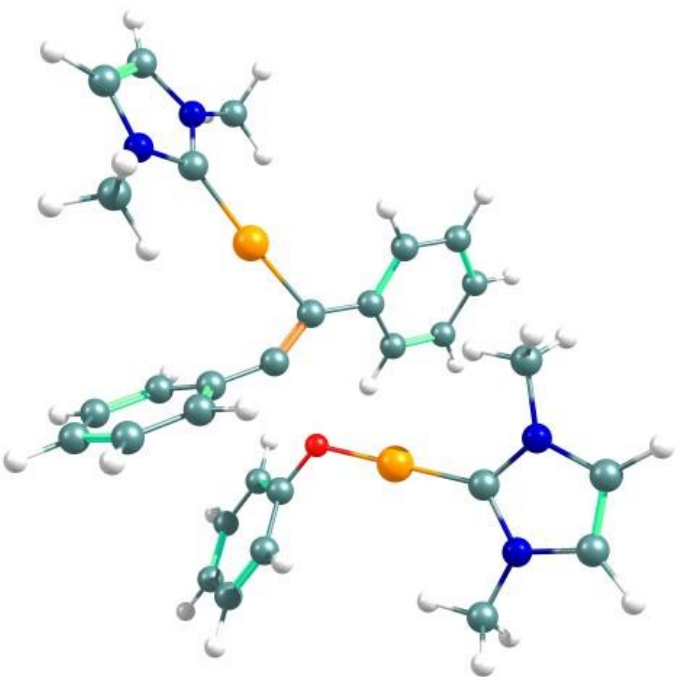
Thermal correction to Energy=	0.568352	1	0.629615000	4.522149000	3.847625000
Thermal correction to Enthalpy=	0.569296	1	2.878381000	5.180650000	0.189998000
Thermal correction to Gibbs Free Energy=	0.448373	1	2.012799000	6.031616000	2.390594000
Sum of electronic and zero-point Energies=	-1787.674415	8	0.960203000	1.060059000	0.890674000
Sum of electronic and thermal Energies=	-1787.635628	6	-0.634203000	-1.716482000	1.520169000
Sum of electronic and thermal Enthalpies=	-1787.634684	6	-1.047131000	-3.048133000	1.254656000
Sum of electronic and thermal Free Energies=	-1787.755608	6	0.327054000	-1.504131000	2.543735000
		6	-0.510033000	-4.130047000	1.970709000
		1	-1.801327000	-3.223018000	0.469155000
		6	0.848588000	-2.586940000	3.268741000
		1	0.654956000	-0.478180000	2.760792000
		6	0.438103000	-3.903018000	2.984687000
		1	-0.844308000	-5.155506000	1.745846000
		1	1.584311000	-2.399906000	4.067168000
		1	0.849005000	-4.748104000	3.559246000
		6	-1.286180000	1.806753000	-0.311766000
		6	-0.880608000	2.026014000	-1.655456000
		6	-2.060044000	2.800224000	0.342941000
		6	-1.265206000	3.193520000	-2.330014000
		1	-0.263538000	1.265054000	-2.158353000
		6	-2.439658000	3.966772000	-0.339364000
		1	-2.363884000	2.640742000	1.388345000
		6	-2.045790000	4.165726000	-1.674545000
		1	-0.950035000	3.351426000	-3.373565000
		1	-3.041226000	4.729879000	0.178678000
		1	-2.340447000	5.084947000	-2.204937000
		1	4.870621000	0.947463000	-0.724703000
		1	5.843299000	0.730274000	-2.231621000
		1	6.473877000	0.123991000	-0.648037000
		1	1.468029000	-2.741936000	-0.680680000
		1	2.375955000	-4.295859000	-0.762796000
		1	1.688431000	-3.571399000	-2.271403000
		1	-4.684353000	-2.145414000	1.675209000
		1	-5.980248000	-3.293530000	1.165257000
		1	-6.403172000	-1.811082000	2.108632000
		1	-4.663393000	0.078644000	-3.590480000
		1	-3.700661000	0.793758000	-2.240052000
		1	-5.248255000	1.565192000	-2.745073000

## XXVII [Au(IME)(OPh)(PhCCPh)(IME)(Cu)]<sup>+</sup> min

	6	5.121091000	-0.757258000	-0.458188000
	7	5.880468000	-1.469057000	0.436930000
	7	5.976283000	-0.509950000	-1.503537000
	6	7.172438000	-1.660233000	-0.036957000
	6	7.232448000	-1.053823000	-1.267176000
	6	5.400696000	-1.940705000	1.733452000
	6	5.611473000	0.226635000	-2.711596000
	1	7.936723000	-2.202365000	0.529834000
	1	8.058345000	-0.967948000	-1.981207000
	29	3.306408000	-0.193788000	-0.290441000
	6	0.539932000	-0.042552000	0.558779000
	6	1.540066000	0.536581000	-0.155160000
	6	-4.083810000	-1.051037000	-0.905607000
	7	-5.392382000	-0.693018000	-0.727564000
	7	-4.108844000	-2.128252000	-1.748909000
	6	-6.225692000	-1.535087000	-1.453288000
	6	-5.417679000	-2.438139000	-2.096552000
	6	-5.866209000	0.411587000	0.107128000
	6	-2.934708000	-2.854974000	-2.234099000
	1	-7.315176000	-1.426131000	-1.449707000
1	-5.665061000	-3.269534000	-2.764708000	
79	-2.486504000	-0.198404000	-0.109096000	
6	-0.771267000	1.867565000	1.510480000	
6	0.108343000	2.041323000	2.590075000	
6	-1.729454000	2.838516000	1.181807000	
6	0.009606000	3.214430000	3.358384000	
1	0.861278000	1.273483000	2.820193000	
6	-1.820085000	4.001794000	1.965245000	
1	-2.379476000	2.687117000	0.304936000	
6	-0.952518000	4.193798000	3.054643000	
1	0.693681000	3.357667000	4.209406000	
1	-2.566213000	4.769871000	1.708590000	
Zero-point correction=	0.531274 (Hartree/Particle)			
Thermal correction to Energy=	0.569918			
Thermal correction to Enthalpy=	0.570862			
Thermal correction to Gibbs Free Energy=	0.450346			
Sum of electronic and zero-point Energies=	-1787.684895			

Sum of electronic and thermal Energies=	-1787.646252	1	-1.022174000	5.108502000	3.662709000
Sum of electronic and thermal Enthalpies=	-1787.645307	8	-0.740085000	0.683163000	0.745652000
Sum of electronic and thermal Free Energies=	-1787.765824	6	1.348560000	1.823628000	-0.875327000
		6	0.366801000	1.960930000	-1.891722000
		6	2.193703000	2.935037000	-0.621631000
		6	0.233039000	3.157561000	-2.614957000
		1	-0.282168000	1.102016000	-2.130611000
		6	2.042369000	4.138988000	-1.327792000
		1	2.972110000	2.846231000	0.154013000
		6	1.063707000	4.256608000	-2.331437000
		1	-0.527098000	3.232233000	-3.409672000
		1	2.701543000	4.991432000	-1.097964000
		1	0.955095000	5.196156000	-2.895579000
		6	0.480225000	-1.365270000	1.214131000
		6	-0.356591000	-1.606230000	2.336074000
		6	1.261366000	-2.446412000	0.725754000
		6	-0.386070000	-2.865563000	2.958511000
		1	-0.973660000	-0.790187000	2.742241000
		6	1.233275000	-3.700477000	1.353108000
		1	1.881955000	-2.286557000	-0.172351000
		6	0.410311000	-3.917965000	2.475018000
		1	-1.033512000	-3.021427000	3.835971000
		1	1.845292000	-4.523894000	0.950995000
		1	0.384336000	-4.904827000	2.963058000
		1	-4.991500000	0.891380000	0.583428000
		1	-6.545872000	0.029496000	0.893939000
		1	-6.400980000	1.157161000	-0.513751000
		1	-2.041872000	-2.478893000	-1.701486000
		1	-2.806858000	-2.695649000	-3.323245000
		1	-3.050888000	-3.936916000	-2.029022000
		1	4.319300000	-1.719430000	1.806994000
		1	5.934277000	-1.425350000	2.557470000
		1	5.555138000	-3.034040000	1.827119000
		1	4.577588000	0.601804000	-2.591662000
		1	5.659706000	-0.433822000	-3.600716000
		1	6.293928000	1.087281000	-2.858130000

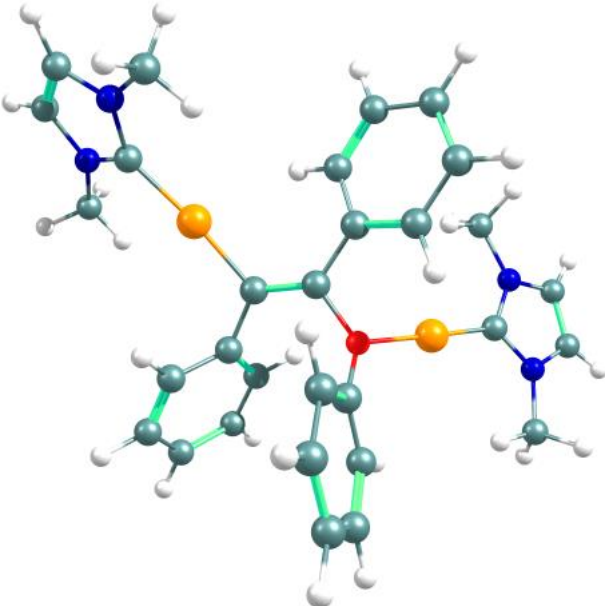
## XXIV+XXVI-XXVIII TS

	6	-4.527883000	-0.660959000	-0.432600000
	7	-5.545682000	-1.317315000	0.212211000
	7	-5.136547000	-0.052990000	-1.501047000
	6	-6.757793000	-1.124590000	-0.438018000
	6	-6.498572000	-0.324572000	-1.523029000
	6	-5.383076000	-2.107582000	1.430866000
	6	-4.444932000	0.760671000	-2.498511000
	1	-7.696253000	-1.561847000	-0.081134000
	1	-7.167265000	0.068769000	-2.295942000
	29	-2.690464000	-0.618352000	0.053377000
	6	-0.496961000	0.512126000	0.311254000
	6	-0.830516000	-0.703596000	0.635154000
	6	3.864779000	-1.232294000	-1.104271000
	7	3.694249000	-2.519061000	-1.550044000
	7	5.162062000	-0.924272000	-1.431930000
	6	4.854596000	-2.999470000	-2.143528000
	6	5.783111000	-1.991549000	-2.067776000
	6	2.456177000	-3.285134000	-1.427017000
	6	5.815632000	0.349009000	-1.136866000
	1	4.928184000	-4.007818000	-2.564075000
1	6.823476000	-1.951788000	-2.407178000	
29	2.629761000	-0.144172000	-0.232900000	
6	1.741178000	2.188523000	1.133800000	
6	1.365747000	2.610392000	2.432332000	
6	2.436571000	3.090373000	0.292163000	
6	1.706723000	3.895692000	2.882486000	
1	0.819917000	1.909361000	3.082903000	
6	2.778692000	4.371933000	0.754244000	
1	2.700510000	2.767047000	-0.728532000	
6	2.416973000	4.781218000	2.050469000	
1	1.419865000	4.207577000	3.899595000	
1	3.327144000	5.060414000	0.091455000	
1	2.685236000	5.786300000	2.410550000	
8	1.427912000	0.926695000	0.718103000	

Zero-point correction= 0.529443 (Hartree/Particle)  
 Thermal correction to Energy= 0.568137  
 Thermal correction to Enthalpy= 0.569081

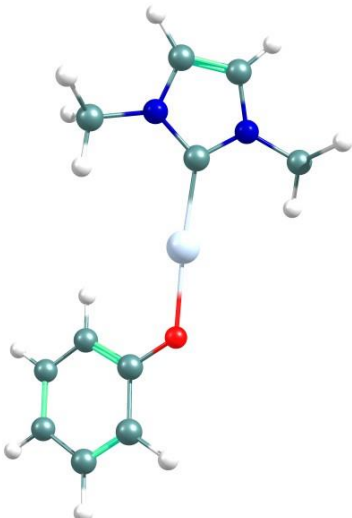
Thermal correction to Gibbs Free Energy=	0.449090	6	-0.226986000	-1.875290000	1.284540000
Sum of electronic and zero-point Energies=	-1849.259365	6	-0.721730000	-3.173915000	0.996355000
Sum of electronic and thermal Energies=	-1849.220671	6	0.831487000	-1.753010000	2.224268000
Sum of electronic and thermal Enthalpies=	-1849.219726	6	-0.170992000	-4.311100000	1.608695000
Sum of electronic and thermal Free Energies=	-1849.339718	1	-1.550183000	-3.278513000	0.276068000
		6	1.369072000	-2.891739000	2.844879000
		1	1.216517000	-0.751487000	2.461280000
		6	0.875877000	-4.174009000	2.538375000
		1	-0.569908000	-5.309513000	1.368475000
		1	2.181621000	-2.775555000	3.579748000
		1	1.299295000	-5.063186000	3.031524000
		6	-0.890990000	1.776373000	-0.281888000
		6	-0.594550000	2.055271000	-1.643367000
		6	-1.545879000	2.767321000	0.495880000
		6	-0.972289000	3.278678000	-2.214329000
		1	-0.067457000	1.296248000	-2.242260000
		6	-1.918537000	3.990142000	-0.083855000
		1	-1.765307000	2.561796000	1.554209000
		6	-1.635714000	4.248110000	-1.436846000
		1	-0.742661000	3.482816000	-3.272087000
		1	-2.428166000	4.750312000	0.528464000
		1	-1.925018000	5.211025000	-1.886423000
		1	5.083998000	1.011717000	-0.637503000
		1	6.164395000	0.830405000	-2.072255000
		1	6.680300000	0.192778000	-0.461329000
		1	1.742877000	-2.711512000	-0.805778000
		1	2.656239000	-4.256167000	-0.933445000
		1	2.009895000	-3.466390000	-2.425713000
		1	-4.317559000	-2.077947000	1.726916000
		1	-5.682589000	-3.159731000	1.253086000
		1	-5.998498000	-1.686109000	2.250496000
		1	-4.437240000	0.248106000	-3.481661000
		1	-3.403279000	0.922325000	-2.162946000
		1	-4.944868000	1.743542000	-2.602662000

## XXVIII [Cu(IMe)(OPh)(PhCCPh)(IMe)(Cu)]<sup>+</sup> min

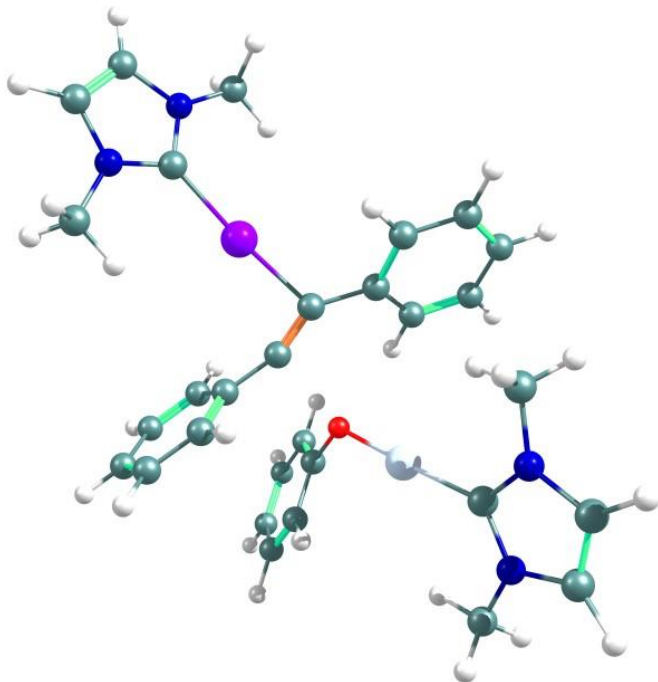
	6	4.685193000	-0.812157000	-0.305219000
	7	5.374494000	-1.572772000	0.606096000
	7	5.604388000	-0.552128000	-1.291255000
	6	6.686902000	-1.780575000	0.200053000
	6	6.831802000	-1.135144000	-1.002964000
	6	4.808952000	-2.073646000	1.856108000
	6	5.325853000	0.232959000	-2.491838000
	1	7.404517000	-2.360542000	0.789951000
	1	7.699248000	-1.046606000	-1.665543000
	29	2.879056000	-0.204473000	-0.223706000
	6	0.047418000	-0.031509000	0.389088000
	6	1.128429000	0.572046000	-0.170558000
	6	-4.274359000	-1.094346000	-0.857243000
	7	-5.560338000	-0.639548000	-0.997154000
	7	-4.305811000	-2.381269000	-1.329518000
	6	-6.375717000	-1.620295000	-1.546441000
	6	-5.582270000	-2.720525000	-1.757521000
	6	-6.023183000	0.693219000	-0.615808000
	6	-3.150636000	-3.276227000	-1.393930000
	1	-7.442258000	-1.461667000	-1.737415000
1	-5.823288000	-3.705531000	-2.170828000	
29	-2.793321000	-0.198668000	-0.170047000	
6	-1.309936000	1.844530000	1.338718000	
6	-0.568808000	1.930531000	2.527082000	
6	-2.192276000	2.864116000	0.948562000	
6	-0.732261000	3.063482000	3.343519000	
1	0.129595000	1.127044000	2.803616000	
6	-2.350191000	3.986002000	1.780038000	
1	-2.723552000	2.785215000	-0.013117000	
6	-1.622486000	4.089084000	2.978641000	
1	-0.156730000	3.139281000	4.279326000	
1	-3.035892000	4.792605000	1.477069000	
1	-1.743612000	4.971964000	3.624480000	
8	-1.230336000	0.701693000	0.516701000	
6	1.039072000	1.920917000	-0.790433000	
6	0.149407000	2.175871000	-1.867409000	
Zero-point correction=	0.531422 (Hartree/Particle)			
Thermal correction to Energy=	0.569836			
Thermal correction to Enthalpy=	0.570780			
Thermal correction to Gibbs Free Energy=	0.451639			
Sum of electronic and zero-point Energies=	-1849.270446			
Sum of electronic and thermal Energies=	-1849.232032			
Sum of electronic and thermal Enthalpies=	-1849.231088			

Sum of electronic and thermal Free Energies=	-1849.350229	6	1.896549000	2.973979000	-0.379284000
		6	0.117911000	3.429218000	-2.500396000
		1	-0.504481000	1.364235000	-2.226575000
		6	1.846685000	4.233776000	-0.996945000
		1	2.603636000	2.793084000	0.446943000
		6	0.960121000	4.467756000	-2.063775000
		1	-0.569208000	3.596122000	-3.345883000
		1	2.513278000	5.038491000	-0.647617000
		1	0.932307000	5.451352000	-2.558339000
		6	-0.107478000	-1.411599000	0.895700000
		6	-1.032706000	-1.729665000	1.927368000
		6	0.658072000	-2.473245000	0.343013000
		6	-1.163734000	-3.046473000	2.401767000
		1	-1.628821000	-0.929068000	2.393176000
		6	0.527683000	-3.785182000	0.822575000
		1	1.350964000	-2.247582000	-0.485190000
		6	-0.383676000	-4.080617000	1.855251000
		1	-1.874516000	-3.261310000	3.215491000
		1	1.132108000	-4.590332000	0.374661000
		1	-0.486783000	-5.111611000	2.228404000
		1	4.292291000	0.621509000	-2.421139000
		1	5.418122000	-0.396727000	-3.399555000
		1	6.028883000	1.086319000	-2.565862000
		1	3.729891000	-1.830362000	1.871422000
		1	5.301833000	-1.595429000	2.726573000
		1	4.935594000	-3.172442000	1.923919000
		1	-2.307562000	-2.812276000	-0.847774000
		1	-2.853032000	-3.450016000	-2.447495000
		1	-3.395301000	-4.245092000	-0.916943000
		1	-5.168363000	1.254420000	-0.194759000
		1	-6.819602000	0.620557000	0.151232000
		1	-6.414013000	1.234254000	-1.500474000

## XXIX[Ag(IMe)(OPh)]

 <p>Zero-point correction= 0.215674 (Hartree/Particle)  Thermal correction to Energy= 0.231534  Thermal correction to Enthalpy= 0.232479  Thermal correction to Gibbs Free Energy= 0.168465  Sum of electronic and zero-point Energies= -758.165155  Sum of electronic and thermal Energies= -758.149294  Sum of electronic and thermal Enthalpies= -758.148350  Sum of electronic and thermal Free Energies= -758.212364</p>	6	-2.244612000	0.097657000	-0.009554000
	7	-3.314390000	-0.696597000	0.317814000
	7	-2.789997000	1.342348000	-0.196198000
	6	-4.497338000	0.034126000	0.333832000
	6	-4.165054000	1.325270000	0.009693000
	6	-3.226184000	-2.125938000	0.603759000
	6	-2.026618000	2.534305000	-0.556348000
	1	-5.466690000	-0.416712000	0.570742000
	1	-4.787695000	2.220516000	-0.089419000
	47	-0.280189000	-0.443893000	-0.165278000
	6	2.737173000	-0.440471000	-0.113686000
	6	2.758353000	0.839807000	0.515208000
	6	3.998790000	-1.015793000	-0.453833000
	6	3.965356000	1.505440000	0.780023000
	1	1.791527000	1.295446000	0.798874000
	6	5.198276000	-0.342502000	-0.184483000
	1	3.998317000	-2.005562000	-0.937499000
	6	5.199412000	0.924271000	0.433303000
	1	3.940848000	2.494516000	1.268694000
	1	6.154859000	-0.816357000	-0.463509000
1	6.145583000	1.447792000	0.642147000	
8	1.623500000	-1.115140000	-0.387754000	
1	-3.632595000	-2.343235000	1.611817000	
1	-2.160164000	-2.419845000	0.570699000	
1	-3.787877000	-2.709679000	-0.153245000	
1	-2.419748000	2.974767000	-1.494362000	
1	-0.972027000	2.236389000	-0.708107000	
1	-2.078078000	3.288740000	0.254483000	

## XXIX+XXII-XXX TS



Zero-point correction= 0.528944 (Hartree/Particle)  
 Thermal correction to Energy= 0.568077  
 Thermal correction to Enthalpy= 0.569021  
 Thermal correction to Gibbs Free Energy= 0.446920  
 Sum of electronic and zero-point Energies= -1737.288125  
 Sum of electronic and thermal Energies= -1737.248993  
 Sum of electronic and thermal Enthalpies= -1737.248049  
 Sum of electronic and thermal Free Energies= -1737.370150

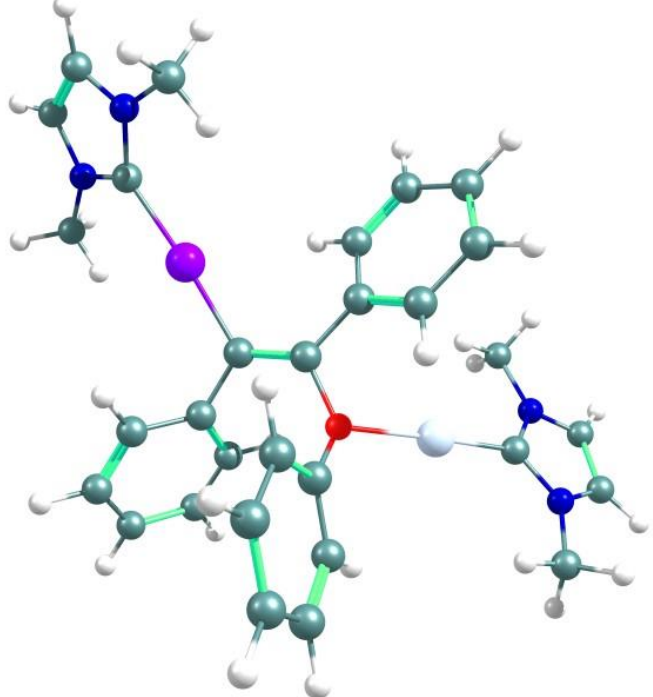
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7	-5.724883000	-0.997699000	0.273913000
7	-5.361680000	0.114224000	-1.558433000
6	-6.957068000	-0.834792000	-0.346859000
6	-6.728142000	-0.132310000	-1.503044000
6	-5.532129000	-1.693906000	1.545860000
6	-4.702919000	0.845119000	-2.639914000
1	-7.886572000	-1.226066000	0.079662000
1	-7.419330000	0.208859000	-2.280767000
79	-2.747669000	-0.365883000	-0.013343000
6	-0.322086000	0.735315000	0.241944000
6	-0.709289000	-0.451210000	0.585100000
6	4.317263000	-1.629557000	-1.012280000
7	4.054537000	-2.934016000	-1.335132000
7	5.603303000	-1.419046000	-1.434656000
6	5.152051000	-3.525574000	-1.949932000
6	6.132174000	-2.567470000	-2.012014000
6	2.788846000	-3.621178000	-1.084018000
6	6.338570000	-0.163688000	-1.291508000
1	5.149462000	-4.567868000	-2.285685000
1	7.151423000	-2.612090000	-2.409871000
47	3.076953000	-0.284859000	-0.089039000
6	2.224841000	2.303160000	1.203943000
6	1.849076000	2.921424000	2.429445000
6	2.977486000	3.067934000	0.270987000
6	2.240065000	4.238140000	2.715868000
1	1.264668000	2.333665000	3.154887000
6	3.361379000	4.384953000	0.565947000
1	3.251793000	2.602921000	-0.691713000
6	2.997176000	4.979464000	1.789121000
1	1.953909000	4.690841000	3.679095000
1	3.951323000	4.956429000	-0.169001000
1	3.303929000	6.011406000	2.019144000
8	1.851690000	1.032816000	0.962996000
6	-0.192442000	-1.638849000	1.284803000
6	-0.709749000	-2.924977000	0.984256000
6	0.806214000	-1.525040000	2.287301000
6	-0.236140000	-4.064688000	1.654050000
1	-1.492227000	-3.018506000	0.213676000
6	1.264960000	-2.667753000	2.962273000
1	1.208028000	-0.528221000	2.518702000
6	0.750634000	-3.939999000	2.649055000
1	-0.650197000	-5.055124000	1.406567000
1	2.031145000	-2.561178000	3.746754000
1	1.110778000	-4.831166000	3.187019000
6	-0.371990000	2.022480000	-0.372663000
6	-0.024482000	2.173471000	-1.746007000
6	-0.733545000	3.174675000	0.380010000
6	-0.068076000	3.435617000	-2.348836000
1	0.271227000	1.283965000	-2.323354000
6	-0.769967000	4.434328000	-0.235458000
1	-0.999906000	3.062264000	1.440545000
6	-0.441277000	4.567652000	-1.595863000
1	0.194094000	3.543597000	-3.413049000
1	-1.053043000	5.320074000	0.353669000
1	-0.469875000	5.559628000	-2.073508000
1	5.685510000	0.568198000	-0.780788000
1	6.623250000	0.232625000	-2.286544000
1	7.251597000	-0.320036000	-0.683455000
1	2.150035000	-2.975540000	-0.452809000
1	2.974172000	-4.573128000	-0.549526000
1	2.265870000	-3.831684000	-2.038644000
1	-4.455050000	-1.672225000	1.795945000
1	-5.867338000	-2.746518000	1.460802000
1	-6.103856000	-1.188975000	2.349468000
1	-4.858195000	0.323356000	-3.605051000
1	-3.620641000	0.893720000	-2.419729000
1	-5.107435000	1.874325000	-2.708448000

6	4.714163000	-0.897988000	-0.188974000
7	5.327828000	-1.687504000	0.748564000
7	5.681223000	-0.663653000	-1.132099000
6	6.649098000	-1.940093000	0.398785000
6	6.871918000	-1.293590000	-0.790876000

	6	4.690037000	-2.180414000	1.967419000
	6	5.490891000	0.139010000	-2.339014000
	1	7.316280000	-2.550207000	1.016555000
	1	7.770571000	-1.232390000	-1.413515000
	79	2.790803000	-0.180894000	-0.181743000
	6	-0.178510000	0.112266000	0.406944000
	6	0.911355000	0.670800000	-0.192097000
	6	-4.887663000	-1.181695000	-0.816127000
	7	-6.194131000	-0.806344000	-0.661876000
	7	-4.936353000	-2.347425000	-1.530066000
	6	-7.045608000	-1.719975000	-1.271533000
	6	-6.250213000	-2.693720000	-1.821152000
	6	-6.652149000	0.387306000	0.048052000
	6	-3.772281000	-3.125798000	-1.953491000
	1	-8.134917000	-1.607990000	-1.261582000
	1	-6.511048000	-3.595028000	-2.385781000
	47	-3.206816000	-0.215717000	-0.135977000
	6	-1.501672000	2.033832000	1.282278000
	6	-0.652848000	2.234150000	2.382122000
	6	-2.497195000	2.967050000	0.949066000
	6	-0.821730000	3.390203000	3.164561000
	1	0.132734000	1.500245000	2.614655000
	6	-2.656367000	4.114269000	1.744613000
	1	-3.122925000	2.801634000	0.056741000
	6	-1.820646000	4.329892000	2.854679000
	1	-0.161082000	3.552630000	4.030574000
	1	-3.430845000	4.851878000	1.482320000
	1	-1.943087000	5.232135000	3.472874000
	8	-1.425700000	0.869372000	0.496754000
	6	0.817171000	1.993979000	-0.872134000
	6	-0.103855000	2.209441000	-1.929428000
	6	1.691104000	3.056559000	-0.528819000
	6	-0.152518000	3.437829000	-2.608525000
	1	-0.769257000	1.387154000	-2.238728000
	6	1.625726000	4.292014000	-1.192404000
	1	2.425513000	2.901457000	0.278104000
	6	0.705510000	4.488721000	-2.237813000
	1	-0.864026000	3.574698000	-3.438988000
	1	2.306619000	5.106051000	-0.896567000
	1	0.664168000	5.453096000	-2.768081000
	6	-0.363816000	-1.236512000	0.986541000
	6	-1.240818000	-1.444454000	2.087237000
	6	0.295830000	-2.369538000	0.440781000
	6	-1.424853000	-2.725957000	2.634487000
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	1	0.952011000	-2.230312000	-0.433041000
	6	-0.749386000	-3.833058000	2.091902000
	1	-2.092912000	-2.855665000	3.500705000
	1	0.632985000	-4.509842000	0.549687000
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	1	-5.771825000	0.905484000	0.471164000
	1	-7.335620000	0.103764000	0.872514000
	1	-7.178518000	1.071181000	-0.647075000
	1	-2.871473000	-2.715400000	-1.460585000
	1	-3.646400000	-3.067809000	-3.053181000
	1	-3.895390000	-4.184242000	-1.652268000
	1	3.625325000	-1.881880000	1.945503000
	1	5.174346000	-1.740808000	2.862424000
	1	4.761597000	-3.285000000	2.017828000
	1	4.461441000	0.543494000	-2.326223000
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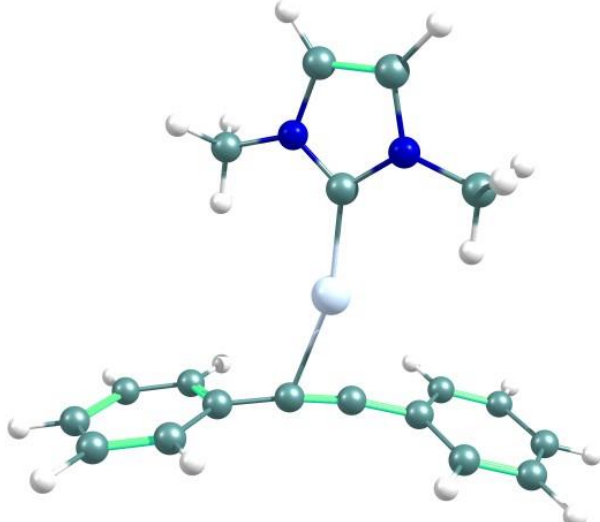
**XXX [Ag(Ime)(OPh)(PhCCPh)(Ime)(Au)]<sup>+</sup> min**



	6	4.714163000	-0.897988000	-0.188974000
	7	5.327828000	-1.687504000	0.748564000
	7	5.681223000	-0.663653000	-1.132099000
	6	6.649098000	-1.940093000	0.398785000
	6	6.871918000	-1.293590000	-0.790876000
	6	4.690037000	-2.180414000	1.967419000
	6	5.490891000	0.139010000	-2.339014000
	1	7.316280000	-2.550207000	1.016555000
	1	7.770571000	-1.232390000	-1.413515000
	79	2.790803000	-0.180894000	-0.181743000
	6	-0.178510000	0.112266000	0.406944000
	6	0.911355000	0.670800000	-0.192097000
	6	-4.887663000	-1.181695000	-0.816127000
	7	-6.194131000	-0.806344000	-0.661876000
	7	-4.936353000	-2.347425000	-1.530066000
	6	-7.045608000	-1.719975000	-1.271533000
	6	-6.250213000	-2.693720000	-1.821152000
	6	-6.652149000	0.387306000	0.048052000
	6	-3.772281000	-3.125798000	-1.953491000
	1	-8.134917000	-1.607990000	-1.261582000
	1	-6.511048000	-3.595028000	-0.385781000
	47	-3.206816000	-0.215717000	-0.135977000
	6	-1.501672000	2.033832000	1.282278000
	6	-0.652848000	2.234150000	2.382122000
	6	-2.497195000	2.967050000	0.949066000
6	-0.821730000	3.390203000	3.164561000	
1	0.132734000	1.500245000	2.614655000	
6	-2.656367000	4.114269000	1.744613000	
1	-3.122925000	2.801634000	0.056741000	
6	-1.820646000	4.329892000	2.854679000	
1	-0.161082000	3.552630000	4.030574000	
1	-3.430845000	4.851878000	1.482320000	
1	-1.943087000	5.232135000	3.472874000	
8	-1.425700000	0.869372000	0.496754000	
6	0.817171000	1.993979000	-0.872134000	
6	-0.103855000	2.209441000	-1.929428000	
6	1.691104000	3.056559000	-0.528819000	
6	-0.152518000	3.437829000	-2.608525000	
1	-0.769257000	1.387154000	-2.238728000	
6	1.625726000	4.292014000	-1.192404000	
1	2.425513000	2.901457000	0.278104000	
6	0.705510000	4.488721000	-2.237813000	
1	-0.864026000	3.574698000	-3.438988000	
1	2.306619000	5.106051000	-0.896567000	
1	0.664168000	5.453096000	-2.768081000	
6	-0.363816000	-1.236512000	0.986541000	
6	-1.240818000	-1.444454000	2.087237000	
6	0.295830000	-2.369538000	0.440781000	
6	-1.424853000	-2.725957000	2.634487000	
1	-1.747791000	-0.583694000	2.552209000	
6	0.110559000	-3.646498000	0.992342000	
1	0.952011000	-2.230312000	-0.433041000	
6	-0.749386000	-3.833058000	2.091902000	
1	-2.092912000	-2.855665000	3.500705000	
1	0.632985000	-4.509842000	0.549687000	
1	-0.893749000	-4.836970000	2.521143000	
1	-5.771825000	0.905484000	0.471164000	
1	-7.335620000	0.103764000	0.872514000	
1	-7.178518000	1.071181000	-0.647075000	
1	-2.871473000	-2.715400000	-1.460585000	
1	-3.646400000	-3.067809000	-3.053181000	
1	-3.895390000	-4.184242000	-1.652268000	
1	3.625325000	-1.881880000	1.945503000	
1	5.174346000	-1.740808000	2.862424000	
1	4.761597000	-3.285000000	2.017828000	
1	4.461441000	0.543494000	-2.326223000	
1	5.628784000	-0.485698000	-3.244099000	
1	6.213613000	0.978716000	-2.358866000	

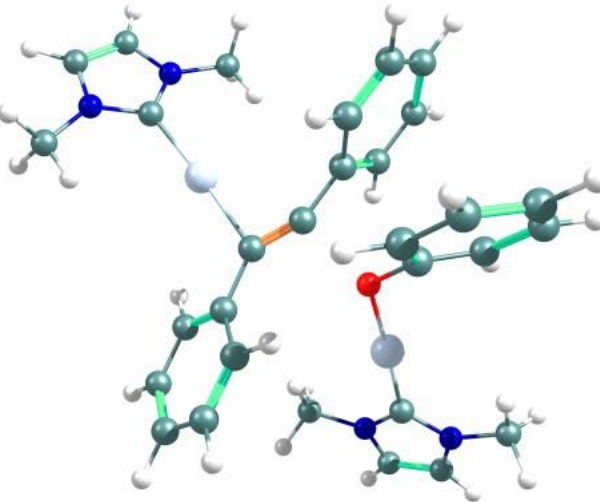
Zero-point correction= 0.531108 (Hartree/Particle)  
 Thermal correction to Energy= 0.570008  
 Thermal correction to Enthalpy= 0.570953  
 Thermal correction to Gibbs Free Energy= 0.448562  
 Sum of electronic and zero-point Energies= -1737.309810  
 Sum of electronic and thermal Energies= -1737.270910  
 Sum of electronic and thermal Enthalpies= -1737.269966  
 Sum of electronic and thermal Free Energies= -1737.392357

**XXXI [Ag(IMe)(PhCCPh)]<sup>+</sup>**

	6	-0.158906000	-2.561434000	0.003948000
	7	-1.206049000	-3.328951000	0.434199000
	7	0.779843000	-3.455769000	-0.431706000
	6	-0.927856000	-4.680227000	0.270447000
	6	0.328150000	-4.760455000	-0.276656000
	6	-2.456463000	-2.818217000	0.996359000
	1	-1.635977000	-5.466575000	0.552663000
	1	0.928261000	-5.630349000	-0.564066000
	47	-0.025477000	-0.485959000	0.007639000
	6	0.732561000	1.696298000	0.044534000
	6	-0.516394000	1.772038000	-0.036894000
	6	2.161930000	1.853758000	0.110880000
	6	2.916684000	2.020150000	-1.082338000
	6	2.824507000	1.876596000	1.368099000
	6	4.302837000	2.212604000	-1.010501000
1	2.403193000	2.011905000	-2.055867000	
6	4.211142000	2.070394000	1.423127000	
1	2.240525000	1.754102000	2.292933000	
6	4.952370000	2.237174000	0.238128000	
1	4.881515000	2.351229000	-1.936837000	
1	4.718522000	2.096448000	2.399839000	
1	6.041445000	2.391412000	0.288195000	
6	-1.916799000	2.096189000	-0.111240000	
6	-2.568756000	2.173621000	-1.371898000	
6	-2.649958000	2.371527000	1.075186000	
6	-3.923197000	2.526018000	-1.437265000	
1	-2.000174000	1.967455000	-2.291488000	
6	-4.004158000	2.722274000	0.992994000	
1	-2.143578000	2.320888000	2.051157000	
6	-4.643114000	2.799237000	-0.258925000	
1	-4.421352000	2.593217000	-2.416752000	
1	-4.565363000	2.944446000	1.913816000	
1	-5.706661000	3.078335000	-0.316788000	
1	-2.578095000	-3.165190000	2.041584000	
1	-3.317494000	-3.164611000	0.391541000	
1	-2.427747000	-1.713058000	0.982128000	
6	2.086309000	-3.107742000	-0.990404000	
1	2.202809000	-2.008633000	-0.963591000	
1	2.161240000	-3.455910000	-2.039647000	
1	2.894478000	-3.570799000	-0.390779000	

Zero-point correction= 0.311901 (Hartree/Particle)  
 Thermal correction to Energy= 0.334393  
 Thermal correction to Enthalpy= 0.335337  
 Thermal correction to Gibbs Free Energy= 0.253492  
 Sum of electronic and zero-point Energies= -990.296676  
 Sum of electronic and thermal Energies= -990.274184  
 Sum of electronic and thermal Enthalpies= -990.273239  
 Sum of electronic and thermal Free Energies= -990.355085

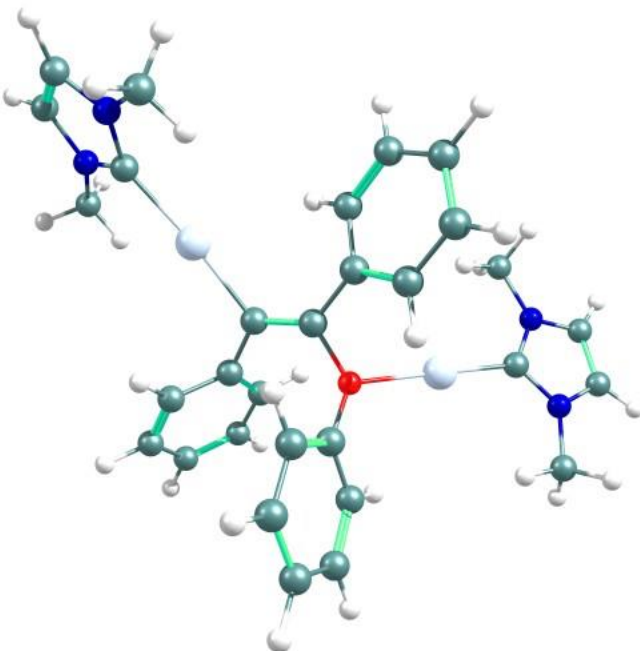
## XXIX+XXXI-XXXII TS

	6	-4.956733000	-0.639918000	-0.444127000
	7	-5.938928000	-1.286825000	0.256946000
	7	-5.607236000	-0.072450000	-1.506760000
	6	-7.177135000	-1.126821000	-0.353915000
	6	-6.967196000	-0.357648000	-1.470679000
	6	-5.728693000	-2.045659000	1.488871000
	6	-4.968563000	0.732555000	-2.546258000
	1	-8.095854000	-1.565812000	0.049221000
	1	-7.667350000	0.004680000	-2.230786000
	47	-2.923652000	-0.536261000	0.021002000
	6	-0.504200000	0.695445000	0.274821000
	6	-0.853389000	-0.505929000	0.610829000
	6	4.141783000	-1.482441000	-1.043840000
	7	3.941590000	-2.794626000	-1.379756000
	7	5.432643000	-1.219905000	-1.418701000
	6	5.082704000	-3.340122000	-1.956390000
	6	6.026261000	-2.344338000	-1.980024000
	6	2.695356000	-3.531803000	-1.177660000
	6	6.112896000	0.062679000	-1.246670000
	1	5.132809000	-4.380144000	-2.295415000
	1	7.060057000	-2.347372000	-2.341145000
	47	2.811712000	-0.196116000	-0.164321000
	6	1.820975000	2.338229000	1.169193000
	6	1.410561000	2.865125000	2.421616000
	6	2.580434000	3.165413000	0.302280000
6	1.777384000	4.165935000	2.800398000	
1	0.817088000	2.227078000	3.095252000	

Zero-point correction= 0.528372 (Hartree/Particle)  
 Thermal correction to Energy= 0.567755  
 Thermal correction to Enthalpy= 0.568699

Thermal correction to Gibbs Free Energy=	0.444926	6	2.945624000	4.464138000	0.691708000
Sum of electronic and zero-point Energies=	-1748.469790	1	2.877985000	2.767316000	-0.682855000
Sum of electronic and thermal Energies=	-1748.430407	6	2.547969000	4.972451000	1.942028000
Sum of electronic and thermal Enthalpies=	-1748.429463	1	1.463167000	4.553056000	3.783185000
Sum of electronic and thermal Free Energies=	-1748.553236	1	3.543418000	5.088452000	0.008068000
		1	2.836312000	5.990563000	2.245639000
		8	1.479829000	1.069713000	0.833462000
		6	-0.282082000	-1.667091000	1.308062000
		6	-0.706303000	-2.980548000	0.977291000
		6	0.680127000	-1.512100000	2.341797000
		6	-0.179372000	-4.099880000	1.641937000
		1	-1.462009000	-3.113134000	0.185228000
		6	1.192043000	-2.633709000	3.013315000
		1	1.012996000	-0.498270000	2.604207000
		6	0.769889000	-3.930977000	2.666328000
		1	-0.524054000	-5.109946000	1.368404000
		1	1.927890000	-2.491588000	3.820926000
		1	1.170994000	-4.806397000	3.201031000
		6	-0.759655000	1.957721000	-0.376328000
		6	-0.474795000	2.115640000	-1.760044000
		6	-1.260363000	3.067156000	0.354690000
		6	-0.710596000	3.342028000	-2.395568000
		1	-0.070352000	1.260492000	-2.323453000
		6	-1.489635000	4.292387000	-0.290133000
		1	-1.476810000	2.952536000	1.426786000
		6	-1.218451000	4.432744000	-1.662479000
		1	-0.492554000	3.452846000	-3.469535000
		1	-1.879570000	5.145968000	0.285750000
		1	-1.397709000	5.397031000	-2.163560000
		1	5.414878000	0.766994000	-0.757250000
		1	6.416283000	0.473536000	-2.230191000
		1	7.009659000	-0.060713000	-0.607670000
		1	2.008659000	-2.914959000	-0.568203000
		1	2.898195000	-4.478058000	-0.639527000
		1	2.216869000	-3.758204000	-2.151797000
		1	-4.654062000	-2.005989000	1.746925000
		1	-6.030003000	-3.102548000	1.346724000
		1	-6.317209000	-1.605262000	2.318100000
		1	-5.104749000	0.258666000	-3.538774000
		1	-3.888212000	0.803623000	-2.321319000
		1	-5.401780000	1.752244000	-2.564054000

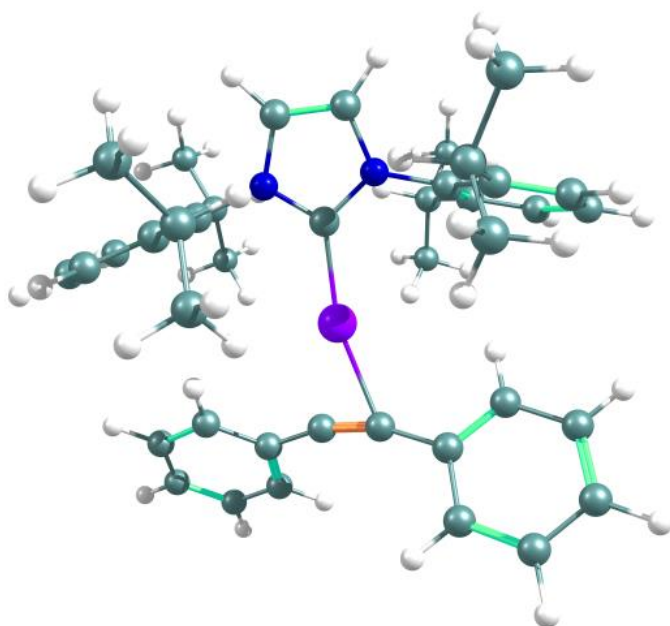
**XXXII [Ag(IMe)(OPh)(PhCCPh)(IMe)(Ag)]<sup>+</sup> min**



Zero-point correction= 0.530415 (Hartree/Particle)  
 Thermal correction to Energy= 0.569525  
 Thermal correction to Enthalpy= 0.570470  
 Thermal correction to Gibbs Free Energy= 0.447354  
 Sum of electronic and zero-point Energies= -1748.483353  
 Sum of electronic and thermal Energies= -1748.444243  
 Sum of electronic and thermal Enthalpies= -1748.443299  
 Sum of electronic and thermal Free Energies= -1748.566414

6	5.031834000	-0.941136000	-0.232356000
7	5.661879000	-1.735792000	0.688793000
7	5.993104000	-0.684276000	-1.174463000
6	6.985126000	-1.969375000	0.331587000
6	7.194520000	-1.303713000	-0.849966000
6	5.037782000	-2.253570000	1.904201000
6	5.788996000	0.131341000	-2.370134000
1	7.662684000	-2.580164000	0.937503000
1	8.089507000	-1.223203000	-1.475890000
47	3.062865000	-0.225684000	-0.206851000
6	0.067502000	0.096755000	0.390233000
6	1.152093000	0.652239000	-0.209010000
6	-4.659850000	-1.181893000	-0.817683000
7	-5.965064000	-0.806266000	-0.653387000
7	-4.714290000	-2.344509000	-1.536401000
6	-6.821266000	-1.716484000	-1.261509000
6	-6.030294000	-2.688471000	-1.820536000
6	-6.417403000	0.384392000	0.065166000
6	-3.553592000	-3.121811000	-1.970633000
1	-7.910387000	-1.603634000	-1.244009000
1	-6.295552000	-3.587065000	-2.387417000
47	-2.975018000	-0.219310000	-0.143954000
6	-1.264090000	2.019466000	1.269965000
6	-0.412426000	2.224726000	2.367125000
6	-2.256317000	2.955582000	0.933537000
6	-0.574695000	3.386419000	3.142396000
1	0.370330000	1.488869000	2.603057000
6	-2.409367000	4.108520000	1.721883000
1	-2.884689000	2.787241000	0.043519000
6	-1.570436000	4.328247000	2.828723000
1	0.088419000	3.551795000	4.006014000
1	-3.181527000	4.847446000	1.456377000
1	-1.687882000	5.235025000	3.441241000
8	-1.193036000	0.850475000	0.494188000
6	1.075404000	1.976911000	-0.877986000
6	0.159803000	2.214146000	-1.937167000
6	1.962090000	3.028030000	-0.527436000
6	0.130708000	3.447038000	-2.609152000
1	-0.517892000	1.404100000	-2.252238000
6	1.913764000	4.268999000	-1.181533000
1	2.693657000	2.859899000	0.280134000
6	1.000390000	4.485048000	-2.229440000
1	-0.577229000	3.598472000	-3.440265000
1	2.603790000	5.072310000	-0.877291000
1	0.973677000	5.453124000	-2.753762000
6	-0.113997000	-1.254174000	0.969267000
6	-0.984564000	-1.471177000	2.072486000
6	0.554420000	-2.381019000	0.421988000
6	-1.153121000	-2.754548000	2.620937000
1	-1.499772000	-0.615655000	2.537855000
6	0.385089000	-3.660142000	0.973623000
1	1.203050000	-2.235884000	-0.456953000
6	-0.468513000	-3.855125000	2.076742000
1	-1.816872000	-2.890793000	3.489508000
1	0.913911000	-4.518306000	0.528374000
1	-0.601051000	-4.860269000	2.506859000
1	-5.533706000	0.901066000	0.483077000
1	-7.094008000	0.097373000	0.894089000
1	-6.949581000	1.070968000	-0.622830000
1	-2.649668000	-2.714702000	-1.480748000
1	-3.433937000	-3.058226000	-3.070721000
1	-3.676011000	-4.181706000	-1.674216000
1	3.966508000	-1.979113000	1.890232000
1	5.514279000	-1.813458000	2.803244000
1	5.131455000	-3.356956000	1.944434000
1	4.758148000	0.531683000	-2.347301000
1	5.922740000	-0.480667000	-3.284569000
1	6.506157000	0.975931000	-2.386712000

# V [Au(IPr) (PhCCPh)]



Zero-point correction= 0.740376 (Hartree/Particle)  
 Thermal correction to Energy= 0.786913  
 Thermal correction to Enthalpy= 0.787857  
 Thermal correction to Gibbs Free Energy= 0.652947  
 Sum of electronic and zero-point Energies= -1833.283807  
 Sum of electronic and thermal Energies= -1833.237270  
 Sum of electronic and thermal Enthalpies= -1833.236326  
 Sum of electronic and thermal Free Energies= -1833.371237

6	-0.000202000	-1.411872000	0.000160000
7	-1.053044000	-2.239443000	-0.278790000
7	1.052467000	-2.239600000	0.279316000
6	-0.664001000	-3.572228000	-0.174731000
6	0.663145000	-3.572328000	0.175582000
6	-2.394380000	-1.803186000	-0.625150000
6	2.393930000	-1.803520000	0.625423000
1	-1.362662000	-4.394060000	-0.359750000
1	1.361630000	-4.394266000	0.360794000
6	-2.683262000	-1.520100000	-1.987159000
6	-4.001352000	-1.119871000	-2.292407000
6	-4.982177000	-1.024880000	-1.294619000
6	-4.664786000	-1.319708000	0.039052000
6	-3.362361000	-1.714021000	0.410830000
6	-1.646813000	-1.645097000	-3.104891000
1	-4.267083000	-0.893020000	-3.336814000
1	-6.008140000	-0.725938000	-1.561662000
1	-5.446328000	-1.246701000	0.811384000
6	-3.050621000	-2.039782000	1.872339000
6	2.683047000	-1.520144000	1.987322000
6	4.001276000	-1.120175000	2.292306000
6	4.982004000	-1.025678000	1.294372000
6	4.664364000	-1.320721000	-0.039192000
6	3.361793000	-1.714804000	-0.410704000
6	1.646703000	-1.644575000	3.105216000
1	4.267193000	-0.893117000	3.336621000
1	6.008072000	-0.726919000	1.561219000
1	5.445815000	-1.248082000	-0.811650000
6	3.049768000	-2.040768000	-1.872104000
1	-0.698155000	-2.001826000	-2.651329000
6	-1.353129000	-0.277222000	-3.757737000
6	-2.073158000	-2.693921000	-4.155422000
1	-1.963215000	-2.251289000	1.949602000
6	-3.344620000	-0.843480000	2.802232000
6	-3.799692000	-3.309508000	2.334535000
1	0.697820000	-2.000911000	2.651819000
6	2.072741000	-2.693501000	4.155767000
6	1.353734000	-0.276512000	3.757991000
1	1.962284000	-2.251947000	-1.949180000
6	3.344011000	-0.844731000	-2.802261000
6	3.798382000	-3.310817000	-2.334140000
1	-0.569547000	-0.377677000	-4.536956000
1	-2.256336000	0.144807000	-4.246178000
1	-0.996766000	0.460427000	-3.007851000
1	-1.280636000	-2.819748000	-4.921948000
1	-2.261931000	-3.684611000	-3.693240000
1	-3.000075000	-2.389645000	-4.684887000
1	-3.038193000	-1.079398000	3.842312000
1	-2.799020000	0.067086000	2.479810000
1	-4.426691000	-0.597534000	2.826988000
1	-3.528447000	-3.562625000	3.380383000
1	-4.899949000	-3.165627000	2.300388000
1	-3.558951000	-4.185681000	1.697783000
1	1.280320000	-2.818838000	4.922480000
1	2.260908000	-3.684342000	3.693660000
1	2.999929000	-2.389639000	4.684997000
1	0.570176000	-0.376546000	4.537287000
1	2.257188000	0.145115000	4.246321000
1	0.997665000	0.461258000	3.008089000
1	3.037367000	-1.080739000	-3.842257000
1	2.798718000	0.066057000	-2.479919000
1	4.426153000	-0.599122000	-2.827208000
1	3.526923000	-3.564063000	-3.379902000
1	4.898690000	-3.167274000	-2.300165000
1	3.557449000	-4.186785000	-1.697177000
79	0.000114000	0.614989000	-0.000007000
6	-0.628135000	2.757328000	0.079098000
6	0.628887000	2.757130000	-0.079354000
6	-1.972470000	3.164156000	0.404480000
6	-2.154880000	4.319982000	1.212189000
6	-3.106855000	2.465254000	-0.083005000
6	-3.448973000	4.764900000	1.512200000

	1	-1.275807000	4.859023000	1.596332000
	6	-4.395450000	2.920162000	0.229249000
	1	-2.968511000	1.571571000	-0.710988000
	6	-4.570209000	4.067958000	1.023663000
	1	-3.584173000	5.662802000	2.134944000
	1	-5.271142000	2.375855000	-0.155911000
	1	-5.584730000	4.422818000	1.263255000
	6	1.973248000	3.163819000	-0.404832000
	6	3.107624000	2.464221000	0.081645000
	6	2.155674000	4.320254000	-1.211679000
	6	4.396229000	2.919013000	-0.230768000
	1	2.969325000	1.570078000	0.708986000
	6	3.449769000	4.765043000	-1.511854000
	1	1.276605000	4.859856000	-1.595045000
	6	4.571006000	4.067383000	-1.024338000
	1	5.271911000	2.374142000	0.153616000
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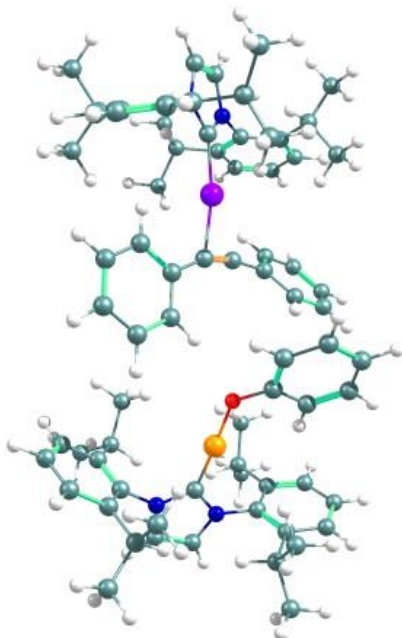
## VIII [Au(IPr)(OPh)]

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	6	-0.576229000	0.671090000	0.007980000
	7	0.026835000	1.910870000	0.015358000
	6	-0.918350000	2.936095000	0.013400000
	1	-0.628386000	3.991337000	0.019272000
	6	-2.151184000	2.335335000	0.003882000
	1	-3.160761000	2.757676000	-0.000646000
	7	-1.925080000	0.959539000	0.000570000
	6	1.457769000	2.129284000	0.023611000
	6	2.124711000	2.228462000	1.273494000
	6	3.514345000	2.467896000	1.250233000
	1	4.063726000	2.543597000	2.201689000
	6	4.207910000	2.603187000	0.039747000
	1	5.293763000	2.788498000	0.046186000
	6	3.524011000	2.495158000	-1.179021000
	1	4.080927000	2.592314000	-2.124119000
	6	2.134655000	2.256050000	-1.218547000
	6	1.403428000	2.043642000	2.608654000
	1	0.316444000	1.965803000	2.396752000
	6	1.832536000	0.721121000	3.281993000
	1	1.652813000	-0.147785000	2.614929000
	1	1.264108000	0.558424000	4.221814000
	1	2.912968000	0.730064000	3.538864000
	6	1.599653000	3.249788000	3.550927000
	1	1.274416000	4.199177000	3.076947000
	1	2.662195000	3.370666000	3.850502000
	1	1.010129000	3.112926000	4.481630000
	6	1.423840000	2.098691000	-2.562901000
1	0.334775000	2.021819000	-2.361665000	

Zero-point correction= 0.644114 (Hartree/Particle)

Thermal correction to Energy=	0.684093	6	1.633024000	3.320184000	-3.482210000
Thermal correction to Enthalpy=	0.685037	1	1.051625000	3.201722000	-4.420530000
Thermal correction to Gibbs Free Energy=	0.565784	1	2.698676000	3.442112000	-3.770031000
Sum of electronic and zero-point Energies=	-1662.734983	1	1.307037000	4.262508000	-2.994851000
Sum of electronic and thermal Energies=	-1662.695004	6	1.852670000	0.786445000	-3.256269000
Sum of electronic and thermal Enthalpies=	-1662.694060	1	1.290694000	0.642851000	-4.203049000
Sum of electronic and thermal Free Energies=	-1662.813313	1	1.664332000	-0.093244000	-2.606102000
		1	2.935060000	0.795366000	-3.504826000
		6	-2.973601000	-0.038278000	-0.013149000
		6	-3.465020000	-0.492874000	-1.265634000
		6	-4.504434000	-1.445726000	-1.248443000
		1	-4.905680000	-1.821517000	-2.202985000
		6	-5.028789000	-1.926859000	-0.041034000
		1	-5.839365000	-2.672724000	-0.051892000
		6	-4.518188000	-1.466327000	1.180257000
		1	-4.930691000	-1.858643000	2.123277000
		6	-3.479147000	-0.513886000	1.225785000
		6	-2.897768000	-0.010136000	-2.600956000
		1	-2.111970000	0.742321000	-2.381631000
		6	-2.218866000	-1.167494000	-3.365260000
		1	-1.420943000	-1.639000000	-2.755250000
		1	-1.760910000	-0.796990000	-4.306350000
		1	-2.949386000	-1.958568000	-3.636780000
		6	-3.974104000	0.685678000	-3.461506000
		1	-4.436768000	1.541304000	-2.926955000
		1	-4.789637000	-0.014478000	-3.741113000
		1	-3.530575000	1.070676000	-4.403745000
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		1	-2.140503000	0.703993000	2.377293000
		6	-2.253858000	-1.222391000	3.326682000
		1	-1.807032000	-0.867070000	4.278914000
		1	-1.448110000	-1.681389000	2.717327000
		1	-2.985155000	-2.019784000	3.576780000
		6	-4.014039000	0.625469000	3.436177000
		1	-3.581146000	0.995060000	4.389455000
		1	-4.830810000	-0.081045000	3.695208000
		1	-4.472920000	1.489177000	2.911467000
		6	2.073671000	-3.188693000	-0.001136000
		6	2.269838000	-4.600046000	0.050607000
		6	3.237478000	-2.370231000	-0.088765000
		6	3.557669000	-5.153278000	0.016893000
		1	1.376578000	-5.241391000	0.118037000
		6	4.521817000	-2.935107000	-0.121919000
		1	3.104333000	-1.274923000	-0.130477000
		6	4.698341000	-4.330760000	-0.069459000
		1	3.674190000	-6.249627000	0.058835000
		1	5.400927000	-2.271731000	-0.190166000
		1	5.707816000	-4.770528000	-0.095777000

**V+VIII [Au(IPr)(PhCCPh)] + [Au(IPr)(OPh)]**



Zero-point correction= 1.386016 (Hartree/Particle)  
 Thermal correction to Energy= 1.474500  
 Thermal correction to Enthalpy= 1.475445  
 Thermal correction to Gibbs Free Energy= 1.242979  
 Sum of electronic and zero-point Energies= -3496.033521  
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 Sum of electronic and thermal Free Energies= -3496.176558

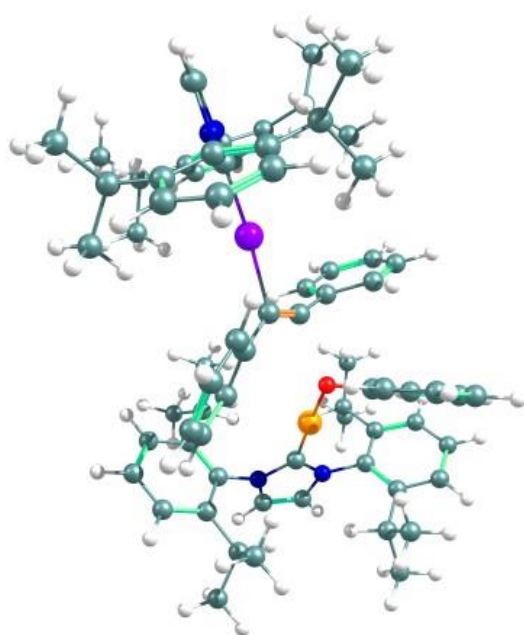
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6	-7.766386000	0.717985000	-0.088625000
6	-5.995263000	-2.126644000	1.280601000
6	-6.005594000	2.291886000	-0.950792000
1	-8.579924000	-1.134524000	0.896728000
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6	-5.718353000	-2.112594000	2.673867000
6	-5.333463000	-3.334970000	3.263596000
6	-5.239440000	-4.510075000	2.504411000
6	-5.521228000	-4.489028000	1.131245000
6	-5.906285000	-3.297564000	0.482013000
6	-5.837184000	-0.854736000	3.536094000
1	-5.113750000	-3.367020000	4.342286000
1	-4.949293000	-5.454994000	2.990447000
1	-5.444662000	-5.419535000	0.547609000
6	-6.228676000	-3.310803000	-1.012993000
6	-5.787374000	2.314693000	-2.353828000
6	-5.384412000	3.542576000	-2.919846000
6	-5.220729000	4.688904000	-2.130242000
6	-5.453958000	4.634625000	-0.748348000
6	-5.850922000	3.435520000	-0.120594000
6	-5.987533000	1.091816000	-3.250119000
1	-5.201597000	3.601287000	-4.004040000
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1	-6.409020000	-2.262222000	-1.331268000
6	-5.048603000	-3.841620000	-1.853949000
6	-7.522982000	-4.106300000	-1.295414000
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1	-5.284791000	-3.769977000	-2.935817000
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1	-4.833628000	-4.908176000	-1.634978000
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6	6.024942000	2.637820000	1.359799000



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	1	1.449484000	-3.315131000	-5.069058000
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## V+VIII-XVI TS

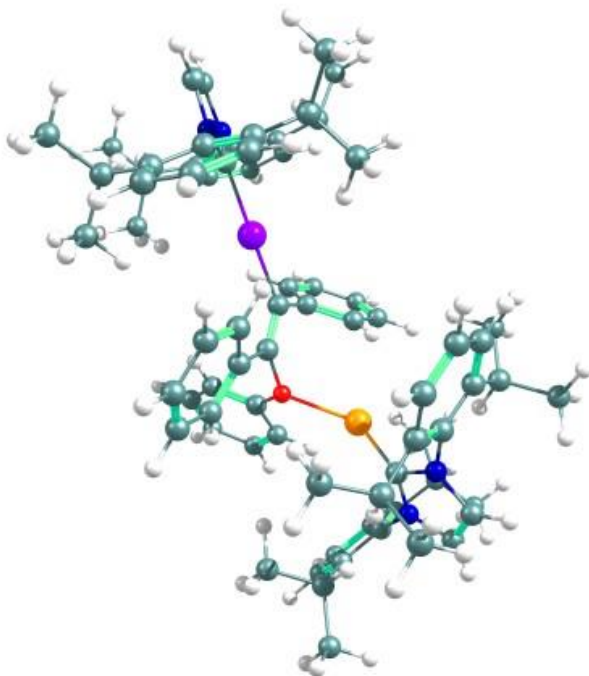
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6	-6.042136000	-5.005210000	0.251445000	
1	-5.948515000	-0.987440000	-2.225644000	
6	-6.960767000	-0.585551000	-4.079541000	
6	-4.434513000	-0.704937000	-3.726933000	
1	-5.761776000	2.208842000	1.313434000	
6	-4.617481000	4.020670000	1.150100000	
6	-7.161750000	3.833676000	1.112377000	
1	-3.167033000	1.500952000	4.197483000	
1	-2.305064000	-0.029358000	4.556419000	
1	-2.524708000	0.496162000	2.851794000	
1	-5.277383000	0.752851000	5.470915000	
1	-6.054077000	-0.820326000	5.094644000	
1	-4.476168000	-0.774011000	5.940182000	
1	-4.210768000	-4.607834000	-1.818499000	
1	-3.062992000	-3.543810000	-0.934038000	
1	-3.299503000	-5.242745000	-0.415781000	
1	-6.449516000	-5.278840000	-0.744069000	
1	-5.621106000	-5.927889000	0.703423000	
1	-6.889810000	-4.678904000	0.888695000	

Zero-point correction= 1.386120 (Hartree/Particle)  
 Thermal correction to Energy= 1.473475  
 Thermal correction to Enthalpy= 1.474419  
 Thermal correction to Gibbs Free Energy= 1.246942  
 Sum of electronic and zero-point Energies= -3496.021522  
 Sum of electronic and thermal Energies= -3495.934167  
 Sum of electronic and thermal Enthalpies= -3495.933223  
 Sum of electronic and thermal Free Energies= -3496.160699

	1	-6.989892000	-1.656923000	-4.367618000
	1	-7.940554000	-0.326377000	-3.628175000
	1	-6.856207000	0.002962000	-5.015071000
	1	-4.436207000	-1.767836000	-4.046909000
	1	-4.210324000	-0.085372000	-4.620858000
	1	-3.606885000	-0.564628000	-2.999334000
	1	-4.627285000	4.197666000	2.245776000
	1	-3.657923000	3.530995000	0.885923000
	1	-4.636093000	5.015086000	0.656711000
	1	-7.199325000	4.043016000	2.201838000
	1	-7.289166000	4.800848000	0.581845000
	1	-8.033864000	3.196685000	0.857525000
	79	-2.855502000	0.068956000	-0.125563000
	6	-0.180869000	-0.399725000	-0.636415000
	6	-0.881943000	0.689521000	-0.586158000
	6	4.978691000	0.260577000	0.693777000
	7	6.115374000	-0.494801000	0.508622000
	7	5.321280000	1.139277000	1.696828000
	6	7.131909000	-0.099266000	1.373855000
	6	6.630333000	0.931828000	2.125847000
	6	6.271690000	-1.538136000	-0.486118000
	6	4.473779000	2.195221000	2.212432000
	1	8.114316000	-0.581401000	1.374079000
	1	7.082802000	1.534418000	2.919458000
	6	6.704054000	-1.172143000	-1.789079000
	6	6.877247000	-2.211481000	-2.726778000
	6	6.638547000	-3.549109000	-2.382342000
	6	6.221631000	-3.879252000	-1.085016000
	6	6.029988000	-2.884389000	-0.103925000
	6	7.018241000	0.271377000	-2.184229000
	1	7.211743000	-1.964999000	-3.746582000
	1	6.785439000	-4.343699000	-3.130878000
	1	6.046345000	-4.934730000	-0.824181000
	6	5.613697000	-3.277093000	1.313968000
	6	3.609304000	1.908863000	3.301600000
	6	2.822800000	2.968395000	3.800183000
	6	2.902805000	4.254252000	3.247664000
	6	3.774827000	4.508960000	2.179554000
	6	4.582649000	3.488872000	1.634616000
	6	3.513540000	0.521220000	3.935624000
	1	2.140129000	2.782892000	4.644274000
	1	2.283662000	5.067726000	3.657422000
	1	3.837580000	5.526018000	1.761080000
	6	5.535062000	3.804224000	0.479967000
	1	6.712824000	0.926575000	-1.341588000
	6	6.216284000	0.723717000	-3.421891000
	6	8.536767000	0.466504000	-2.393334000
	1	5.405627000	-2.342132000	1.875657000
	6	4.316309000	-4.110546000	1.326614000
	6	6.759938000	-4.012088000	2.044270000
	1	4.231806000	-0.141270000	3.409344000
	6	3.916210000	0.544837000	5.425708000
	6	2.109118000	-0.086993000	3.737208000
	1	6.057929000	2.864333000	0.205744000
	6	4.773119000	4.278564000	-0.775513000
	6	6.616162000	4.822935000	0.902648000
	1	6.412083000	1.794779000	-3.636725000
	1	6.499764000	0.150353000	-4.329336000
	1	5.125112000	0.593759000	-3.271284000
	1	8.764750000	1.526778000	-2.630047000
	1	9.116333000	0.185549000	-1.489737000
	1	8.911376000	-0.152171000	-3.235915000
	1	4.006336000	-4.324448000	2.370985000
	1	3.485105000	-3.576738000	0.822392000
	1	4.449244000	-5.088407000	0.817562000
	1	6.471588000	-4.246549000	3.090351000
	1	7.009023000	-4.970295000	1.541405000
	1	7.686453000	-3.402523000	2.074835000
	1	3.900434000	-0.480918000	5.849848000
	1	4.937043000	0.955676000	5.566756000
	1	3.220089000	1.164388000	6.029413000
	1	2.069526000	-1.118426000	4.145867000
	1	1.328107000	0.509053000	4.254581000
	1	1.843352000	-0.130078000	2.660282000
	1	5.477223000	4.437758000	-1.618485000

	1	4.015905000	3.534607000	-1.097659000
	1	4.250192000	5.241926000	-0.597686000
	1	7.331904000	4.996942000	0.072427000
	1	6.170910000	5.804877000	1.168318000
	1	7.192915000	4.469375000	1.782063000
	29	3.380525000	0.124990000	-0.256587000
	6	1.952796000	-0.249452000	-2.622231000
	6	1.241176000	0.495926000	-3.598166000
	6	2.755264000	-1.339567000	-3.049177000
	6	1.343980000	0.162223000	-4.956923000
	1	0.621676000	1.342819000	-3.265992000
	6	2.857942000	-1.658079000	-4.414685000
	1	3.299787000	-1.926249000	-2.290935000
	6	2.151848000	-0.914033000	-5.376022000
	1	0.792495000	0.757469000	-5.702826000
	1	3.493510000	-2.502612000	-4.726148000
	1	2.230382000	-1.167273000	-6.444674000
	8	1.835447000	0.074458000	-1.308648000
	6	-0.644513000	2.133055000	-0.759326000
	6	-1.558212000	2.922971000	-1.501154000
	6	0.483219000	2.763537000	-0.179045000
	6	-1.333317000	4.296706000	-1.683332000
	1	-2.445678000	2.443975000	-1.944123000
	6	0.689858000	4.141474000	-0.346068000
	1	1.194443000	2.164101000	0.407204000
	6	-0.211026000	4.912819000	-1.102592000
	1	-2.046580000	4.889730000	-2.276907000
	1	1.568199000	4.613252000	0.120650000
	1	-0.040803000	5.992910000	-1.235316000
	6	0.023331000	-1.818782000	-0.561755000
	6	0.289990000	-2.446513000	0.685883000
	6	-0.050036000	-2.617175000	-1.737212000
	6	0.465339000	-3.834258000	0.754103000
	1	0.338751000	-1.830294000	1.595837000
	6	0.136048000	-4.005146000	-1.656793000
	1	-0.263500000	-2.135036000	-2.701908000
	6	0.392554000	-4.615968000	-0.416176000
	1	0.654099000	-4.313853000	1.727024000
	1	0.075769000	-4.615564000	-2.571226000
	1	0.531217000	-5.707222000	-0.358181000

**XVI [Au(IPr)(PhCCPh)(OPh)(IPr)Cu]<sup>+</sup> min**



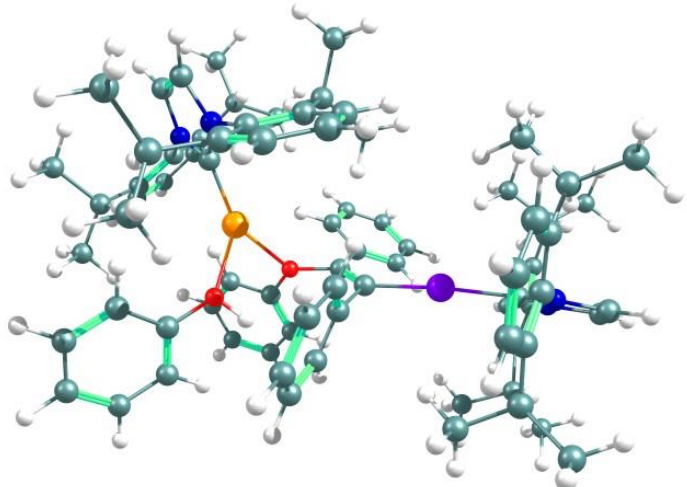
Zero-point correction= 1.388538 (Hartree/Particle)  
 Thermal correction to Energy= 1.475401  
 Thermal correction to Enthalpy= 1.476346  
 Thermal correction to Gibbs Free Energy= 1.252367  
 Sum of electronic and zero-point Energies= -3496.039637  
 Sum of electronic and thermal Energies= -3495.952773  
 Sum of electronic and thermal Enthalpies= -3495.951829  
 Sum of electronic and thermal Free Energies= -3496.175808

6	4.613761000	0.072358000	0.164471000
7	5.371580000	1.208582000	0.015137000
7	5.520570000	-0.895283000	0.525675000
6	6.716539000	0.954259000	0.280965000
6	6.810086000	-0.374869000	0.602901000
6	4.881982000	2.515772000	-0.373677000
6	5.202904000	-2.286175000	0.786486000
1	7.477503000	1.737979000	0.215884000
1	7.669580000	-0.994352000	0.876962000
6	4.453834000	3.409945000	0.642783000
6	4.041874000	4.697163000	0.239016000
6	4.067895000	5.078505000	-1.110188000
6	4.498040000	4.172680000	-2.090371000
6	4.914907000	2.869220000	-1.748552000
6	4.443963000	3.035182000	2.125416000
1	3.707048000	5.419489000	1.000396000
1	3.755745000	6.094616000	-1.399619000
1	4.516536000	4.483994000	-3.146660000
6	5.387257000	1.907502000	-2.839806000
6	5.277494000	-3.209928000	-0.289439000
6	5.001718000	-4.562321000	0.000936000
6	4.672776000	-4.973432000	1.300485000
6	4.607071000	-4.036451000	2.341035000
6	4.871291000	-2.670207000	2.112325000
6	5.623933000	-2.790101000	-1.718762000
1	5.051158000	-5.308438000	-0.807747000
1	4.469035000	-6.036440000	1.505111000
1	4.346677000	-4.371889000	3.357088000
6	4.791469000	-1.672499000	3.267911000
1	4.813664000	1.992456000	2.213965000
6	3.013755000	3.054872000	2.705099000
6	5.399481000	3.931968000	2.942117000
1	5.652865000	0.946667000	-2.351549000
6	4.262588000	1.603872000	-3.852068000
6	6.658110000	2.430803000	-3.543856000
1	5.873818000	-1.708491000	-1.703566000
6	6.862671000	-3.537454000	-2.256623000
6	4.407596000	-2.958900000	-2.654968000
1	5.049671000	-0.669720000	2.867628000
6	3.356538000	-1.578267000	3.829771000
6	5.815218000	-2.000473000	4.376236000
1	3.022954000	2.736338000	3.768454000
1	2.570515000	4.072408000	2.665643000
1	2.345030000	2.367107000	2.147307000
1	5.425184000	3.607634000	4.003366000
1	6.435949000	3.891864000	2.548231000
1	5.077385000	4.994518000	2.927063000
1	4.606696000	0.858846000	-4.599532000
1	3.363148000	1.198120000	-3.345848000
1	3.955066000	2.514134000	-4.408536000
1	7.018015000	1.695875000	-4.293812000
1	6.465933000	3.384334000	-4.079424000
1	7.481792000	2.613456000	-2.823139000
1	7.130643000	-3.166311000	-3.267739000
1	7.743921000	-3.398134000	-1.597022000
1	6.679258000	-4.628956000	-2.344197000
1	4.652515000	-2.609444000	-3.679833000
1	4.097306000	-4.022712000	-2.728163000
1	3.539189000	-2.372419000	-2.288111000
1	3.303380000	-0.806437000	4.626110000
1	2.630634000	-1.309058000	3.034664000
1	3.027880000	-2.540450000	4.275614000
1	5.779193000	-1.232856000	5.177208000
1	5.606124000	-2.982962000	4.849392000
1	6.851781000	-2.033885000	3.981633000
79	2.596063000	-0.219387000	-0.041737000
6	-0.310507000	-0.178500000	-1.034690000
6	0.601556000	-0.740961000	-0.192443000
6	-4.695093000	0.644869000	0.508083000
7	-5.967177000	0.142827000	0.362426000
7	-4.857288000	1.768728000	1.283315000
6	-6.898881000	0.937243000	1.023101000
6	-6.198143000	1.963733000	1.603467000
6	-6.310194000	-1.058031000	-0.374728000
6	-3.793901000	2.656221000	1.716175000

	1	-7.967972000	0.703763000	1.018358000
	1	-6.531881000	2.812176000	2.208349000
	6	-6.411410000	-2.283644000	0.337915000
	6	-6.771342000	-3.430816000	-0.400263000
	6	-7.021145000	-3.359875000	-1.778288000
	6	-6.919000000	-2.134413000	-2.451000000
	6	-6.567361000	-0.951655000	-1.767733000
	6	-6.185185000	-2.387290000	1.847272000
	1	-6.862974000	-4.398097000	0.118119000
	1	-7.305812000	-4.268202000	-2.332443000
	1	-7.123361000	-2.091352000	-3.532255000
	6	-6.494266000	0.372800000	-2.528628000
	6	-3.438565000	3.745465000	0.876551000
	6	-2.421803000	4.607500000	1.337669000
	6	-1.800243000	4.400393000	2.576327000
	6	-2.183950000	3.324306000	3.388976000
	6	-3.192324000	2.426091000	2.983394000
	6	-4.152948000	4.036104000	-0.444162000
	1	-2.115439000	5.461386000	0.714203000
	1	-1.011167000	5.089514000	2.916045000
	1	-1.692687000	3.180787000	4.363361000
	6	-3.645937000	1.303064000	3.919065000
	1	-5.806245000	-1.405567000	2.202030000
	6	-5.116725000	-3.441152000	2.203852000
	6	-7.514430000	-2.665644000	2.585037000
	1	-6.192789000	1.163177000	-1.809526000
	6	-5.419359000	0.332852000	-3.635212000
	6	-7.874087000	0.772426000	-3.096202000
	1	-4.727145000	3.127557000	-0.724993000
	6	-5.167272000	5.190096000	-0.269196000
	6	-3.174763000	4.328857000	-1.597962000
	1	-4.197465000	0.556709000	3.307694000
	6	-2.472181000	0.564570000	4.591949000
	6	-4.624068000	1.849494000	4.985890000
	1	-4.936439000	-3.449998000	3.298973000
	1	-5.434449000	-4.465534000	1.917707000
	1	-4.150166000	-3.233383000	1.700751000
	1	-7.353935000	-2.692111000	3.682941000
	1	-8.276659000	-1.888578000	2.370241000
	1	-7.943094000	-3.644782000	2.284602000
	1	-5.345160000	1.318224000	-4.140368000
	1	-4.420610000	0.084472000	-3.219242000
	1	-5.656976000	-0.423602000	-4.412304000
	1	-7.817570000	1.763596000	-3.592310000
	1	-8.231761000	0.042167000	-3.852076000
	1	-8.643725000	0.832703000	-2.299446000
	1	-5.715403000	5.375227000	-1.216519000
	1	-5.915986000	4.969266000	0.519229000
	1	-4.653630000	6.133005000	0.013934000
	1	-3.731408000	4.442412000	-2.551154000
	1	-2.615383000	5.273936000	-1.436381000
	1	-2.433483000	3.515150000	-1.730050000
	1	-2.849324000	-0.305125000	5.168669000
	1	-1.735828000	0.192814000	3.851291000
	1	-1.930260000	1.214385000	5.310227000
	1	-4.986377000	1.030793000	5.642075000
	1	-4.123962000	2.603954000	5.629017000
	1	-5.510182000	2.336237000	4.529994000
	29	-3.154257000	-0.061191000	0.268275000
	6	-1.709192000	-2.038880000	-1.908843000
	6	-0.696274000	-2.428677000	-2.799549000
	6	-2.867864000	-2.813496000	-1.740872000
	6	-0.859833000	-3.617767000	-3.531626000
	1	0.208092000	-1.813915000	-2.913552000
	6	-3.015302000	-3.998324000	-2.481060000
	1	-3.648821000	-2.491309000	-1.030947000
	6	-2.013166000	-4.406472000	-3.378307000
	1	-0.069263000	-3.925941000	-4.233681000
	1	-3.923155000	-4.605584000	-2.344560000
	1	-2.129656000	-5.336830000	-3.954743000
	8	-1.622173000	-0.835199000	-1.180012000
	6	0.209934000	-1.902892000	0.658110000
	6	-0.790466000	-1.769561000	1.653932000
	6	0.857805000	-3.157373000	0.537369000
	6	-1.132391000	-2.845719000	2.490175000

	1	-1.282351000	-0.790919000	1.788668000
	6	0.497962000	-4.240005000	1.355689000
	1	1.654566000	-3.277302000	-0.213213000
	6	-0.496036000	-4.090758000	2.339364000
	1	-1.896905000	-2.707447000	3.271420000
	1	1.009732000	-5.207280000	1.230491000
	1	-0.765403000	-4.936011000	2.992073000
	6	-0.219780000	1.012986000	-1.903490000
	6	-0.980018000	1.109961000	-3.099230000
	6	0.634690000	2.095197000	-1.569794000
	6	-0.857491000	2.224250000	-3.945047000
	1	-1.656996000	0.291247000	-3.384931000
	6	0.751822000	3.207398000	-2.415899000
	1	1.207230000	2.051674000	-0.630000000
	6	0.012159000	3.276814000	-3.611378000
	1	-1.445091000	2.265869000	-4.875846000
	1	1.426681000	4.029612000	-2.131531000
	1	0.106606000	4.151093000	-4.274563000

## XVI-XXXIII+XXXIV TS

	6	4.779312000	0.211035000	-0.088526000
	7	5.820348000	-0.687337000	-0.101851000
	7	5.388874000	1.433585000	-0.255797000
	6	7.043671000	-0.041030000	-0.270153000
	6	6.771204000	1.297999000	-0.367400000
	6	5.711736000	-2.127225000	0.027193000
	6	4.714887000	2.715062000	-0.318982000
	1	7.988290000	-0.592379000	-0.305172000
	1	7.429428000	2.161578000	-0.503781000
	6	5.643571000	-2.905368000	-1.159177000
	6	5.597148000	-4.306865000	-1.008949000
	6	5.616334000	-4.902676000	0.260688000
	6	5.684534000	-4.106507000	1.412531000
	6	5.744075000	-2.699640000	1.326257000
	6	5.595275000	-2.279370000	-2.553980000
	1	5.547842000	-4.943616000	-1.905978000
	1	5.583643000	-5.999807000	0.353485000
	1	5.704586000	-4.587836000	2.402844000
	6	5.839612000	-1.858328000	2.599838000
	6	4.481217000	3.421545000	0.889855000
6	3.858367000	4.683060000	0.789237000	
6	3.499832000	5.219661000	-0.455086000	
6	3.758158000	4.503785000	-1.632846000	
6	4.373224000	3.235152000	-1.595375000	
6	4.903409000	2.884277000	2.257389000	
1	3.660395000	5.260438000	1.705908000	
1	3.025662000	6.212621000	-0.508218000	
1	3.486996000	4.943501000	-2.605853000	
6	4.679094000	2.493625000	-2.897517000	
1	5.831412000	-1.199614000	-2.447282000	
6	4.172721000	-2.377143000	-3.148040000	
6	6.649414000	-2.880247000	-3.506610000	
1	5.983314000	-0.800485000	2.295570000	
6	4.525285000	-1.920542000	3.408023000	
6	7.055904000	-2.255430000	3.462873000	
1	5.339957000	1.875825000	2.102632000	
6	6.001638000	3.767814000	2.889522000	
6	3.698246000	2.715712000	3.204817000	
1	5.095640000	1.500145000	-2.631046000	
6	3.403717000	2.236328000	-3.725319000	
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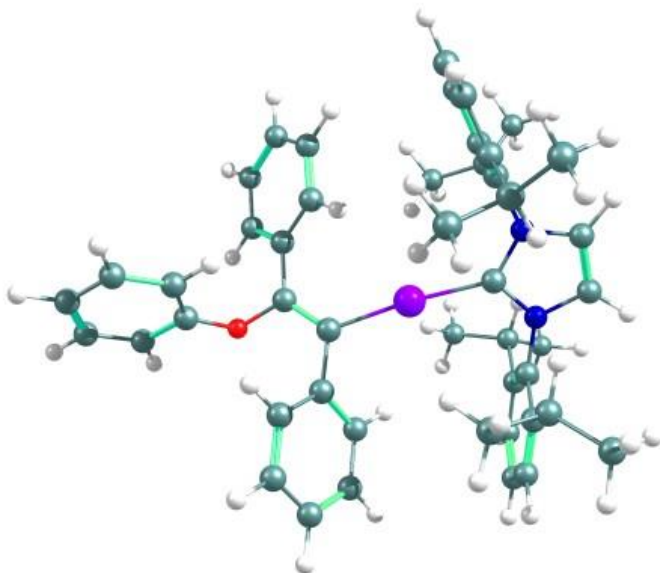
Zero-point correction= 1.491824 (Hartree/Particle)  
 Thermal correction to Energy= 1.584625  
 Thermal correction to Enthalpy= 1.585569  
 Thermal correction to Gibbs Free Energy= 1.352491  
 Sum of electronic and zero-point Energies= -3803.186491  
 Sum of electronic and thermal Energies= -3803.093690  
 Sum of electronic and thermal Enthalpies= -3803.092746  
 Sum of electronic and thermal Free Energies= -3803.325824

	1	3.865913000	-3.435296000	-3.286037000
	1	3.424563000	-1.894802000	-2.485388000
	1	6.642686000	-2.341085000	-4.476636000
	1	7.673240000	-2.810879000	-3.084734000
	1	6.448272000	-3.949467000	-3.727623000
	1	4.595942000	-1.284199000	4.314920000
	1	3.668636000	-1.559820000	2.799792000
	1	4.301555000	-2.956488000	3.740158000
	1	7.144974000	-1.579587000	4.338744000
	1	6.963925000	-3.290260000	3.854196000
	1	8.003599000	-2.197046000	2.888922000
	1	6.337862000	3.337704000	3.856004000
	1	6.888694000	3.857534000	2.228949000
	1	5.631671000	4.794820000	3.093155000
	1	4.024480000	2.270478000	4.167935000
	1	3.218453000	3.689669000	3.436032000
	1	2.925687000	2.054288000	2.761895000
	1	3.641390000	1.641712000	-4.631881000
	1	2.653380000	1.675151000	-3.131582000
	1	2.938054000	3.185271000	-4.066055000
	1	6.003739000	2.662725000	-4.642369000
	1	5.393651000	4.238112000	-4.046881000
	1	6.685211000	3.385662000	-3.148386000
	79	2.785086000	-0.134927000	0.256934000
	6	-0.044697000	-1.385673000	0.560132000
	6	0.787495000	-0.329794000	0.780805000
	6	-4.137965000	0.427505000	-1.302070000
	7	-5.288234000	-0.204164000	-1.734345000
	7	-4.037641000	1.530901000	-2.125910000
	6	-5.881954000	0.494628000	-2.785022000
	6	-5.090887000	1.582795000	-3.036809000
	6	-5.764227000	-1.505272000	-1.299220000
	6	-2.926160000	2.460903000	-2.157444000
	1	-6.801971000	0.147711000	-3.264753000
	1	-5.174826000	2.377450000	-3.783962000
	6	-6.546047000	-1.605021000	-0.114861000
	6	-6.990687000	-2.891002000	0.257099000
	6	-6.690426000	-4.020225000	-0.518740000
	6	-5.948316000	-3.885921000	-1.698323000
	6	-5.470539000	-2.627750000	-2.122670000
	6	-6.970479000	-0.371722000	0.685296000
	1	-7.597000000	-3.008796000	1.167089000
	1	-7.051659000	-5.012679000	-0.206335000
	1	-5.737824000	-4.776913000	-2.310070000
	6	-4.733670000	-2.513654000	-3.460262000
	6	-1.762050000	2.087844000	-2.883532000
	6	-0.708750000	3.024162000	-2.942128000
	6	-0.816058000	4.278460000	-2.326600000
	6	-1.984358000	4.625883000	-1.634338000
	6	-3.067105000	3.728147000	-1.529821000
	6	-1.641537000	0.764241000	-3.640350000
	1	0.209843000	2.767458000	-3.491253000
	1	0.017646000	4.994953000	-2.391678000
	1	-2.060578000	5.619615000	-1.167027000
	6	-4.348074000	4.154279000	-0.810460000
	1	-6.151534000	0.375694000	0.601817000
	6	-7.182084000	-0.652837000	2.183181000
	6	-8.244610000	0.255843000	0.070322000
	1	-4.309657000	-1.490122000	-3.532031000
	6	-3.555379000	-3.499062000	-3.582956000
	6	-5.719558000	-2.691785000	-4.638173000
	1	-2.501750000	0.126677000	-3.348662000
	6	-1.737617000	1.000295000	-5.164984000
	6	-0.361054000	-0.010866000	-3.272800000
	1	-4.929786000	3.232090000	-0.594463000
	6	-4.067632000	4.855301000	0.534148000
	6	-5.218019000	5.054740000	-1.718201000
	1	-7.370726000	0.295746000	2.723782000
	1	-8.059251000	-1.308838000	2.364432000
	1	-6.292467000	-1.125692000	2.646635000
	1	-8.535137000	1.171187000	0.627018000
	1	-8.102755000	0.538207000	-0.992497000
	1	-9.095596000	-0.455813000	0.119248000
	1	-3.026835000	-3.346876000	-4.546810000
	1	-2.817885000	-3.357785000	-2.768904000



	1	-3.893351000	-4.556247000	-3.561296000
	1	-5.198425000	-2.553122000	-5.608280000
	1	-6.164333000	-3.709126000	-4.637182000
	1	-6.556939000	-1.965684000	-4.594184000
	1	-1.698132000	0.034972000	-5.711646000
	1	-2.681234000	1.512743000	-5.444584000
	1	-0.896202000	1.626829000	-5.529432000
	1	-0.352712000	-1.000350000	-3.774259000
	1	0.553701000	0.527271000	-3.598147000
	1	-0.279176000	-0.181673000	-2.179907000
	1	-5.017677000	5.040510000	1.076733000
	1	-3.410061000	4.246346000	1.186475000
	1	-3.584824000	5.844476000	0.390343000
	1	-6.159144000	5.337820000	-1.202197000
	1	-4.680025000	5.990347000	-1.979496000
	1	-5.491799000	4.552359000	-2.667968000
	29	-3.043176000	0.061388000	0.180604000
	6	-1.892439000	-2.181999000	1.933875000
	6	-1.034739000	-2.746653000	2.895243000
	6	-3.263465000	-2.493600000	1.926902000
	6	-1.568230000	-3.618863000	3.861107000
	1	0.040993000	-2.519023000	2.874379000
	6	-3.783955000	-3.359882000	2.901874000
	1	-3.914922000	-2.068594000	1.142541000
	6	-2.939853000	-3.925401000	3.874361000
	1	-0.895816000	-4.065614000	4.610453000
	1	-4.857669000	-3.602857000	2.887394000
	1	-3.348212000	-4.610083000	4.633305000
	8	-1.433865000	-1.267377000	0.975139000
	8	-2.853977000	0.846439000	2.129800000
	1	-1.934279000	0.691693000	2.474917000
	6	-3.725512000	1.142383000	3.172317000
	6	-3.526589000	0.595031000	4.453637000
	6	-4.808034000	2.001287000	2.919222000
	6	-4.413181000	0.932029000	5.490799000
	1	-2.688181000	-0.095660000	4.632698000
	6	-5.689943000	2.325459000	3.964399000
	1	-4.937193000	2.419568000	1.910801000
	6	-5.495663000	1.797455000	5.253236000
	1	-4.255805000	0.506091000	6.494219000
	1	-6.532960000	3.007226000	3.769406000
	1	-6.185993000	2.058911000	6.069662000
	6	0.232977000	-2.686916000	-0.097886000
	6	1.526761000	-3.262175000	-0.082306000
	6	-0.806896000	-3.414412000	-0.730228000
	6	1.773920000	-4.503576000	-0.687087000
	1	2.344263000	-2.724401000	0.424800000
	6	-0.558909000	-4.657517000	-1.332869000
	1	-1.824677000	-2.996805000	-0.745230000
	6	0.733098000	-5.209645000	-1.316116000
	1	2.789678000	-4.925922000	-0.648871000
	1	-1.385557000	-5.202434000	-1.815193000
	1	0.925031000	-6.190376000	-1.779299000
	6	0.321948000	0.858586000	1.554032000
	6	0.142847000	2.118133000	0.925120000
	6	0.129885000	0.793523000	2.962997000
	6	-0.209527000	3.256224000	1.667987000
	1	0.298072000	2.198931000	-0.161894000
	6	-0.204170000	1.944181000	3.707531000
	1	0.300137000	-0.161511000	3.484591000
	6	-0.379705000	3.180522000	3.063154000
	1	-0.343961000	4.217233000	1.147235000
	1	-0.323722000	1.868845000	4.800072000
	1	-0.642106000	4.077907000	3.644472000

XXXIII [Au(IPr)(PhCCPh)(OPh)]



Zero-point correction= 0.833458 (Hartree/Particle)  
 Thermal correction to Energy= 0.885387  
 Thermal correction to Enthalpy= 0.886331  
 Thermal correction to Gibbs Free Energy= 0.740863  
 Sum of electronic and zero-point Energies= -2140.051192  
 Sum of electronic and thermal Energies= -2139.999262  
 Sum of electronic and thermal Enthalpies= -2139.998318  
 Sum of electronic and thermal Free Energies= -2140.143787

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7	2.741611000	1.512513000	0.463404000
7	3.188445000	-0.535061000	-0.093319000
6	4.131605000	1.390388000	0.468766000
6	4.413401000	0.096111000	0.117439000
6	2.057128000	2.749215000	0.776994000
6	3.062367000	-1.925060000	-0.482818000
1	4.785075000	2.231407000	0.720088000
1	5.364802000	-0.431413000	-0.001038000
6	1.680094000	2.997434000	2.122940000
6	1.053798000	4.230216000	2.401529000
6	0.825914000	5.173782000	1.389935000
6	1.212342000	4.900253000	0.070132000
6	1.836976000	3.682764000	-0.270057000
6	1.905434000	1.981518000	3.243366000
1	0.741633000	4.455511000	3.433369000
1	0.340692000	6.132546000	1.633103000
1	1.021606000	5.646445000	-0.716903000
6	2.216740000	3.390907000	-1.722370000
6	3.045011000	-2.243164000	-1.866719000
6	2.958343000	-3.606659000	-2.215716000
6	2.896100000	-4.605094000	-1.233406000
6	2.912785000	-4.259248000	0.124646000
6	2.998846000	-2.912732000	0.534693000
6	3.080101000	-1.174046000	-2.959436000
1	2.935938000	-3.890863000	-3.279710000
1	2.828859000	-5.663885000	-1.530102000
1	2.851656000	-5.051628000	0.886946000
6	2.992031000	-2.566389000	2.024106000
1	2.540172000	1.166734000	2.836288000
6	0.569415000	1.340192000	3.679317000
6	2.661744000	2.591841000	4.441628000
1	2.841736000	2.473324000	-1.727746000
6	0.958777000	3.089855000	-2.566121000
6	3.064069000	4.518943000	-2.346358000
1	3.267658000	-0.196520000	-2.467670000
6	4.226585000	-1.405462000	-3.965888000
6	1.712019000	-1.070694000	-3.668812000
1	3.154969000	-1.472212000	2.117038000
6	1.618285000	-2.875111000	2.658531000
6	4.139721000	-3.264311000	2.784306000
1	0.740547000	0.579215000	4.469390000
1	-0.129113000	2.101048000	4.087759000
1	0.070294000	0.839616000	2.822477000
1	2.879315000	1.809620000	5.198714000
1	3.626154000	3.045181000	4.131422000
1	2.067241000	3.380862000	4.948902000
1	1.242776000	2.829492000	-3.607498000
1	0.381122000	2.243762000	-2.139586000
1	0.280457000	3.967619000	-2.607604000
1	3.387476000	4.235663000	-3.369839000
1	2.491087000	5.465854000	-2.436788000
1	3.973784000	4.731897000	-1.747043000
1	4.267701000	-0.574933000	-4.701352000
1	5.212712000	-1.463857000	-3.459921000
1	4.087831000	-2.345419000	-4.540790000
1	1.726556000	-0.261637000	-4.429026000
1	1.454321000	-2.017772000	-4.188580000
1	0.902139000	-0.848142000	-2.942532000
1	1.611960000	-2.582287000	3.729620000
1	0.805067000	-2.324569000	2.141728000
1	1.377739000	-3.957365000	2.602381000
1	4.151313000	-2.942810000	3.846926000
1	4.026199000	-4.369001000	2.777051000
1	5.130474000	-3.026217000	2.344057000
79	0.148392000	-0.163383000	-0.023950000
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6	-1.785755000	-0.862113000	-0.156865000
6	-5.240045000	-0.595602000	-0.262363000
6	-6.395812000	-1.183248000	-0.823002000
6	-5.345316000	0.182383000	0.910444000
6	-7.644098000	-0.988914000	-0.215209000
1	-6.285562000	-1.793982000	-1.732047000
6	-6.605495000	0.370549000	1.505561000
1	-4.444269000	0.634796000	1.349922000

	6	-7.759778000	-0.208537000	0.951443000
	1	-8.539239000	-1.453532000	-0.659719000
	1	-6.679831000	0.981383000	2.420026000
	1	-8.742231000	-0.055596000	1.424657000
	8	-4.054208000	-0.865309000	-0.897200000
	6	-1.946232000	-2.310964000	0.168424000
	6	-1.127602000	-3.291540000	-0.448901000
	6	-2.885862000	-2.758652000	1.132968000
	6	-1.260596000	-4.654947000	-0.139487000
	1	-0.379527000	-2.966870000	-1.190086000
	6	-3.007566000	-4.119783000	1.455724000
	1	-3.525286000	-2.020676000	1.642317000
	6	-2.200099000	-5.078716000	0.817704000
	1	-0.618483000	-5.392351000	-0.648373000
	1	-3.745345000	-4.434157000	2.212152000
	1	-2.300170000	-6.147369000	1.067488000
	6	-2.952047000	1.294664000	-0.920758000
	6	-3.793227000	1.728769000	-1.977385000
	6	-2.228253000	2.277724000	-0.202184000
	6	-3.890689000	3.087325000	-2.313725000
	1	-4.368957000	0.980511000	-2.542396000
	6	-2.332648000	3.637609000	-0.535528000
	1	-1.591202000	1.962852000	0.639605000
	6	-3.162647000	4.051360000	-1.593315000
	1	-4.545650000	3.396298000	-3.144551000
	1	-1.766820000	4.380579000	0.048197000
	1	-3.250672000	5.119998000	-1.847602000

### XXXIV [Cu(IPr)(OHPH)]<sup>+</sup>

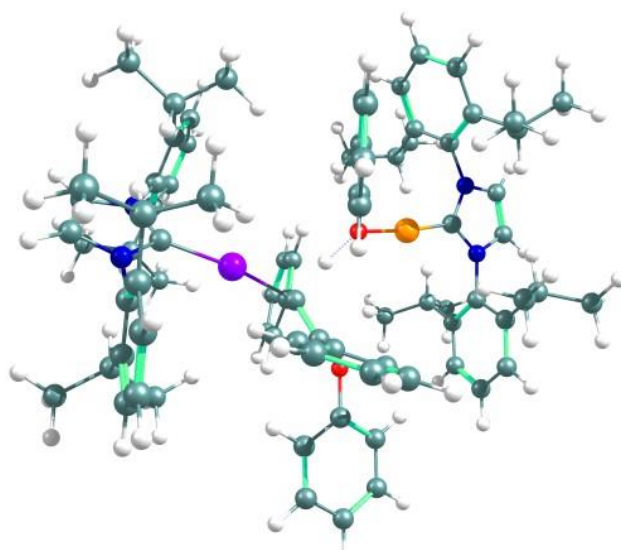
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	6	-2.221529000	-2.269020000	-0.001700000
	6	-0.994928000	-2.887846000	-0.001969000
	6	-3.002741000	0.129530000	0.000048000
	6	1.398260000	-2.099636000	-0.001430000
	1	-3.236614000	-2.678633000	-0.002097000
	1	-0.721050000	-3.947651000	-0.002747000
	6	-3.484583000	0.606754000	-1.248527000
	6	-4.478814000	1.607043000	-1.214439000
	6	-4.970819000	2.102380000	0.001361000
	6	-4.478985000	1.605260000	1.216503000
	6	-3.484710000	0.604990000	1.249245000
	6	-2.976664000	0.084169000	-2.593583000
	1	-4.878879000	2.001496000	-2.161682000
	1	-5.750699000	2.879995000	0.001877000
	1	-4.879230000	1.998223000	2.164291000
	6	-2.976848000	0.080599000	2.593617000
	6	2.066497000	-2.211384000	1.247685000
	6	3.459431000	-2.432416000	1.213780000
	6	4.149166000	-2.540795000	-0.002206000
	6	3.459189000	-2.429632000	-1.217808000
	6	2.066255000	-2.208524000	-1.250934000
	6	1.342122000	-2.107259000	2.590660000
	1	4.012916000	-2.527470000	2.160923000
	1	5.235684000	-2.721203000	-0.002523000
	1	4.012488000	-2.522531000	-2.165279000
	6	1.341636000	-2.101528000	-2.593551000
	1	-2.212729000	-0.695938000	-2.391117000
	6	-2.282729000	1.200228000	-3.404019000
	6	-4.108623000	-0.581402000	-3.406571000
	1	-2.213320000	-0.699653000	2.390181000
	6	-2.282320000	1.195582000	3.405037000
	6	-4.108927000	-0.585332000	3.406135000
	1	0.265653000	-1.928164000	2.384262000
	6	1.441361000	-3.424128000	3.391601000
	6	1.851273000	-0.905978000	3.416406000
	1	0.265132000	-1.923239000	-2.386614000
	6	1.850245000	-0.898234000	-3.416682000
	6	1.441153000	-3.416560000	-3.397504000
	1	-1.886441000	0.800564000	-4.360333000
	1	-2.985583000	2.022666000	-3.652614000
	1	-1.432830000	1.641205000	-2.840997000

Zero-point correction=	0.656292 (Hartree/Particle)
Thermal correction to Energy=	0.697001
Thermal correction to Enthalpy=	0.697945
Thermal correction to Gibbs Free Energy=	0.577929
Sum of electronic and zero-point Energies=	-1663.120103
Sum of electronic and thermal Energies=	-1663.079395
Sum of electronic and thermal Enthalpies=	-1663.078451
Sum of electronic and thermal Free Energies=	-1663.198466

1	-3.711142000	-1.003613000	-4.352659000
1	-4.590116000	-1.405105000	-2.840734000
1	-4.901328000	0.147585000	-3.675140000
1	-1.886015000	0.794917000	4.360929000
1	-1.432326000	1.636737000	2.842286000
1	-2.984857000	2.018057000	3.654404000
1	-3.711405000	-1.008641000	4.351720000
1	-4.901298000	0.143665000	3.675663000
1	-4.590854000	-1.408286000	2.839580000
1	0.861973000	-3.349403000	4.335136000
1	1.045723000	-4.285663000	2.815519000
1	2.491488000	-3.658401000	3.664837000
1	1.274870000	-0.810263000	4.359721000
1	2.920546000	-1.020235000	3.692036000
1	1.749233000	0.046789000	2.855127000
1	1.273858000	-0.800824000	-4.359833000
1	1.747626000	0.053290000	-2.853389000
1	2.919600000	-1.011310000	-3.692479000
1	0.861604000	-3.339837000	-4.340779000
1	2.491305000	-3.649913000	-3.671421000
1	1.045842000	-4.279510000	-2.823325000
29	0.184524000	1.021427000	0.001220000
6	2.330351000	3.178428000	0.002462000
6	3.298801000	2.167082000	0.002042000
6	2.669353000	4.537592000	0.002687000
6	4.654399000	2.538311000	0.001846000
1	2.998432000	1.106334000	0.001863000
6	4.030721000	4.890258000	0.002494000
1	1.888845000	5.316910000	0.003006000
6	5.023256000	3.895255000	0.002077000
1	5.426213000	1.753573000	0.001525000
1	4.310526000	5.954828000	0.002676000
1	6.086558000	4.178208000	0.001930000
8	0.969498000	2.793664000	0.002687000
1	0.386252000	3.579123000	0.003136000

### XXXIII+XXXIV-XXXV (TS)

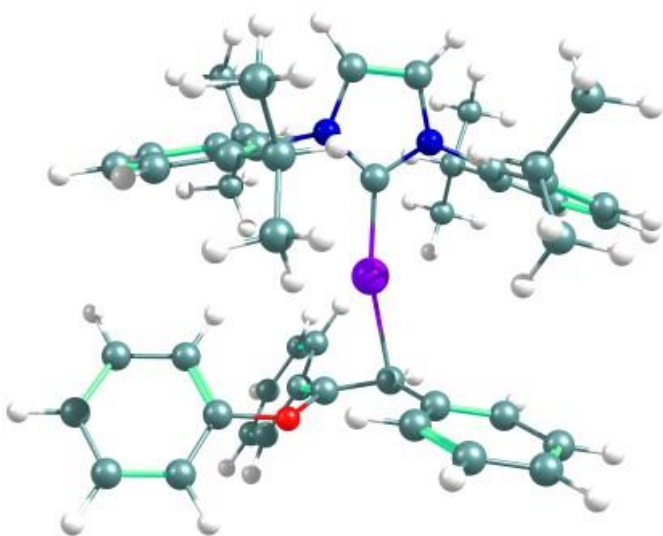
	6	4.760349000	-0.451014000	0.022012000
	7	5.519243000	-1.598900000	-0.049015000
	7	5.668303000	0.531447000	0.342284000
	6	6.859123000	-1.336079000	0.221008000
	6	6.953543000	0.009004000	0.467294000
	6	5.024539000	-2.913145000	-0.409611000
	6	5.387554000	1.946231000	0.487307000
	1	7.619060000	-2.123247000	0.209413000
	1	7.812837000	0.640382000	0.712832000
	6	5.067668000	-3.298814000	-1.776464000
	6	4.627133000	-4.600697000	-2.094011000
	6	4.171710000	-5.476570000	-1.099022000
	6	4.144497000	-5.067633000	0.242177000
	6	4.571695000	-3.778420000	0.622329000
	6	5.597940000	-2.381599000	-2.880175000
	1	4.649479000	-4.935068000	-3.142944000
	1	3.840389000	-6.491568000	-1.369865000
	1	3.792705000	-5.768204000	1.015459000
	6	4.580350000	-3.375642000	2.097441000
	6	5.186688000	2.467610000	1.792637000
	6	5.008366000	3.862125000	1.909732000
	6	5.028032000	4.693911000	0.781263000
	6	5.219240000	4.147447000	-0.495749000
	6	5.412764000	2.762096000	-0.675786000
	6	5.191942000	1.589976000	3.044279000
	1	4.857516000	4.303968000	2.907174000
	1	4.902146000	5.781893000	0.898107000
	1	5.235692000	4.813799000	-1.372414000
	6	5.657618000	2.203528000	-2.078697000
	1	5.785911000	-1.384459000	-2.429382000
	6	4.571326000	-2.179476000	-4.013489000
	6	6.945790000	-2.900879000	-3.429464000
	1	4.748888000	-2.279279000	2.146789000
	6	3.231260000	-3.655933000	2.789344000
	6	5.744930000	-4.061483000	2.847350000
	1	5.230370000	0.530647000	2.713531000

Zero-point correction= 1.486158 (Hartree/Particle)  
 Thermal correction to Energy= 1.580033  
 Thermal correction to Enthalpy= 1.580978  
 Thermal correction to Gibbs Free Energy= 1.338641  
 Sum of electronic and zero-point Energies= -3803.192635  
 Sum of electronic and thermal Energies= -3803.098759  
 Sum of electronic and thermal Enthalpies= -3803.097815

Sum of electronic and thermal Free Energies=	-3803.340152	6	6.449490000	1.853315000	3.902644000
		6	3.901448000	1.760663000	3.871583000
		1	5.829344000	1.110900000	-1.984216000
		6	4.420445000	2.388259000	-2.982865000
		6	6.923221000	2.811791000	-2.720600000
		1	4.964155000	-1.462200000	-4.763860000
		1	4.356237000	-3.128008000	-4.548412000
		1	3.608562000	-1.786387000	-3.628560000
		1	7.349776000	-2.204241000	-4.193353000
		1	7.705617000	-3.005786000	-2.627746000
		1	6.829853000	-3.894694000	-3.911055000
		1	3.249175000	-3.275277000	3.831545000
		1	2.392356000	-3.163018000	2.256714000
		1	3.008884000	-4.742346000	2.842582000
		1	5.774877000	-3.734367000	3.907692000
		1	5.632878000	-5.166289000	2.837398000
		1	6.726998000	-3.822261000	2.390140000
		1	6.468259000	1.180009000	4.784955000
		1	7.384874000	1.687939000	3.328999000
		1	6.469920000	2.898148000	4.278182000
		1	3.898219000	1.056895000	4.729430000
		1	3.812039000	2.785491000	4.289098000
		1	2.994992000	1.561609000	3.265044000
		1	4.597908000	1.939985000	-3.982546000
		1	3.522592000	1.903476000	-2.546030000
		1	4.186090000	3.462799000	-3.136319000
		1	7.121650000	2.343088000	-3.706963000
		1	6.814221000	3.903687000	-2.889647000
		1	7.819044000	2.659601000	-2.084074000
		29	2.927925000	-0.346599000	-0.301478000
		6	0.133002000	4.590705000	0.771957000
		6	1.224424000	5.432985000	1.052137000
		6	-1.164154000	5.116827000	0.623636000
		6	1.013342000	6.815671000	1.170487000
		1	2.222815000	4.987896000	1.175713000
		6	-1.357040000	6.504573000	0.740046000
		1	-2.013895000	4.447741000	0.423975000
		6	-0.274668000	7.359204000	1.010566000
		1	1.866594000	7.476900000	1.390051000
		1	-2.371144000	6.918137000	0.622776000
		1	-0.434569000	8.444394000	1.102053000
		8	0.395541000	3.226759000	0.737545000
		6	-0.630401000	1.090441000	0.590476000
		6	-0.378267000	2.340748000	0.019772000
		6	-4.216883000	-0.957510000	0.157680000
		7	-4.593348000	-2.099498000	0.827143000
		7	-5.379287000	-0.509064000	-0.425970000
		6	-5.953113000	-2.351763000	0.662932000
		6	-6.449542000	-1.348970000	-0.126945000
		6	-3.734770000	-2.942099000	1.637951000
		6	-5.530173000	0.679955000	-1.240013000
		1	-6.440463000	-3.215735000	1.124400000
		1	-7.459317000	-1.153365000	-0.500180000
		6	-3.603284000	-2.638755000	3.018982000
		6	-2.792234000	-3.495559000	3.791253000
		6	-2.157111000	-4.605804000	3.217611000
		6	-2.326771000	-4.891564000	1.855431000
		6	-3.124487000	-4.071444000	1.030974000
		6	-4.356020000	-1.484695000	3.682904000
		1	-2.662777000	-3.291441000	4.865193000
		1	-1.531927000	-5.263258000	3.842430000
		1	-1.836075000	-5.776608000	1.421704000
		6	-3.366058000	-4.447917000	-0.431408000
		6	-5.509771000	0.536668000	-2.652809000
		6	-5.722592000	1.700134000	-3.422143000
		6	-5.944334000	2.943853000	-2.813577000
		6	-5.967870000	3.049916000	-1.415935000
		6	-5.773201000	1.920853000	-0.593067000
		6	-5.289977000	-0.808949000	-3.345886000
		1	-5.722474000	1.626896000	-4.521317000
		1	-6.109469000	3.838312000	-3.434661000
		1	-6.157653000	4.029525000	-0.949944000
		6	-5.864344000	2.060909000	0.927249000
		1	-4.735499000	-0.821781000	2.877026000
		6	-3.454182000	-0.623360000	4.586471000

	6	-5.580795000	-2.017314000	4.462502000
	1	-3.807621000	-3.563931000	-0.937972000
	6	-2.067269000	-4.796532000	-1.181383000
	6	-4.389987000	-5.602678000	-0.532454000
	1	-5.132487000	-1.574826000	-2.558267000
	6	-6.532045000	-1.233199000	-4.159969000
	6	-4.019481000	-0.795853000	-4.220789000
	1	-5.672894000	1.062314000	1.371920000
	6	-4.785392000	3.013670000	1.482411000
	6	-7.280948000	2.496347000	1.363574000
	1	-4.022997000	0.247515000	4.973389000
	1	-3.089769000	-1.189689000	5.468985000
	1	-2.570483000	-0.241230000	4.037926000
	1	-6.151635000	-1.179271000	4.914549000
	1	-6.273538000	-2.587021000	3.809284000
	1	-5.266584000	-2.694358000	5.284709000
	1	-2.282520000	-4.980845000	-2.254100000
	1	-1.327476000	-3.973674000	-1.123391000
	1	-1.593076000	-5.717838000	-0.782007000
	1	-4.597929000	-5.848797000	-1.594831000
	1	-4.005110000	-6.521484000	-0.041629000
	1	-5.354873000	-5.347613000	-0.047985000
	1	-6.378198000	-2.236577000	-4.608795000
	1	-7.443206000	-1.278378000	-3.528419000
	1	-6.736556000	-0.525140000	-4.990373000
	1	-3.847606000	-1.796758000	-4.668287000
	1	-4.106426000	-0.069263000	-5.056163000
	1	-3.122776000	-0.531413000	-3.624588000
	1	-4.850832000	3.070692000	2.588787000
	1	-3.766930000	2.658015000	1.220191000
	1	-4.906909000	4.045030000	1.089026000
	1	-7.351932000	2.533519000	2.470604000
	1	-7.533685000	3.507083000	0.979664000
	1	-8.057689000	1.794868000	0.995282000
	79	-2.403614000	-0.019927000	0.186182000
	1	0.159450000	0.252120000	-0.239638000
	8	1.089926000	-0.389165000	-0.775755000
	6	-0.283941000	0.867882000	2.037881000
	6	0.294954000	-0.360528000	2.449525000
	6	-0.574711000	1.822890000	3.048220000
	6	0.595647000	-0.611446000	3.799169000
	1	0.505381000	-1.130619000	1.691088000
	6	-0.278698000	1.570337000	4.396292000
	1	-1.054282000	2.774709000	2.775467000
	6	0.315770000	0.354107000	4.781218000
	1	1.045635000	-1.575489000	4.084002000
	1	-0.521053000	2.330706000	5.156019000
	1	0.545851000	0.157362000	5.840207000
	6	-0.640503000	2.732173000	-1.389841000
	6	-1.849917000	2.424299000	-2.055122000
	6	0.368610000	3.426841000	-2.108500000
	6	-2.038528000	2.783081000	-3.400022000
	1	-2.653683000	1.909817000	-1.501922000
	6	0.179636000	3.776004000	-3.452509000
	1	1.315860000	3.675289000	-1.607642000
	6	-1.026201000	3.457053000	-4.104420000
	1	-2.993761000	2.543143000	-3.890494000
	1	0.978897000	4.303338000	-3.996528000
	1	-1.178442000	3.742357000	-5.157347000
	6	0.764800000	-1.179414000	-1.861245000
	6	0.107683000	-0.621377000	-2.978857000
	6	1.124726000	-2.545622000	-1.871320000
	6	-0.169729000	-1.425134000	-4.098041000
	1	-0.160329000	0.445104000	-2.968561000
	6	0.851657000	-3.335452000	-3.001177000
	1	1.633638000	-2.974826000	-0.993316000
	6	0.202381000	-2.781624000	-4.119043000
	1	-0.669115000	-0.977180000	-4.971730000
	1	1.149628000	-4.395735000	-3.002650000
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**XXXV [Au(PhCHCPh-OPh)]<sup>+</sup> min**

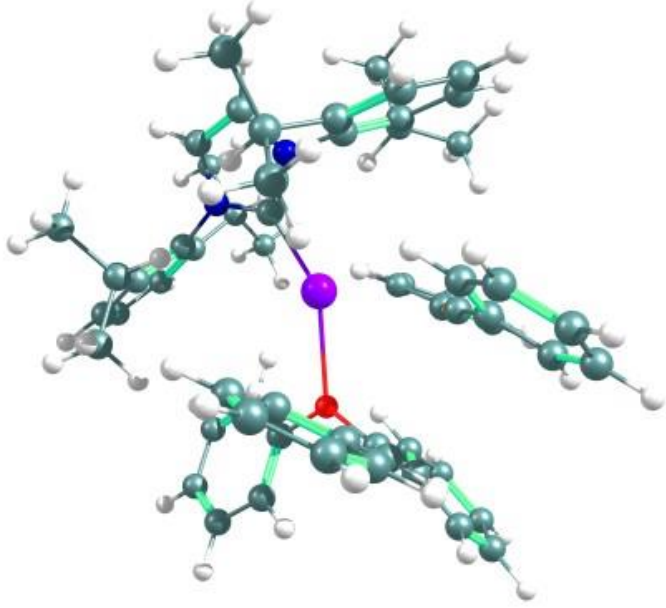


Zero-point correction= 0.846629 (Hartree/Particle)  
 Thermal correction to Energy= 0.898805  
 Thermal correction to Enthalpy= 0.899749  
 Thermal correction to Gibbs Free Energy= 0.754419  
 Sum of electronic and zero-point Energies= -2140.461810  
 Sum of electronic and thermal Energies= -2140.409634  
 Sum of electronic and thermal Enthalpies= -2140.408690  
 Sum of electronic and thermal Free Energies= -2140.554021

6	-1.247577000	1.269841000	-0.217057000
7	-2.599261000	1.406632000	-0.036719000
7	-0.830993000	2.463426000	-0.743205000
6	-3.022408000	2.667445000	-0.444764000
6	-1.908919000	3.333676000	-0.890109000
6	-3.487256000	0.378338000	0.477563000
6	0.528405000	2.815723000	-1.111144000
1	-4.071325000	2.973002000	-0.383120000
1	-1.784526000	4.341536000	-1.297874000
6	-3.719156000	0.319491000	1.877874000
6	-4.610030000	-0.671870000	2.339085000
6	-5.237375000	-1.555708000	1.449540000
6	-4.989321000	-1.467499000	0.072723000
6	-4.109617000	-0.497771000	-0.451375000
6	-3.084867000	1.300734000	2.864753000
1	-4.821437000	-0.748280000	3.416903000
1	-5.932792000	-2.318371000	1.833935000
1	-5.494076000	-2.163889000	-0.614652000
6	-3.891425000	-0.395990000	-1.961674000
6	0.976542000	2.502771000	-2.421950000
6	2.279834000	2.915108000	-2.769769000
6	3.088398000	3.613101000	-1.862218000
6	2.614711000	3.908345000	-0.575965000
6	1.322372000	3.518304000	-0.165711000
6	0.108164000	1.778452000	-3.451229000
1	2.664812000	2.692877000	-3.777190000
1	4.096542000	3.937668000	-2.164330000
1	3.257412000	4.464271000	0.124599000
6	0.822373000	3.884049000	1.232833000
1	-2.294242000	1.863261000	2.323692000
6	-2.401945000	0.583785000	4.047603000
6	-4.125645000	2.329154000	3.363177000
1	-3.055620000	0.314448000	-2.136375000
6	-3.475676000	-1.743127000	-2.586782000
6	-5.143573000	0.181135000	-2.660313000
1	-0.856759000	1.521723000	-2.965607000
6	-0.214574000	2.691628000	-4.654963000
6	0.753484000	0.452898000	-3.906814000
1	-0.174358000	3.414725000	1.372758000
6	1.742870000	3.323244000	2.336747000
6	0.637103000	5.410938000	1.378971000
1	-1.880106000	1.318832000	4.694856000
1	-3.134239000	0.049099000	4.687723000
1	-1.655932000	-0.160426000	3.699228000
1	-3.651134000	3.072033000	4.037681000
1	-4.593368000	2.882098000	2.522814000
1	-4.941166000	1.832374000	3.929655000
1	-3.250864000	-1.610659000	-3.665366000
1	-2.574364000	-2.164877000	-2.097153000
1	-4.284748000	-2.499547000	-2.514390000
1	-4.964367000	0.296270000	-3.749526000
1	-6.019052000	-0.489749000	-2.533065000
1	-5.424160000	1.174754000	-2.254177000
1	-0.889597000	2.172225000	-5.366375000
1	-0.711978000	3.630840000	-4.336652000
1	0.703843000	2.972341000	-5.211738000
1	0.081099000	-0.084548000	-4.607082000
1	1.714517000	0.625111000	-4.434953000
1	0.955869000	-0.215133000	-3.044197000
1	1.323966000	3.547272000	3.339786000
1	1.857479000	2.222949000	2.250689000
1	2.756691000	3.773659000	2.297471000
1	0.220113000	5.659530000	2.376958000
1	1.603537000	5.947760000	1.277338000
1	-0.051990000	5.817885000	0.610697000
79	-0.195379000	-0.406922000	0.220856000
6	3.786357000	-1.473575000	-0.591664000
6	3.902701000	-0.103474000	-0.310857000
6	4.812959000	-2.189683000	-1.227982000
6	5.099043000	0.550388000	-0.654812000
1	3.075007000	0.446608000	0.161302000
6	5.997998000	-1.517859000	-1.569233000
1	4.673370000	-3.259619000	-1.443538000
6	6.146724000	-0.149590000	-1.278143000
1	5.204005000	1.623427000	-0.433881000

	1	6.810925000	-2.071286000	-2.064309000
	1	7.079145000	0.372355000	-1.542141000
	8	2.609946000	-2.197112000	-0.330686000
	6	0.487529000	-2.474513000	0.670425000
	6	1.827395000	-2.009929000	0.748592000
	1	0.037519000	-2.618855000	1.668491000
	6	-0.113421000	-3.348461000	-0.377914000
	6	-1.210533000	-4.159003000	0.015935000
	6	0.341616000	-3.442708000	-1.719466000
	6	-1.810389000	-5.052660000	-0.882637000
	1	-1.585538000	-4.093562000	1.050205000
	6	-0.266134000	-4.335007000	-2.615656000
	1	1.179589000	-2.821204000	-2.059472000
	6	-1.338210000	-5.147358000	-2.203776000
	1	-2.649391000	-5.682088000	-0.547215000
	1	0.106568000	-4.399185000	-3.650049000
	1	-1.804833000	-5.850761000	-2.910864000
	6	2.444841000	-1.629869000	2.051787000
	6	3.703883000	-2.185492000	2.392417000
	6	1.766474000	-0.839339000	3.009001000
	6	4.256700000	-1.961143000	3.661746000
	1	4.240846000	-2.819717000	1.672193000
	6	2.326595000	-0.615069000	4.275430000
	1	0.798917000	-0.381164000	2.742463000
	6	3.573695000	-1.174798000	4.606169000
	1	5.229503000	-2.409986000	3.915287000
	1	1.789136000	0.008627000	5.006323000
	1	4.014364000	-0.995682000	5.599188000

## XXXV-XXXVI TS

	6	-3.006158000	-0.657398000	-1.234571000
	6	-3.308268000	0.505669000	-1.883095000
	6	2.143089000	0.380261000	0.283770000
	7	3.244687000	-0.361533000	-0.080988000
	7	2.656797000	1.518806000	0.861090000
	6	4.417049000	0.309571000	0.259493000
	6	4.048327000	1.486182000	0.851126000
	6	3.294699000	-1.658015000	-0.739858000
	6	1.935259000	2.671911000	1.377427000
	1	5.403282000	-0.111771000	0.044704000
	1	4.644544000	2.307305000	1.259598000
	6	3.297243000	-1.696466000	-2.160934000
	6	3.476097000	-2.955320000	-2.770275000
	6	3.656888000	-4.115722000	-2.006286000
	6	3.654685000	-4.045406000	-0.607037000
6	3.479741000	-2.816414000	0.063489000	
6	3.189868000	-0.437141000	-3.022398000	
1	3.483322000	-3.026536000	-3.868017000	
1	3.807121000	-5.084765000	-2.507650000	
1	3.805617000	-4.963705000	-0.019540000	
6	3.565078000	-2.765089000	1.590221000	
6	1.466815000	2.645136000	2.720439000	
6	0.845801000	3.815105000	3.203623000	
6	0.726019000	4.961388000	2.405087000	
6	1.223773000	4.964584000	1.096175000	
6	1.839484000	3.820669000	0.545468000	
6	1.691851000	1.446649000	3.645241000	
1	0.460089000	3.833553000	4.233269000	
1	0.244985000	5.864315000	2.812360000	
1	1.137642000	5.876496000	0.485279000	
6	2.418283000	3.879758000	-0.870301000	
1	2.719279000	0.356697000	-2.402860000	
6	2.297233000	-0.638572000	-4.261923000	
6	4.594875000	0.058155000	-3.440296000	
1	3.117629000	-1.803831000	1.923644000	
6	2.773236000	-3.901669000	2.266863000	
6	5.038326000	-2.787959000	2.061369000	
1	1.712125000	0.534449000	3.010287000	
6	3.063125000	1.558348000	4.355220000	
6	0.571311000	1.257523000	4.684424000	
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6	1.396398000	4.392441000	-1.904854000	

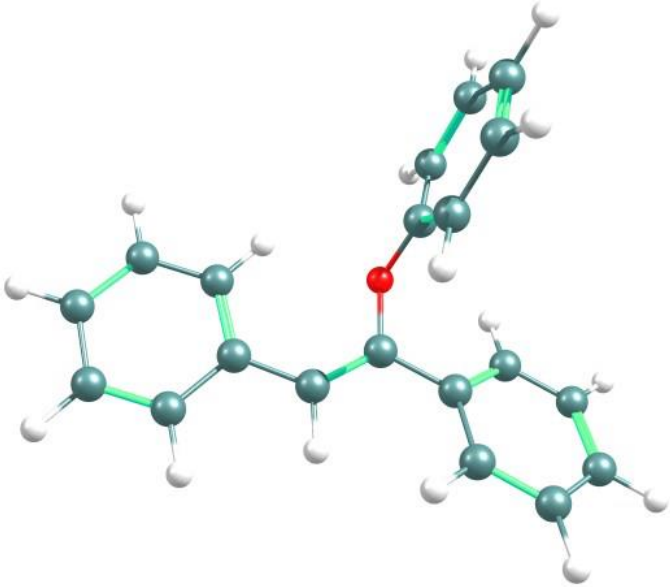
Zero-point correction= 1.033527 (Hartree/Particle)  
 Thermal correction to Energy= 1.098026  
 Thermal correction to Enthalpy= 1.098970  
 Thermal correction to Gibbs Free Energy= 0.926557  
 Sum of electronic and zero-point Energies= -2679.311128  
 Sum of electronic and thermal Energies= -2679.246629  
 Sum of electronic and thermal Enthalpies= -2679.245685  
 Sum of electronic and thermal Free Energies= -2679.418098



	6	3.704890000	4.737087000	-0.901345000
	1	2.170842000	0.323017000	-4.800380000
	1	2.745902000	-1.347838000	-4.987986000
	1	1.293150000	-1.022496000	-3.990792000
	1	4.518551000	0.991037000	-4.036826000
	1	5.242709000	0.268241000	-2.565123000
	1	5.111648000	-0.701019000	-4.064282000
	1	2.760084000	-3.752440000	3.366151000
	1	1.725296000	-3.948668000	1.907117000
	1	3.235580000	-4.894015000	2.085103000
	1	5.096812000	-2.721014000	3.167664000
	1	5.536251000	-3.730601000	1.751506000
	1	5.626282000	-1.947553000	1.641328000
	1	3.235436000	0.676922000	5.007495000
	1	3.907858000	1.617417000	3.639497000
	1	3.100555000	2.465064000	4.994864000
	1	0.708900000	0.295821000	5.218884000
	1	0.583083000	2.057693000	5.453620000
	1	-0.430938000	1.245181000	4.212113000
	1	1.834944000	4.360204000	-2.923549000
	1	0.473929000	3.777767000	-1.916928000
	1	1.106990000	5.446570000	-1.711488000
	1	4.148791000	4.738781000	-1.918518000
	1	3.489377000	5.791023000	-0.626666000
	1	4.474647000	4.362809000	-0.195775000
	79	0.205802000	-0.096245000	0.067161000
	6	-1.372083000	-2.292569000	-1.918983000
	6	-2.085220000	-2.616711000	-3.085199000
	6	-0.340633000	-3.116651000	-1.444405000
	6	-1.759685000	-3.797461000	-3.774891000
	1	-2.887981000	-1.957030000	-3.445365000
	6	-0.027284000	-4.293586000	-2.145465000
	1	0.205353000	-2.836665000	-0.528216000
	6	-0.736689000	-4.640672000	-3.308496000
	1	-2.318500000	-4.057100000	-4.687532000
	1	0.775203000	-4.944762000	-1.767938000
	1	-0.494114000	-5.568121000	-3.849337000
	8	-1.662998000	-1.112746000	-1.198123000
	1	-4.348082000	0.835863000	-1.735528000
	6	-1.700644000	-1.250006000	3.007021000
	6	-2.796982000	-1.520556000	3.874146000
	6	-0.550568000	-2.075970000	3.085913000
	6	-2.733438000	-2.577476000	4.790980000
	1	-3.694762000	-0.887619000	3.817362000
	6	-0.499682000	-3.134655000	4.005178000
	1	0.301354000	-1.869621000	2.418379000
	6	-1.586456000	-3.389570000	4.860649000
	1	-3.588693000	-2.769705000	5.457560000
	1	0.398079000	-3.768587000	4.056289000
	1	-1.539246000	-4.220920000	5.581068000
	6	-2.539367000	1.382247000	-2.765753000
	6	-1.207384000	1.145933000	-3.204437000
	6	-3.206383000	2.531954000	-3.273671000
	6	-0.591912000	2.014044000	-4.118288000
	1	-0.661007000	0.263937000	-2.843580000
	6	-2.585835000	3.398697000	-4.182244000
	1	-4.239030000	2.735021000	-2.947548000
	6	-1.272453000	3.141258000	-4.614082000
	1	0.433066000	1.800140000	-4.457680000
	1	-3.133030000	4.274960000	-4.563938000
	1	-0.783998000	3.810843000	-5.339184000
	6	-3.986689000	-1.517003000	-0.534260000
	6	-3.561699000	-2.543351000	0.346057000
	6	-5.382969000	-1.359316000	-0.743978000
	6	-4.491985000	-3.366740000	0.999302000
	1	-2.489516000	-2.697953000	0.526561000
	6	-6.309257000	-2.174870000	-0.081365000
	1	-5.752790000	-0.606574000	-1.456338000
	6	-5.869733000	-3.185324000	0.794518000
	1	-4.132375000	-4.157232000	1.676054000
	1	-7.385784000	-2.033012000	-0.265625000
	1	-6.599101000	-3.834368000	1.303792000
	6	-1.813176000	-0.132606000	2.114861000
	6	-2.144146000	0.921764000	1.545440000
	6	-2.691474000	2.145743000	1.047068000

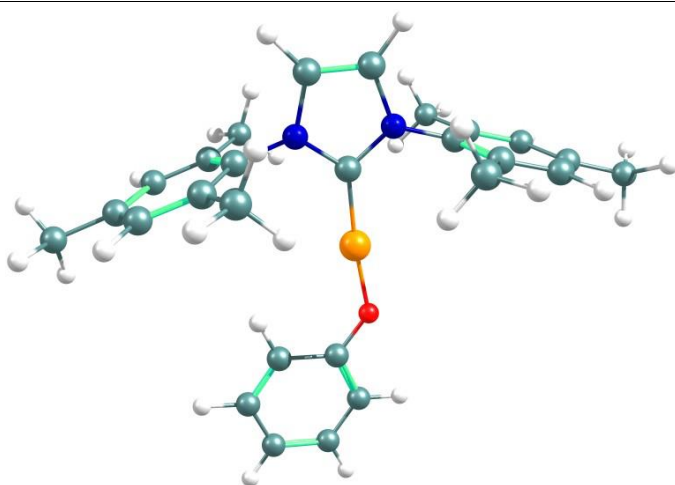
	6	-1.902030000	3.129378000	0.398533000
	6	-4.077447000	2.399591000	1.252606000
	6	-2.483410000	4.330933000	-0.029386000
	1	-0.829011000	2.943538000	0.244068000
	6	-4.645257000	3.606330000	0.823748000
	1	-4.695918000	1.640387000	1.754336000
	6	-3.852116000	4.576141000	0.181424000
	1	-1.858764000	5.084878000	-0.532267000
	1	-5.716938000	3.793806000	0.995254000
	1	-4.302155000	5.524158000	-0.152510000

## XXXVI Product

	6	0.759209000	1.569554000	-0.236727000
	6	1.116155000	1.544829000	1.124908000
	6	1.038454000	2.699915000	-1.030635000
	6	1.764993000	2.659848000	1.683594000
	1	0.879850000	0.664002000	1.739785000
	6	1.681870000	3.806400000	-0.455952000
	1	0.742903000	2.691557000	-2.090918000
	6	2.051646000	3.792327000	0.902058000
	1	2.044416000	2.639535000	2.749179000
	1	1.898414000	4.689016000	-1.078825000
	1	2.559029000	4.661297000	1.348746000
	8	0.079399000	0.536378000	-0.860837000
	6	-1.140554000	-1.315857000	0.014693000
	6	0.057475000	-0.732458000	-0.295662000
	6	1.366113000	-1.426203000	-0.198389000
	6	2.430855000	-1.058745000	-1.058649000
	6	3.662099000	-1.729306000	-1.003980000
	1	2.278196000	-0.248696000	-1.786914000
	6	2.816063000	-3.145880000	0.778832000
	6	3.861289000	-2.777227000	-0.088094000
1	4.473414000	-1.431603000	-1.687264000	
1	2.965531000	-3.955550000	1.510929000	
1	4.829492000	-3.300587000	-0.044114000	
6	-2.507638000	-0.790461000	-0.022158000	
6	-2.868467000	0.513410000	-0.462033000	
6	-3.553682000	-1.650036000	0.414682000	
6	-4.207701000	0.928114000	-0.451197000	
1	-2.088034000	1.195099000	-0.822532000	
6	-4.890975000	-1.231100000	0.424327000	
1	-3.300006000	-2.667899000	0.754669000	
6	-5.226570000	0.064269000	-0.008371000	
1	-4.460312000	1.943364000	-0.797299000	
1	-5.677562000	-1.920663000	0.770468000	
1	-6.276355000	0.398102000	-0.003422000	
1	-1.068241000	-2.371275000	0.323188000	
6	1.585364000	-2.475451000	0.729444000	
1	0.788088000	-2.752377000	1.436881000	

Zero-point correction= 0.291524 (Hartree/Particle)  
 Thermal correction to Energy= 0.308710  
 Thermal correction to Enthalpy= 0.309654  
 Thermal correction to Gibbs Free Energy= 0.244093  
 Sum of electronic and zero-point Energies= -846.066597  
 Sum of electronic and thermal Energies= -846.049412  
 Sum of electronic and thermal Enthalpies= -846.048468  
 Sum of electronic and thermal Free Energies= -846.114029

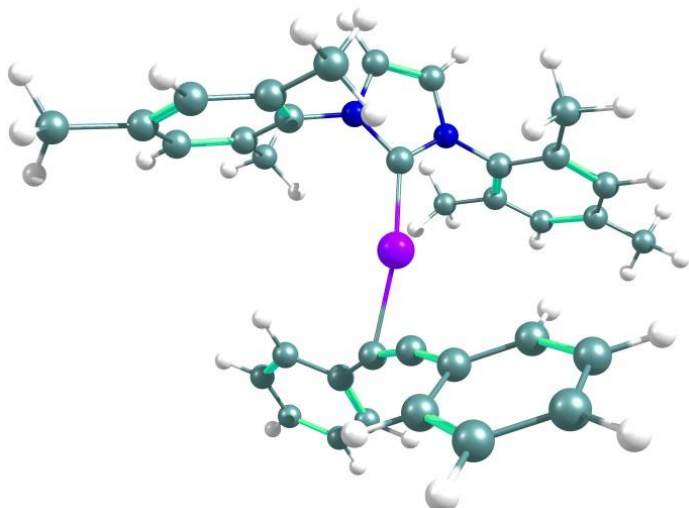
# XXXVII [Au(IMes)(OPh)]



Zero-point correction= 0.477029 (Hartree/Particle)  
 Thermal correction to Energy= 0.510026  
 Thermal correction to Enthalpy= 0.510970  
 Thermal correction to Gibbs Free Energy= 0.405708  
 Sum of electronic and zero-point Energies= -1427.223429  
 Sum of electronic and thermal Energies= -1427.190433  
 Sum of electronic and thermal Enthalpies= -1427.189488  
 Sum of electronic and thermal Free Energies= -1427.294750

29	-0.081215000	0.746589000	-0.090367000
8	0.243645000	2.526984000	-0.194926000
6	-0.584207000	-1.027421000	0.032906000
7	0.222323000	-2.142491000	0.106028000
6	-0.534335000	-3.309691000	0.217570000
1	-0.069759000	-4.298207000	0.290212000
6	-1.851239000	-2.927097000	0.214668000
1	-2.773428000	-3.512676000	0.285436000
7	-1.863569000	-1.536498000	0.100669000
6	1.666934000	-2.109287000	0.063234000
6	2.315364000	-2.250948000	-1.188636000
6	3.722167000	-2.238372000	-1.202038000
1	4.241307000	-2.343816000	-2.169386000
6	4.481326000	-2.086697000	-0.022656000
6	5.992008000	-2.055143000	-0.080801000
6	3.793988000	-1.946686000	1.198403000
1	4.369617000	-1.822591000	2.130632000
6	2.386050000	-1.953365000	1.271181000
6	1.524047000	-2.381490000	-2.469266000
6	1.674566000	-1.769104000	2.591011000
6	-3.062747000	-0.730367000	0.060842000
6	-3.582510000	-0.213770000	1.272438000
6	-4.763660000	0.549670000	1.204607000
6	-4.867177000	0.272361000	-1.196109000
6	-3.687096000	-0.496713000	-1.187620000
6	-2.882070000	-0.447774000	2.590486000
6	-3.093822000	-1.025892000	-2.472641000
6	1.377337000	3.222671000	-0.135032000
6	1.326861000	4.643454000	-0.249079000
6	2.660925000	2.627327000	0.040276000
6	2.494890000	5.416635000	-0.189814000
1	0.339613000	5.113191000	-0.385234000
6	3.823228000	3.411420000	0.098478000
1	2.718815000	1.528118000	0.128658000
6	3.755948000	4.813201000	-0.015609000
1	2.420046000	6.513678000	-0.281130000
1	4.800522000	2.917719000	0.235883000
1	4.670585000	5.425177000	0.030888000
1	0.823730000	-3.243125000	-2.442034000
1	2.195940000	-2.514873000	-3.338906000
1	0.908813000	-1.473593000	-2.648334000
1	2.393301000	-1.769159000	3.433011000
1	0.925433000	-2.567151000	2.777044000
1	1.126190000	-0.802344000	2.611079000
1	-3.489213000	-0.069027000	3.435189000
1	-1.901640000	0.075637000	2.614122000
1	-2.675919000	-1.523982000	2.769123000
1	6.442355000	-2.072829000	0.931229000
1	6.350429000	-1.135445000	-0.591667000
1	6.395003000	-2.917844000	-0.651869000
1	-2.922595000	-2.122316000	-2.435697000
1	-2.107927000	-0.554520000	-2.675552000
1	-3.756237000	-0.811382000	-3.333380000
6	-5.420973000	0.806624000	-0.015680000
1	-5.180495000	0.959317000	2.139847000
1	-5.364965000	0.463785000	-2.161340000
6	-6.666410000	1.663158000	-0.057821000
1	-7.294171000	1.517533000	0.844729000
1	-7.285867000	1.443928000	-0.950519000
1	-6.401054000	2.742547000	-0.098648000

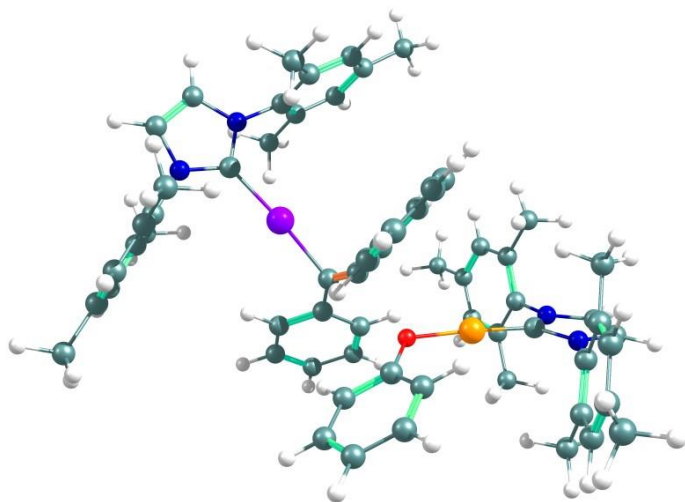
# XXXVIII [Au(IMes)(PhCCPh)]<sup>+</sup>



Zero-point correction= 0.573219 (Hartree/Particle)  
 Thermal correction to Energy= 0.612757  
 Thermal correction to Enthalpy= 0.613701  
 Thermal correction to Gibbs Free Energy= 0.491451  
 Sum of electronic and zero-point Energies= -1597.774781  
 Sum of electronic and thermal Energies= -1597.735244  
 Sum of electronic and thermal Enthalpies= -1597.734299  
 Sum of electronic and thermal Free Energies= -1597.856549

6	-0.000278000	-1.701661000	0.000026000
7	1.070025000	-2.529857000	0.207343000
7	-1.070795000	-2.529587000	-0.207230000
6	0.673990000	-3.861287000	0.129963000
6	-0.675110000	-3.861118000	-0.129751000
6	2.431217000	-2.095868000	0.459235000
6	-2.431875000	-2.095288000	-0.459194000
1	1.382732000	-4.684613000	0.266622000
1	-1.384072000	-4.684263000	-0.266361000
6	2.828078000	-1.833951000	1.792191000
6	4.163755000	-1.438303000	2.004265000
6	5.086956000	-1.309886000	0.946648000
6	4.641265000	-1.583199000	-0.363943000
6	3.319116000	-1.981877000	-0.638503000
6	1.862964000	-1.958185000	2.948745000
1	4.492936000	-1.229465000	3.035409000
6	6.523975000	-0.924866000	1.209643000
1	5.348229000	-1.489273000	-1.204867000
6	2.870088000	-2.269603000	-2.053164000
6	-2.828594000	-1.833254000	-1.792170000
6	-4.164178000	-1.437326000	-2.004319000
6	-5.087417000	-1.308754000	-0.946758000
6	-4.641872000	-1.582180000	0.363856000
6	-3.319822000	-1.981137000	0.638490000
6	-1.863442000	-1.957664000	-2.948673000
1	-4.493256000	-1.228393000	-3.035476000
6	-6.524383000	-0.923423000	-1.209855000
1	-5.348863000	-1.488119000	1.204742000
6	-2.870949000	-2.268994000	2.053173000
79	0.000052000	0.317132000	-0.000017000
6	0.273460000	2.463754000	-0.570472000
6	-0.272626000	2.463833000	0.570503000
6	0.741424000	2.839095000	-1.883199000
6	-0.038283000	3.727920000	-2.670541000
6	1.979554000	2.360214000	-2.385360000
6	0.423627000	4.131934000	-3.930523000
1	-0.999441000	4.096492000	-2.281664000
6	2.429340000	2.773019000	-3.647006000
1	2.583144000	1.674932000	-1.770644000
6	1.654363000	3.656776000	-4.420890000
1	-0.181550000	4.825026000	-4.535222000
1	3.394320000	2.406404000	-4.029924000
1	2.012138000	3.978504000	-5.411392000
6	-0.740487000	2.839302000	1.883229000
6	-1.978727000	2.360717000	2.385401000
6	0.039433000	3.727949000	2.670561000
6	-2.428407000	2.773631000	3.647049000
1	-2.582487000	1.675577000	1.770694000
6	-0.422375000	4.132078000	3.930544000
1	1.000676000	4.096292000	2.281676000
6	-1.653218000	3.657210000	4.420924000
1	-3.393472000	2.407245000	4.029975000
1	0.182970000	4.825029000	4.535236000
1	-2.010908000	3.979027000	5.411427000
1	-1.335996000	-2.934424000	-2.950148000
1	-1.081872000	-1.168312000	-2.910049000
1	-2.391491000	-1.857094000	-3.915942000
1	-3.702134000	-2.122388000	2.768904000
1	-2.036209000	-1.603464000	2.361006000
1	-2.509637000	-3.312674000	2.171326000
1	-6.939481000	-0.304909000	-0.388811000
1	-7.165080000	-1.828997000	-1.289102000
1	-6.632814000	-0.361602000	-2.158540000
1	2.035524000	-1.603828000	-2.360947000
1	2.508467000	-3.313177000	-2.171297000
1	3.701277000	-2.123232000	-2.768937000
1	2.391065000	-1.857613000	3.915985000
1	1.335412000	-2.934888000	2.950305000
1	1.081476000	-1.168753000	2.910103000
1	6.632625000	-0.363102000	2.158338000
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1	7.164520000	-1.830557000	1.288796000

# XXXVII+XXXVIII-XXXIX TS

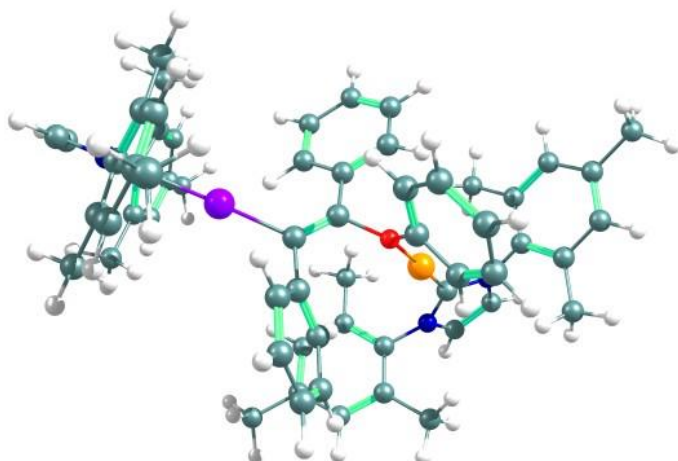


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 Thermal correction to Gibbs Free Energy= 0.922452  
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 Sum of electronic and thermal Energies= -3024.931393  
 Sum of electronic and thermal Enthalpies= -3024.930449  
 Sum of electronic and thermal Free Energies= -3025.133702

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7	5.738079000	-0.567214000	-0.529191000
6	6.512095000	1.155413000	-1.695723000
6	6.880490000	-0.037190000	-1.126880000
6	4.384760000	2.476723000	-1.854614000
6	5.704809000	-1.824694000	0.189695000
1	7.088096000	1.896252000	-2.259492000
1	7.844166000	-0.555633000	-1.094814000
6	4.248895000	3.567498000	-0.962954000
6	3.527311000	4.690029000	-1.414513000
6	2.958683000	4.747278000	-2.703246000
6	3.114043000	3.631402000	-3.551454000
6	3.823702000	2.481778000	-3.154238000
6	4.834840000	3.524975000	0.428981000
1	3.412297000	5.550668000	-0.734959000
6	2.232177000	5.985002000	-3.178269000
1	2.671692000	3.654171000	-4.561295000
6	3.962506000	1.293246000	-4.077322000
6	5.331427000	-2.999012000	-0.506624000
6	5.326930000	-4.208873000	0.214464000
6	5.682647000	-4.272121000	1.577284000
6	6.046904000	-3.074614000	2.227002000
6	6.069633000	-1.835489000	1.557797000
6	4.927190000	-2.959645000	-1.962123000
1	5.035641000	-5.133467000	-0.310776000
6	5.705186000	-5.591930000	2.313310000
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6	6.455364000	-0.566578000	2.283372000
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6	0.131043000	-0.574003000	-0.059309000
6	0.900954000	-0.268728000	0.933041000
6	-4.889448000	0.889284000	0.184423000
7	-6.062845000	0.504111000	-0.419824000
7	-5.141733000	2.163252000	0.636351000
6	-7.021986000	1.512975000	-0.345320000
6	-6.440646000	2.561085000	0.321563000
6	-6.286669000	-0.780185000	-1.049384000
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1	-6.831393000	3.544778000	0.601289000
6	-6.759051000	-1.856755000	-0.261386000
6	-7.003096000	-3.082727000	-0.912623000
6	-6.795779000	-3.252346000	-2.296018000
6	-6.315171000	-2.152589000	-3.037823000
6	-6.054353000	-0.904551000	-2.441374000
6	-6.971353000	-1.714163000	1.227784000
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6	-3.366016000	3.870726000	0.639334000
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6	-2.396718000	4.618741000	2.780519000
6	-3.249053000	3.721917000	3.458416000
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6	-1.106216000	-3.238702000	1.717327000
6	-2.820006000	-3.260573000	-0.020993000
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6	-2.892745000	-4.660887000	0.074108000
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	6	1.704930000	-0.414333000	4.639723000
	1	2.665518000	-1.112456000	2.812958000
	6	-0.392239000	0.779045000	4.343832000
	6	0.608040000	0.270081000	5.192414000
	1	2.491411000	-0.819170000	5.296069000
	1	-1.254479000	1.317611000	4.767645000
	1	0.532989000	0.407402000	6.282631000
	6	-0.246524000	-0.785365000	-1.426581000
	6	-0.633189000	0.315993000	-2.240412000
	6	-0.243823000	-2.093698000	-1.985096000
	6	-0.996134000	0.111184000	-3.577587000
	1	-0.626380000	1.327768000	-1.807291000
	6	-0.611655000	-2.285114000	-3.324735000
	1	0.054059000	-2.945038000	-1.356542000
	6	-0.987038000	-1.188654000	-4.122463000
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	1	-0.603883000	-3.300379000	-3.751097000
	1	-1.269309000	-1.345698000	-5.175583000
	1	-7.492553000	-2.599116000	1.640108000
	1	-7.569855000	-0.814472000	1.480902000
	1	-6.000549000	-1.617877000	1.761068000
	1	-5.459186000	-0.014820000	-4.327834000
	1	-4.508431000	0.548143000	-2.915310000
	1	-6.167092000	1.154263000	-3.169372000
	1	-4.439629000	4.246294000	-1.226052000
	1	-3.199432000	2.972713000	-1.336847000
	1	-2.706790000	4.697462000	-1.255286000
	1	-4.922853000	2.039445000	4.619830000
	1	-4.834044000	0.879050000	3.255771000
	1	-6.128299000	2.104839000	3.296329000
	1	5.906404000	3.235347000	0.420570000
	1	4.304284000	2.779845000	1.061183000
	1	4.752130000	4.510499000	0.925878000
	1	3.478926000	0.391015000	-3.645633000
	1	5.025369000	1.030964000	-4.263536000
	1	3.489455000	1.495836000	-5.057107000
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	1	5.670997000	-2.423510000	-2.587882000
	1	3.956839000	-2.433000000	-2.092061000
	1	6.725958000	-0.779715000	3.335124000
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	1	7.323385000	-0.061670000	1.808930000
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	1	1.414093000	5.735316000	-3.883781000
	1	2.926225000	6.667769000	-3.716049000
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	1	6.701924000	-6.077111000	2.222385000
	1	4.958960000	-6.302250000	1.904531000
	1	-1.061972000	6.335450000	2.941896000
	1	-0.517771000	4.882905000	3.834491000
	1	-1.857363000	5.868347000	4.482207000
	1	-7.129877000	-5.407194000	-2.255977000
	1	-6.364398000	-4.803864000	-3.765192000
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**XXXIX [Au(IMes)(PhCCPh)(OPh)(IMes)Cu]<sup>+</sup> min**



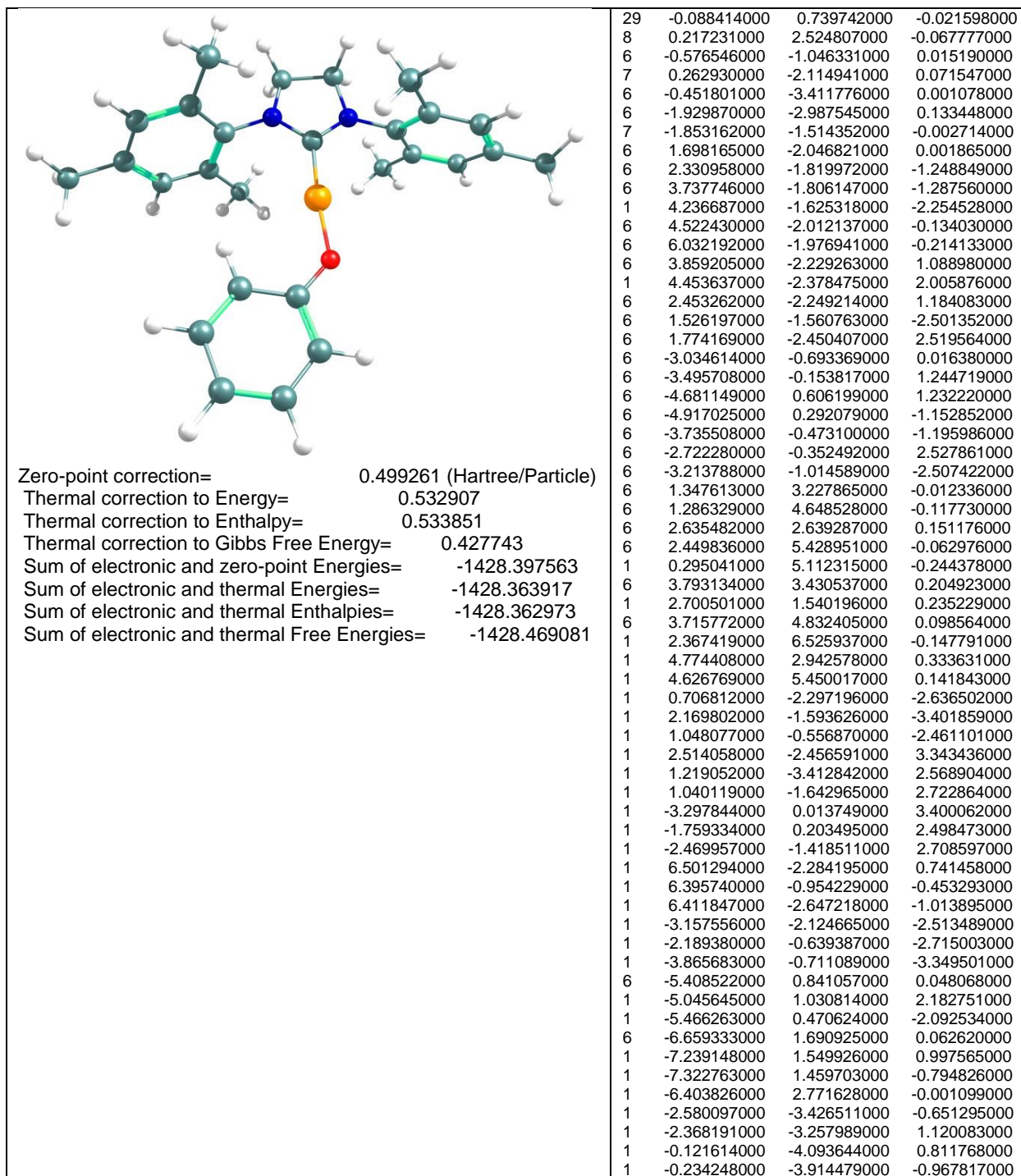
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6	6.407773000	1.632245000	-1.037329000
6	6.767700000	0.333508000	-0.786980000
6	4.259718000	2.919385000	-1.048786000
6	5.550924000	-1.762602000	-0.142509000
1	7.004175000	2.507114000	-1.315408000
1	7.743216000	-0.162936000	-0.804792000
6	3.971399000	3.723947000	0.078804000
6	3.268311000	4.925867000	-0.139845000
6	2.863237000	5.334786000	-1.426141000
6	3.165931000	4.494688000	-2.518404000
6	3.863285000	3.281405000	-2.359480000
6	4.387562000	3.307298000	1.469823000
1	3.041001000	5.567716000	0.727466000
6	2.157391000	6.654754000	-1.639218000
1	2.857182000	4.796088000	-3.533457000
6	4.160021000	2.391393000	-3.544311000
6	5.362895000	-2.696626000	-1.190108000
6	5.356533000	-4.063318000	-0.851897000
6	5.533699000	-4.508243000	0.474815000
6	5.707484000	-3.540161000	1.484272000
6	5.720935000	-2.158845000	1.205014000
6	5.150450000	-2.245328000	-2.616421000
1	5.210913000	-4.804267000	-1.655512000
6	5.567108000	-5.984916000	0.797433000
1	5.840186000	-3.867334000	2.528820000
6	5.878738000	-1.144000000	2.313224000
79	2.570722000	-0.032779000	-0.102392000
6	-0.400291000	-0.642029000	-0.446476000
6	0.675400000	-0.692545000	0.389133000
6	-4.674750000	0.824710000	0.557225000
7	-5.898338000	0.782660000	-0.062538000
7	-4.774542000	1.855392000	1.458365000
6	-6.744584000	1.768440000	0.441542000
6	-6.034960000	2.445996000	1.401124000
6	-6.263867000	-0.149264000	-1.109201000
6	-3.712715000	2.272905000	2.349428000
1	-7.766618000	1.899899000	0.071675000
1	-6.309441000	3.291958000	2.039469000
6	-6.883385000	-1.370154000	-0.749450000
6	-7.252449000	-2.244747000	-1.790499000
6	-7.027623000	-1.933320000	-3.146823000
6	-6.416520000	-0.699888000	-3.454929000
6	-6.023719000	0.213056000	-2.457250000
6	-7.141720000	-1.729969000	0.695928000
1	-7.738743000	-3.199053000	-1.529453000
6	-7.412531000	-2.900010000	-4.242890000
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6	-2.731871000	3.174080000	1.870483000
6	-1.723167000	3.574101000	2.769927000
6	-1.673572000	3.109191000	4.099365000
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6	-3.710461000	1.782989000	3.678967000
6	-2.747361000	3.683521000	0.447663000
1	-0.952677000	4.278526000	2.415957000
1	-2.662757000	1.850434000	5.571079000
6	-4.774277000	0.827119000	4.168584000
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6	-1.657939000	-2.756795000	-0.047446000
6	-0.809428000	-3.503037000	-0.879919000
6	-2.597393000	-3.381478000	0.788015000
6	-0.921340000	-4.904525000	-0.874877000
1	-0.070125000	-2.995140000	-1.516290000
6	-2.700026000	-4.782505000	0.776374000
1	-3.228326000	-2.767897000	1.451487000
6	-1.863687000	-5.548947000	-0.054386000
1	-0.261276000	-5.496760000	-1.527926000
1	-3.432526000	-5.276414000	1.433696000
1	-1.942601000	-6.646754000	-0.057818000
8	-1.629956000	-1.349122000	-0.050764000
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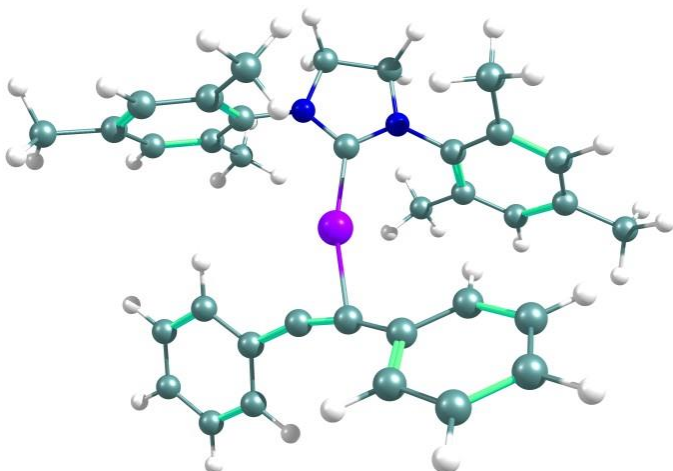
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6	1.303096000	-2.977284000	3.392235000
1	2.140250000	-2.778460000	1.394902000
6	0.378944000	-2.482909000	4.330077000
1	-1.166604000	-0.993830000	4.705357000
1	1.962281000	-3.818983000	3.658340000
1	0.311773000	-2.929862000	5.334527000
6	-0.589993000	0.032169000	-1.748275000
6	-1.526529000	-0.456657000	-2.699040000
6	0.144980000	1.199673000	-2.083624000
6	-1.694316000	0.177114000	-3.941661000
1	-2.112826000	-1.361531000	-2.476968000
6	-0.026193000	1.828165000	-3.325301000
1	0.855080000	1.612235000	-1.349486000
6	-0.943680000	1.320613000	-4.264597000
1	-2.413346000	-0.235951000	-4.666759000
1	0.557584000	2.733667000	-3.554815000
1	-1.076230000	1.817077000	-5.238789000
1	5.089281000	-3.112153000	-3.301987000
1	5.971147000	-1.587790000	-2.972934000
1	4.207253000	-1.665051000	-2.712852000
1	6.669294000	-0.397873000	2.089023000
1	6.137144000	-1.638045000	3.269331000
1	4.934217000	-0.578664000	2.468250000
1	5.469826000	3.066002000	1.524125000
1	3.838191000	2.396166000	1.791632000
1	4.180580000	4.109645000	2.203645000
1	3.795293000	2.847704000	-4.484434000
1	3.670444000	1.400339000	-3.432388000
1	5.247648000	2.200908000	-3.661441000
1	1.385803000	6.584235000	-2.432761000
1	2.877078000	7.440389000	-1.958187000
1	1.670074000	7.015645000	-0.711660000
1	4.859659000	-6.558695000	0.164968000
1	5.318760000	-6.179081000	1.859755000
1	6.579918000	-6.406268000	0.614058000
1	-5.411525000	1.702442000	-3.909239000
1	-4.289478000	1.526055000	-2.526881000
1	-5.839143000	2.386643000	-2.309548000
1	-7.676110000	-2.696027000	0.773424000
1	-7.754407000	-0.961819000	1.213504000
1	-6.193528000	-1.821009000	1.268115000
1	-6.534840000	-3.502821000	-4.564071000
1	-7.787187000	-2.369715000	-5.141742000
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1	-4.837270000	-0.076020000	3.525496000
1	-5.783414000	1.291842000	4.166647000
1	-4.562310000	0.495281000	5.202900000
1	-2.048399000	4.533020000	0.325802000
1	-3.756772000	4.022023000	0.135174000
1	-2.435820000	2.891904000	-0.268368000
6	-0.560367000	3.529300000	5.030930000
1	-0.916356000	3.627948000	6.076269000
1	0.253558000	2.771528000	5.034181000
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**XL [Cu(SIMes)(OPh)]**





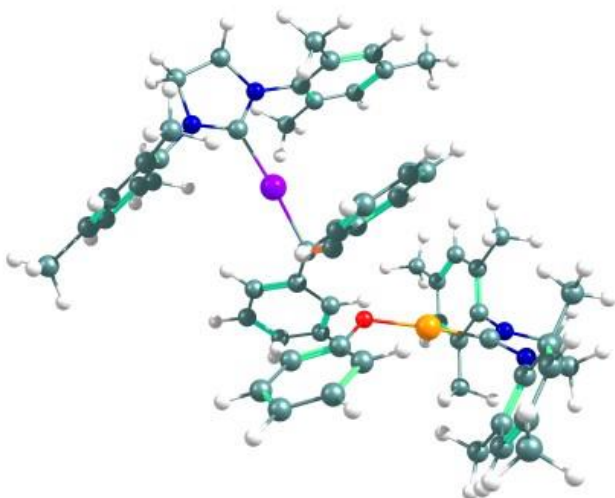
**XLI [Cu(SIMes)(PhCCPh)]<sup>+</sup>**



Zero-point correction= 0.595495 (Hartree/Particle)  
 Thermal correction to Energy= 0.635711  
 Thermal correction to Enthalpy= 0.636655  
 Thermal correction to Gibbs Free Energy= 0.514879  
 Sum of electronic and zero-point Energies= -1598.948360  
 Sum of electronic and thermal Energies= -1598.908144  
 Sum of electronic and thermal Enthalpies= -1598.907200  
 Sum of electronic and thermal Free Energies= -1599.028977

6	0.000034000	-1.738208000	0.000146000
7	-1.081216000	-2.507065000	-0.231917000
7	1.081535000	-2.506806000	0.231942000
6	-0.756550000	-3.956691000	-0.159339000
6	0.757315000	-3.956499000	0.158908000
6	-2.401135000	-2.037357000	-0.573836000
6	2.401334000	-2.036870000	0.573982000
6	-2.676977000	-1.674122000	-1.919451000
6	-3.985452000	-1.264941000	-2.236265000
6	-5.013663000	-1.219482000	-1.270223000
6	-4.696756000	-1.584793000	0.053150000
6	-3.402468000	-2.000087000	0.429205000
6	-1.602785000	-1.704907000	-2.982967000
1	-4.211617000	-0.981202000	-3.277531000
6	-6.416296000	-0.813271000	-1.658653000
1	-5.484344000	-1.552002000	0.824168000
6	-3.113630000	-2.397430000	1.859151000
6	2.677017000	-1.673543000	1.919617000
6	3.985384000	-1.264103000	2.236504000
6	5.013694000	-1.218572000	1.270555000
6	4.696980000	-1.584058000	-0.052804000
6	3.402778000	-1.999592000	-0.428942000
6	1.602785000	-1.704589000	2.983082000
1	4.211411000	-0.980194000	3.277753000
6	6.416247000	-0.812206000	1.659099000
1	5.484618000	-1.551179000	-0.823768000
6	3.114302000	-2.397237000	-1.858885000
79	-0.000182000	0.292912000	0.000143000
6	-0.573749000	2.436773000	0.268311000
6	0.573444000	2.436754000	-0.268769000
6	-1.755636000	2.829395000	0.994098000
6	-1.700392000	4.001885000	1.796210000
6	-2.968322000	2.097910000	0.906494000
6	-2.842386000	4.431093000	2.484857000
1	-0.758436000	4.565877000	1.870509000
6	-4.100888000	2.536876000	1.606059000
1	-3.014152000	1.190756000	0.283861000
6	-4.042667000	3.701540000	2.393130000
1	-2.794685000	5.342059000	3.101452000
1	-5.039962000	1.967398000	1.531509000
1	-4.936451000	4.043679000	2.937781000
6	1.755464000	2.828905000	-0.994572000
6	2.968241000	2.097684000	-0.906146000
6	1.700219000	4.000777000	-1.797605000
6	4.100891000	2.536325000	-1.605787000
1	3.014130000	1.190983000	-0.282859000
6	2.842296000	4.429670000	-2.486307000
1	0.758191000	4.564563000	-1.872556000
6	4.042677000	3.700383000	-2.393751000
1	5.040034000	1.967044000	-1.530581000
1	2.794572000	5.340173000	-3.103582000
1	4.936540000	4.042240000	-2.938451000
1	1.042967000	-2.663207000	2.987784000
1	0.854655000	-0.896275000	2.827690000
1	2.038800000	-1.564520000	3.990694000
1	3.886698000	-1.997979000	-2.544282000
1	2.127234000	-2.027999000	-2.204318000
1	3.116434000	-3.502474000	-1.985781000
1	7.051394000	-0.620091000	0.772274000
1	6.907788000	-1.613038000	2.253011000
1	6.416311000	0.099808000	2.290917000
1	-2.127910000	-2.025212000	2.205283000
1	-3.112314000	-3.502702000	1.985707000
1	-3.887675000	-2.000854000	2.544232000
1	-2.038838000	-1.564622000	-3.990532000
1	-1.042926000	-2.663505000	-2.987934000
1	-0.854687000	-0.896600000	-2.827376000
1	-6.416599000	0.100008000	-2.288661000
1	-7.051976000	-0.623251000	-0.771764000
1	-6.907046000	-1.613193000	-2.254427000
1	1.001270000	-4.445717000	1.124639000
1	1.365537000	-4.444929000	-0.629892000
1	-1.364626000	-4.445613000	0.629265000
1	-1.000317000	-4.445642000	-1.125252000

# XL+XLI-XLII TS

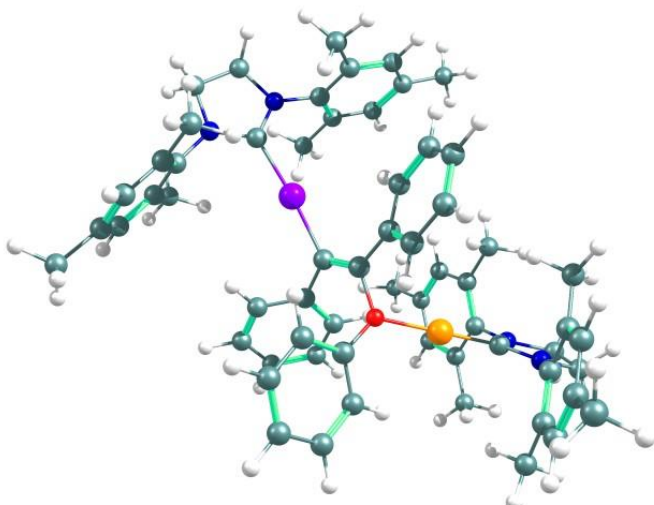


Zero-point correction= 1.095799 (Hartree/Particle)  
 Thermal correction to Energy= 1.170618  
 Thermal correction to Enthalpy= 1.171562  
 Thermal correction to Gibbs Free Energy= 0.968355  
 Sum of electronic and zero-point Energies= -3027.352570  
 Sum of electronic and thermal Energies= -3027.277751  
 Sum of electronic and thermal Enthalpies= -3027.276807  
 Sum of electronic and thermal Free Energies= -3027.480014

6	4.678721000	0.247003000	-0.707506000
7	5.123597000	1.307458000	-1.415485000
7	5.699023000	-0.609807000	-0.487765000
6	6.581660000	1.229344000	-1.690343000
6	6.962838000	-0.156579000	-1.122771000
6	4.353502000	2.468170000	-1.785377000
6	5.608850000	-1.877770000	0.192007000
6	4.211555000	3.529962000	-0.857077000
6	3.502296000	4.675976000	-1.267765000
6	2.945337000	4.790308000	-2.557267000
6	3.097132000	3.705673000	-3.445851000
6	3.795893000	2.537187000	-3.087311000
6	4.770079000	3.428685000	0.543576000
1	3.387023000	5.509131000	-0.554547000
6	2.232946000	6.051731000	-2.989786000
1	2.659751000	3.769846000	-4.456302000
6	3.919119000	1.381781000	-4.053999000
6	5.209618000	-3.027119000	-0.533349000
6	5.179295000	-4.260959000	0.147842000
6	5.531965000	-4.375819000	1.506488000
6	5.920086000	-3.205840000	2.193987000
6	5.968651000	-1.949087000	1.563159000
6	4.790979000	-2.937761000	-1.983011000
1	4.870903000	-5.162722000	-0.406655000
6	5.492542000	-5.708521000	2.218750000
1	6.197743000	-3.273014000	3.259299000
6	6.368833000	-0.711456000	2.334334000
79	2.782556000	-0.020386000	-0.025525000
6	0.116570000	-0.566143000	-0.109089000
6	0.886587000	-0.291941000	0.891552000
6	-4.882127000	0.941761000	0.211748000
7	-6.029444000	0.565924000	-0.403354000
7	-5.045597000	2.192871000	0.706805000
6	-7.109250000	1.575429000	-0.261704000
6	-6.370148000	2.773614000	0.370915000
6	-6.282881000	-0.723614000	-0.991632000
6	-4.038124000	2.952256000	1.399454000
6	-6.583528000	-1.828976000	-0.154902000
6	-6.877454000	-3.063072000	-0.768455000
6	-6.887176000	-3.221994000	-2.168471000
6	-6.572968000	-2.101912000	-2.965777000
6	-6.271006000	-0.846200000	-2.405666000
6	-6.559705000	-1.711754000	1.352023000
1	-7.109491000	-3.928459000	-0.125832000
6	-7.252595000	-4.545770000	-2.800537000
1	-6.560645000	-2.207920000	-4.063506000
6	-5.929313000	0.330451000	-3.291676000
6	-3.127004000	3.742502000	0.655098000
6	-2.180842000	4.510117000	1.363637000
6	-2.124890000	4.516688000	2.771292000
6	-3.051004000	3.719429000	3.476549000
6	-4.012544000	2.929316000	2.818248000
6	-3.159084000	3.758633000	-0.856408000
1	-1.467361000	5.127930000	0.793341000
6	-1.090489000	5.333812000	3.510956000
1	-3.028961000	3.714933000	4.579327000
6	-4.976344000	2.068955000	3.603347000
29	-3.358729000	-0.117871000	0.388617000
6	-1.951414000	-2.536464000	0.718035000
6	-1.125527000	-3.274425000	1.607255000
6	-2.836762000	-3.249208000	-0.133752000
6	-1.197710000	-4.674452000	1.645386000
1	-0.443049000	-2.723824000	2.272111000
6	-2.906710000	-4.651941000	-0.078699000
1	-3.477836000	-2.682578000	-0.829823000
6	-2.087142000	-5.374684000	0.805853000
1	-0.555748000	-5.228859000	2.349265000
1	-3.608551000	-5.183635000	-0.741304000
1	-2.141470000	-6.473694000	0.844893000
8	-1.865591000	-1.185502000	0.690876000
6	0.778634000	-0.142810000	2.350762000

	6	1.764946000	-0.697197000	3.204063000
	6	-0.302642000	0.567692000	2.928408000
	6	1.659830000	-0.566126000	4.597811000
	1	2.609253000	-1.247757000	2.759412000
	6	-0.391460000	0.708794000	4.321765000
	6	0.583669000	0.141151000	5.162344000
	1	2.426831000	-1.016474000	5.247539000
	1	-1.237193000	1.266375000	4.754108000
	1	0.505386000	0.250840000	6.255452000
	6	-0.259966000	-0.741950000	-1.481079000
	6	-0.627382000	0.382618000	-2.272111000
	6	-0.271871000	-2.037550000	-2.068842000
	6	-0.986988000	0.212608000	-3.614889000
	1	-0.608109000	1.384433000	-1.816938000
	6	-0.636348000	-2.193904000	-3.413906000
	1	0.012211000	-2.906939000	-1.458906000
	6	-0.993287000	-1.074824000	-4.188375000
	1	-1.258574000	1.089006000	-4.224270000
	1	-0.640830000	-3.199409000	-3.862783000
	1	-1.274113000	-1.204633000	-5.245574000
	1	-7.049955000	-2.583859000	1.825821000
	1	-7.068562000	-0.794300000	1.712911000
	1	-5.514729000	-1.670351000	1.732526000
	1	-5.787694000	0.007696000	-4.341284000
	1	-4.999547000	0.835540000	-2.957159000
	1	-6.733844000	1.098366000	-3.294142000
	1	-4.111904000	4.174666000	-1.249259000
	1	-3.060087000	2.734672000	-1.275542000
	1	-2.337251000	4.378685000	-1.263896000
	1	-4.827694000	2.197770000	4.692748000
	1	-4.842204000	0.991864000	3.366554000
	1	-6.036224000	2.316142000	3.380989000
	1	5.836483000	3.120653000	0.550922000
	1	4.213714000	2.672524000	1.139567000
	1	4.695643000	4.397615000	1.073717000
	1	3.454765000	0.460938000	-3.641743000
	1	4.978096000	1.135548000	-4.282810000
	1	3.419984000	1.613157000	-5.014564000
	1	4.654572000	-3.945670000	-2.419965000
	1	5.533471000	-2.397680000	-2.607081000
	1	3.828197000	-2.391075000	-2.084585000
	1	6.606955000	-0.959862000	3.386494000
	1	5.554522000	0.044052000	2.338730000
	1	7.264765000	-0.216597000	1.901732000
	1	-1.070430000	1.009424000	2.276664000
	1	1.385664000	5.831925000	-3.670762000
	1	2.923664000	6.726236000	-3.542057000
	1	1.843785000	6.622472000	-2.123116000
	1	4.734831000	-5.705767000	3.031415000
	1	6.469270000	-5.941690000	2.692584000
	1	5.242268000	-6.536833000	1.527459000
	1	-1.535972000	5.868978000	4.374742000
	1	-0.611597000	6.084136000	2.851399000
	1	-0.286288000	4.681020000	3.915084000
	1	-7.043725000	-5.397067000	-2.122385000
	1	-6.702646000	-4.713407000	-3.748684000
	1	-8.337260000	-4.580797000	-3.044438000
	1	7.106991000	2.066405000	-1.182442000
	1	6.777308000	1.323367000	-2.778183000
	1	7.779489000	-0.111833000	-0.373350000
	1	7.270477000	-0.878472000	-1.909244000
	1	-7.916479000	1.172619000	0.388481000
	1	-7.559881000	1.812775000	-1.246471000
	1	-6.869847000	3.163630000	1.280966000
	1	-6.246087000	3.624519000	-0.334018000

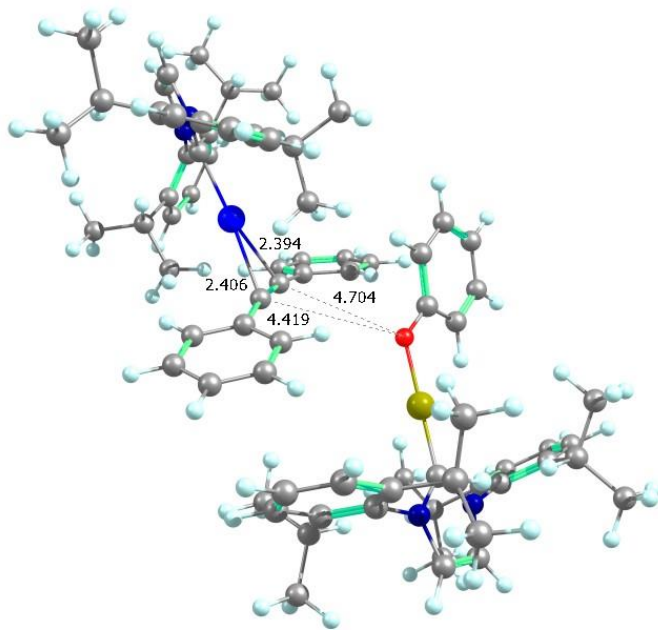
**XLII [Au(SIMes)(PhCCPh)(OPh)(SIMes)Cu]<sup>+</sup> min**



Zero-point correction= 1.098112 (Hartree/Particle)  
 Thermal correction to Energy= 1.172624  
 Thermal correction to Enthalpy= 1.173568  
 Thermal correction to Gibbs Free Energy= 0.971322  
 Sum of electronic and zero-point Energies= -3027.371844  
 Sum of electronic and thermal Energies= -3027.297332  
 Sum of electronic and thermal Enthalpies= -3027.296388  
 Sum of electronic and thermal Free Energies= -3027.498634

6	4.478672000	0.478245000	-0.597168000
7	4.926534000	1.687564000	-1.007372000
7	5.522605000	-0.379093000	-0.541370000
6	6.400049000	1.716254000	-1.195742000
6	6.798210000	0.239702000	-0.981163000
6	4.141952000	2.887578000	-1.137003000
6	5.450591000	-1.774904000	-0.190114000
6	3.871176000	3.673081000	0.011373000
6	3.162070000	4.878848000	-0.162921000
6	2.729096000	5.317843000	-1.429836000
6	3.006656000	4.501350000	-2.546092000
6	3.709453000	3.286816000	-2.427850000
6	4.304064000	3.225634000	1.388189000
1	2.952545000	5.500245000	0.723841000
6	2.019074000	6.642215000	-1.597864000
1	2.670402000	4.822381000	-3.546449000
6	3.972364000	2.423788000	-3.640873000
6	5.160153000	-2.730823000	-1.195919000
6	5.147664000	-4.091386000	-0.831816000
6	5.416166000	-4.517432000	0.485051000
6	5.685558000	-3.534350000	1.459254000
6	5.709771000	-2.160567000	1.149235000
6	4.829200000	-2.306504000	-2.608414000
1	4.921998000	-4.843162000	-1.606611000
6	5.444389000	-5.987791000	0.836037000
1	5.885056000	-3.844899000	2.498473000
6	5.961985000	-1.129274000	2.225048000
79	2.552818000	-0.022304000	-0.103794000
6	-0.395550000	-0.729710000	-0.341613000
6	0.675665000	-0.647994000	0.496068000
6	-4.673762000	0.849585000	0.440918000
7	-5.828956000	0.745234000	-0.251294000
7	-4.762982000	1.885882000	1.305445000
6	-6.837768000	1.749659000	0.173796000
6	-6.051051000	2.615687000	1.183812000
6	-6.115076000	-0.238236000	-1.264754000
6	-3.708276000	2.330361000	2.179088000
6	-6.762762000	-1.447328000	-0.899308000
6	-7.065276000	-2.369204000	-1.919213000
6	-6.757441000	-2.118283000	-3.272836000
6	-6.113654000	-0.906727000	-3.593463000
6	-5.782241000	0.049296000	-2.612512000
6	-7.120114000	-1.748556000	0.539002000
1	-7.560075000	-3.315941000	-1.645428000
6	-7.134121000	-3.112246000	-4.347346000
1	-5.861515000	-0.693048000	-4.645475000
6	-5.063032000	1.322969000	-2.994058000
6	-2.648800000	3.110675000	1.646909000
6	-1.643311000	3.550058000	2.530150000
6	-1.666812000	3.246936000	3.906395000
6	-2.742922000	2.480480000	4.398188000
6	-3.773337000	2.010645000	3.560560000
6	-2.577418000	3.455586000	0.176302000
1	-0.815707000	4.156295000	2.126392000
6	-0.554969000	3.702107000	4.822925000
1	-2.784043000	2.236644000	5.472959000
6	-4.911909000	1.197182000	4.133735000
29	-3.188979000	-0.265830000	0.266643000
6	-1.638563000	-2.782757000	0.353039000
6	-0.718044000	-3.634991000	-0.275646000
6	-2.640000000	-3.285211000	1.199132000
6	-0.819845000	-5.019563000	-0.052882000
1	0.069206000	-3.219751000	-0.921704000
6	-2.730576000	-4.671494000	1.406941000
1	-3.332066000	-2.587260000	1.699017000
6	-1.822065000	-5.543821000	0.782015000
1	-0.102559000	-5.694746000	-0.545258000
1	-3.512469000	-5.068348000	2.073073000
1	-1.891896000	-6.629281000	0.950043000
8	-1.622933000	-1.393367000	0.127932000
6	0.579453000	-1.098535000	1.913149000
6	-0.378617000	-0.542494000	2.799535000
6	1.483657000	-2.059560000	2.433333000
6	-0.435375000	-0.941148000	4.145387000
1	-1.066875000	0.237638000	2.434190000

	6	1.410743000	-2.472304000	3.773058000
	1	2.249136000	-2.486734000	1.765653000
	6	0.452378000	-1.914387000	4.638145000
	1	-1.180026000	-0.481728000	4.815233000
	1	2.115741000	-3.231819000	4.147193000
	1	0.403566000	-2.229596000	5.692408000
	6	-0.576638000	-0.236966000	-1.724308000
	6	-1.435191000	-0.909008000	-2.635274000
	6	0.086909000	0.933773000	-2.176978000
	6	-1.592439000	-0.448915000	-3.953232000
	1	-1.964918000	-1.820444000	-2.318110000
	6	-0.075771000	1.390068000	-3.493429000
	1	0.731238000	1.488868000	-1.476806000
	6	-0.911794000	0.700481000	-4.391584000
	1	-2.248845000	-1.001140000	-4.644175000
	1	0.448507000	2.303607000	-3.815844000
	1	-1.036782000	1.061010000	-5.424797000
	1	4.737857000	-3.184370000	-3.276802000
	1	5.600434000	-1.634647000	-3.040398000
	1	3.865912000	-1.751895000	-2.640304000
	1	6.805705000	-0.452816000	1.972093000
	1	6.200647000	-1.613117000	3.191659000
	1	5.067699000	-0.487228000	2.377120000
	1	5.379921000	2.954147000	1.422970000
	1	3.736377000	2.324930000	1.708631000
	1	4.133217000	4.021802000	2.138193000
	1	3.523730000	2.869009000	-4.549884000
	1	3.547882000	1.405871000	-3.510964000
	1	5.058499000	2.298015000	-3.839408000
	1	1.230490000	6.589171000	-2.376016000
	1	2.731368000	7.435429000	-1.914862000
	1	1.552034000	6.982395000	-0.652121000
	1	4.756453000	-6.576335000	0.196212000
	1	5.168205000	-6.162551000	1.895276000
	1	6.463646000	-6.408976000	0.691240000
	1	-5.123911000	1.500485000	-4.085117000
	1	-3.984531000	1.269793000	-2.727900000
	1	-5.478553000	2.214079000	-2.480329000
	1	-7.419771000	-2.807581000	0.658674000
	1	-7.973236000	-1.128858000	0.892938000
	1	-6.270508000	-1.553791000	1.226241000
	1	-6.548938000	-2.956945000	-5.275219000
	1	-8.209222000	-3.016051000	-4.614955000
	1	-6.978573000	-4.157124000	-4.009689000
	1	-5.201348000	0.360168000	3.466259000
	1	-5.821239000	1.817939000	4.294401000
	1	-4.638702000	0.771534000	5.118808000
	1	-1.851619000	4.272373000	-0.001468000
	1	-3.558632000	3.776297000	-0.229900000
	1	-2.247564000	2.585271000	-0.432924000
	1	6.658153000	2.094943000	-2.205842000
	1	6.862599000	2.402087000	-0.453355000
	1	7.582639000	0.107142000	-0.207842000
	1	7.159346000	-0.251690000	-1.910439000
	1	-7.712146000	1.239403000	0.630847000
	1	-7.204331000	2.322956000	-0.702235000
	1	-6.550531000	2.694056000	2.170522000
	1	-5.865776000	3.648696000	0.818114000
	1	-0.072443000	4.628576000	4.452569000
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**Adduct-IPr**

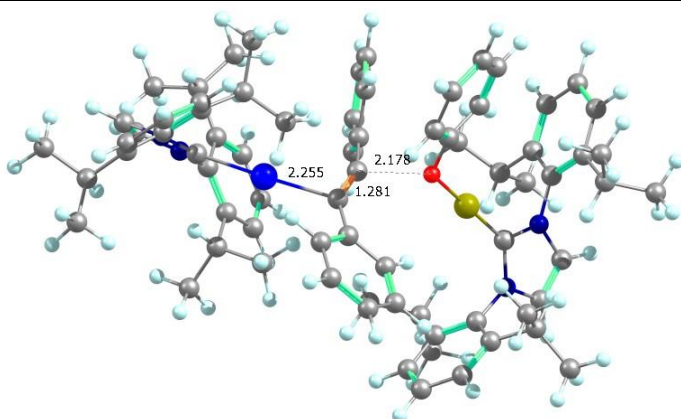
Zero-point correction= 1.336432 (Hartree/Particle)  
 Thermal correction to Energy= 1.425123  
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 Sum of electronic and zero-point Energies= -1629.824084  
 Sum of electronic and thermal Energies= -1629.735393  
 Sum of electronic and thermal Enthalpies= -1629.734449  
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7	-6.433792000	-0.168682000	-0.062492000
7	-5.656545000	1.500510000	-1.169512000
6	-7.522736000	0.396793000	-0.720438000
6	-7.024362000	1.456904000	-1.435084000
6	-6.470066000	-1.322053000	0.825364000
6	-4.728660000	2.465264000	-1.744086000
1	-8.538392000	-0.001929000	-0.631599000
1	-7.517986000	2.179910000	-2.093376000
6	-5.946940000	-1.193252000	2.133720000
6	-6.024434000	-2.299896000	2.991365000
6	-6.610799000	-3.494645000	2.570264000
6	-7.108304000	-3.609846000	1.273054000
6	-7.033960000	-2.537320000	0.371336000
6	-5.322661000	0.087842000	2.669413000
1	-5.635375000	-2.222150000	4.008471000
1	-6.682020000	-4.339156000	3.258955000
1	-7.564073000	-4.550124000	0.951997000
6	-7.564679000	-2.722509000	-1.041680000
6	-3.598039000	1.993603000	-2.450665000
6	-2.747217000	2.935203000	-3.047312000
6	-3.013252000	4.301704000	-2.956029000
6	-4.122199000	4.751653000	-2.239571000
6	-4.989088000	3.849223000	-1.606644000
6	-3.245579000	0.519224000	-2.580662000
1	-1.866111000	2.592879000	-3.595233000
1	-2.350378000	5.019617000	-3.443371000
1	-4.318004000	5.824147000	-2.169310000
6	-6.165103000	4.393598000	-0.810805000
1	-5.342826000	0.910671000	1.901622000
6	-3.851624000	-0.165764000	3.045319000
6	-6.133147000	0.606672000	3.863257000
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6	-7.139725000	-4.073262000	-1.629259000
6	-9.091625000	-2.579224000	-1.031959000
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6	-3.104680000	0.123165000	-4.054903000
6	-1.958100000	0.234664000	-1.792201000
1	-6.554461000	3.603673000	-0.117793000
6	-5.746696000	5.577897000	0.069151000
6	-7.289983000	4.792651000	-1.774227000
1	-3.198926000	0.701815000	2.820737000
1	-3.742428000	-0.301128000	4.136896000
1	-3.450845000	-1.113915000	2.634582000
1	-5.732077000	1.556743000	4.236905000
1	-7.181609000	0.781079000	3.587165000
1	-6.140519000	-0.095113000	4.706184000
1	-7.396418000	-4.133737000	-2.694857000
1	-6.058092000	-4.230346000	-1.545259000
1	-7.635669000	-4.919650000	-1.139385000
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1	-9.569383000	-3.325561000	-0.384749000
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1	-1.056045000	0.289736000	-2.452732000
1	-1.726512000	0.994313000	-1.021622000
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6	5.626593000	2.659328000	0.873252000

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	6	7.158179000	-3.722419000	-1.817625000
	6	6.819206000	-4.711096000	-0.894048000
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	6	6.479834000	-3.024348000	0.825997000
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	1	6.232681000	-5.147291000	1.132967000
	6	6.145748000	-2.686929000	2.270033000
	6	4.962912000	2.935359000	2.090705000
	6	4.330178000	4.178058000	2.232738000
	6	4.351611000	5.114531000	1.197870000
	6	5.013273000	4.827788000	0.004222000
	6	5.668781000	3.600747000	-0.178865000
	6	4.949642000	1.949990000	3.248082000
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	6	9.084132000	-1.424083000	-2.735165000
	1	5.988403000	-1.583217000	2.378520000
	6	4.846761000	-3.372179000	2.711224000
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	6	5.521183000	3.592883000	-2.690511000
	6	7.677451000	4.223609000	-1.516695000
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	1	7.433337000	5.292383000	-1.512275000
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	1	0.411747000	-0.202324000	-2.929689000
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	6	-6.833638000	-1.388672000	0.284648000
	6	-3.635790000	-2.222364000	1.782641000
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	6	-3.265056000	-3.578897000	1.630325000
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	1	-7.534956000	3.400178000	-3.574951000
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	6	-8.472363000	2.738515000	1.200195000
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	1	-1.668549000	1.536464000	3.308611000
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	1	-2.546878000	-6.166019000	0.555600000
	1	-5.531351000	-6.099441000	0.944388000
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	1	-5.722505000	-4.760020000	2.086050000
	1	-3.587211000	-1.108125000	-4.265326000
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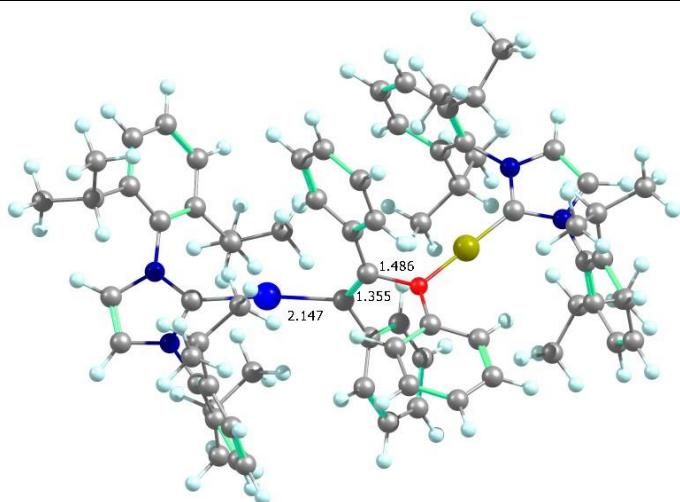


**Ts-IPr**

Zero-point correction= 1.336609 (Hartree/Particle)  
 Thermal correction to Energy= 1.424322  
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 Thermal correction to Gibbs Free Energy= 1.195911  
 Sum of electronic and zero-point Energies= -1629.806642  
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	1	-3.251591000	1.885104000	-1.796455000
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	1	-7.553897000	3.331904000	1.274421000
	1	-9.197815000	3.327359000	0.625999000
	1	-10.093285000	0.506022000	1.273392000
	1	-10.168879000	1.116249000	-0.378003000
	1	-9.341222000	-0.409433000	-0.044255000
	79	-2.842809000	0.328033000	-0.024315000
	6	-0.209467000	0.162264000	-0.753114000
	6	-0.813589000	1.236031000	-0.403810000
	6	4.779004000	0.140662000	0.583714000
	7	5.873681000	-0.660112000	0.343022000
	7	5.156963000	0.802296000	1.731796000
	6	6.877340000	-0.505337000	1.289421000
	6	6.418149000	0.432044000	2.180465000
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	6	6.631826000	-2.057952000	-3.055002000
	6	6.302416000	-3.400126000	-2.870190000
	6	5.824616000	-3.843481000	-1.635382000
	6	5.661206000	-2.952020000	-0.566865000
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	1	5.582063000	-4.898045000	-1.499495000
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	6	2.765062000	2.378408000	4.150814000
	6	2.889911000	3.726735000	3.810190000
	6	3.748708000	4.115252000	2.782513000
	6	4.497711000	3.164939000	2.071994000
	6	3.364891000	-0.060672000	3.886535000
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	1	2.319223000	4.480061000	4.355975000
	1	3.852039000	5.173151000	2.534771000
	6	5.451525000	3.632451000	0.984424000
	1	6.539102000	0.955357000	-1.396229000
	6	6.267366000	0.869745000	-3.524940000
	6	8.428733000	0.407180000	-2.284650000
	1	4.893233000	-2.618002000	1.439456000
	6	3.912258000	-4.337016000	0.602597000
	6	6.296074000	-4.259954000	1.456953000
	1	3.785297000	-0.724483000	3.087555000
	6	4.176758000	-0.287980000	5.167546000
	6	1.896300000	-0.463991000	4.079505000
	1	5.860555000	2.750803000	0.426873000
	6	4.726442000	4.515342000	-0.037462000
	6	6.634530000	4.369420000	1.624549000
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	1	6.670651000	0.399286000	-4.428483000
	1	5.177579000	0.719697000	-3.539632000
	1	8.756977000	1.443546000	-2.429127000
	1	8.881346000	0.042210000	-1.356736000
	1	8.852496000	-0.179423000	-3.108674000
	1	3.488986000	-4.608617000	1.575404000
	1	3.140429000	-3.805916000	0.031767000
	1	4.123968000	-5.273459000	0.072752000
	1	5.981416000	-4.633981000	2.437892000
	1	6.607693000	-5.129377000	0.865118000
	1	7.185132000	-3.638175000	1.609650000
	1	4.119638000	-1.332201000	5.495785000
	1	5.235803000	-0.047226000	5.019883000
	1	3.816882000	0.332493000	5.997349000
	1	1.808864000	-1.543485000	4.245903000
	1	1.446560000	0.031553000	4.948262000
	1	1.295130000	-0.204851000	3.201350000
	1	5.384485000	4.760361000	-0.880751000
	1	3.843861000	4.011370000	-0.452692000
	1	4.394770000	5.467378000	0.390910000
	1	7.359530000	4.684578000	0.863982000

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	1	7.165178000	3.735008000	2.342718000
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	6	1.819019000	0.635298000	-2.867271000
	6	1.021457000	1.524881000	-3.638272000
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	8	1.761008000	0.680780000	-1.521650000
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	6	-1.637771000	3.606601000	-0.427466000
	6	0.646620000	3.141318000	0.282167000
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	1	1.457310000	2.418986000	0.469090000
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	6	0.261363000	-2.096854000	0.148971000
	6	-0.222100000	-1.833518000	-2.239445000
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	1	0.629723000	-4.124489000	0.826447000
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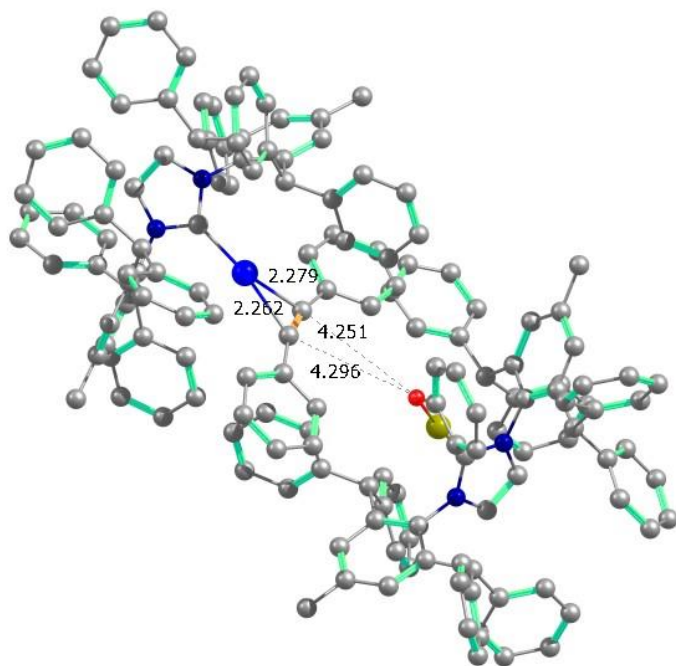
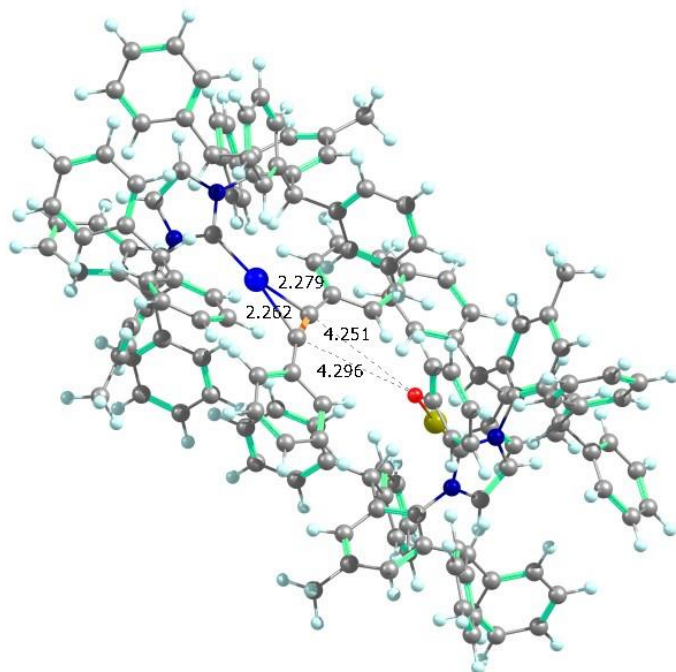
**Int-IPr**

Zero-point correction= 1.339220 (Hartree/Particle)  
 Thermal correction to Energy= 1.425905  
 Thermal correction to Enthalpy= 1.426849  
 Thermal correction to Gibbs Free Energy= 1.201566  
 Sum of electronic and zero-point Energies= -1629.820244  
 Sum of electronic and thermal Energies= -1629.733559  
 Sum of electronic and thermal Enthalpies= -1629.732615  
 Sum of electronic and thermal Free Energies= -1629.957899

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	6	6.814790000	-1.071178000	0.377318000
	6	5.269693000	2.209614000	0.462337000
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	1	7.581220000	-1.850146000	0.385631000
	6	4.277066000	2.669049000	1.358541000
	6	4.030374000	4.048668000	1.431178000
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	6	5.690041000	4.479763000	-0.267256000
	6	5.953552000	3.108264000	-0.392835000
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	1	3.273940000	4.421797000	2.122810000
	1	4.556708000	6.021057000	0.730276000
	1	6.233631000	5.190295000	-0.893690000
	6	6.954739000	2.656494000	-1.445289000
	6	4.520581000	-3.057429000	-1.313356000
	6	4.038134000	-4.361484000	-1.487201000
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	6	4.041760000	-4.726232000	0.909169000
	6	4.519909000	-3.428202000	1.128515000
	6	4.601584000	-2.084275000	-2.477802000
	1	3.809836000	-4.728872000	-2.488722000
	1	3.488093000	-6.222137000	-0.543618000
	1	3.814249000	-5.375680000	1.755866000
	6	4.584892000	-2.824047000	2.520871000
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	1	3.087505000	3.166855000	3.877477000
	1	7.337141000	2.927213000	-3.574746000
	1	5.665615000	3.262500000	-3.106929000
	1	6.944181000	4.430077000	-2.747258000
	1	9.125157000	2.601835000	-1.685109000
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	1	8.587711000	2.360861000	-0.014762000
	1	4.980017000	-2.047867000	-4.623645000
	1	5.673419000	-3.449309000	-3.805916000
	1	3.934058000	-3.376794000	-4.125180000
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	6	1.051448000	2.543695000	-2.892523000
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	1	0.556655000	3.157244000	-4.925810000



**Adduct-IPr\***

Zero-point correction= 2.250372 (Hartree/Particle)  
 Thermal correction to Energy= 2.399935  
 Thermal correction to Enthalpy= 2.400880  
 Thermal correction to Gibbs Free Energy= 2.017537  
 Sum of electronic and zero-point Energies= -1628.104247  
 Sum of electronic and thermal Energies= -1627.954684  
 Sum of electronic and thermal Enthalpies= -1627.953740  
 Sum of electronic and thermal Free Energies= -1628.337082

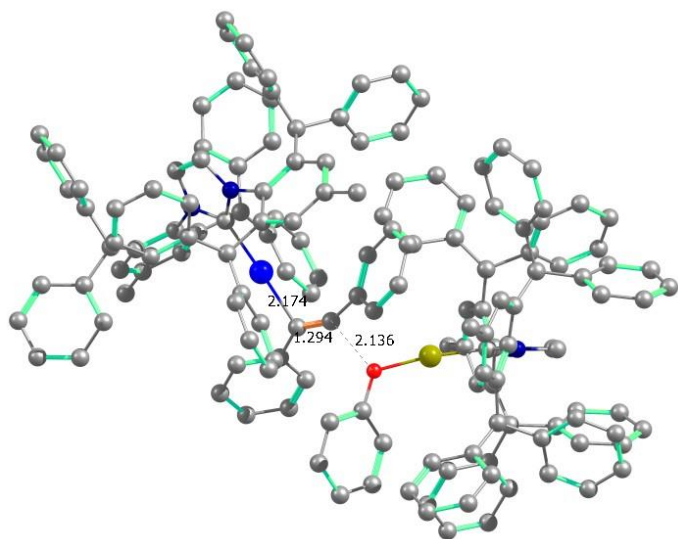
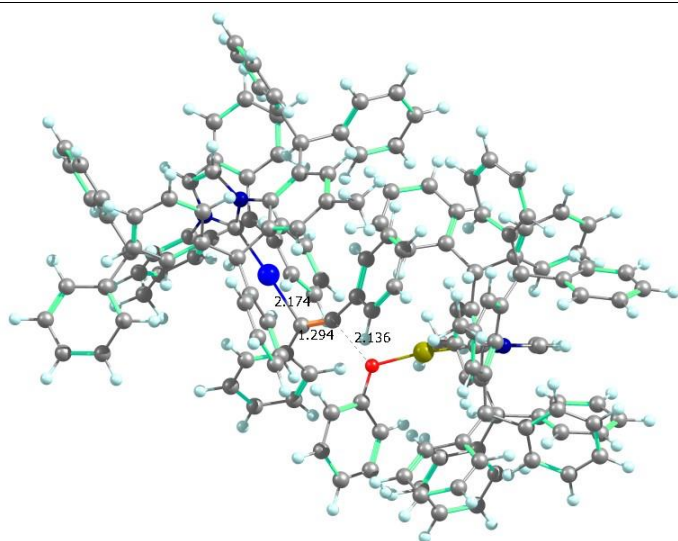
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7	6.426919000	-0.171624000	-1.228235000
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6	6.142665000	1.298073000	1.998697000
6	5.977624000	-0.907048000	-2.403439000
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1	8.410808000	0.380265000	-1.959692000
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6	5.801796000	1.073028000	4.380655000
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6	1.488858000	-2.960405000	2.646054000
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6	1.485590000	-4.141313000	3.402441000
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6	3.472830000	-4.902049000	2.246808000
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	6	-0.946734000	3.522255000	1.189469000
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	1	2.068024000	2.172879000	2.138270000
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**Ts-IPr\***

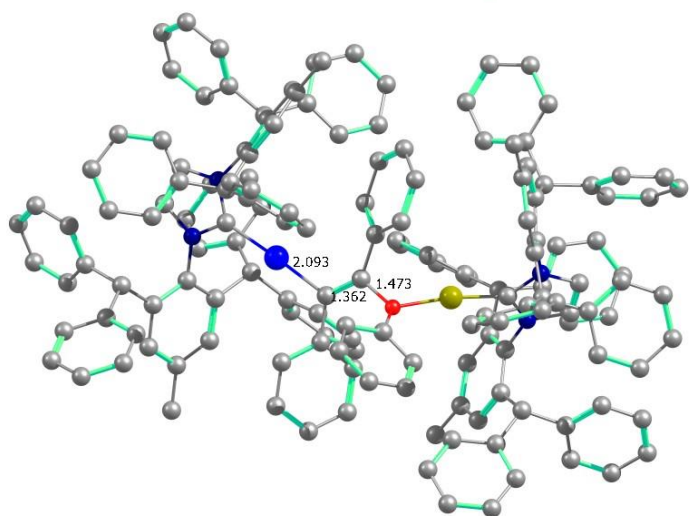
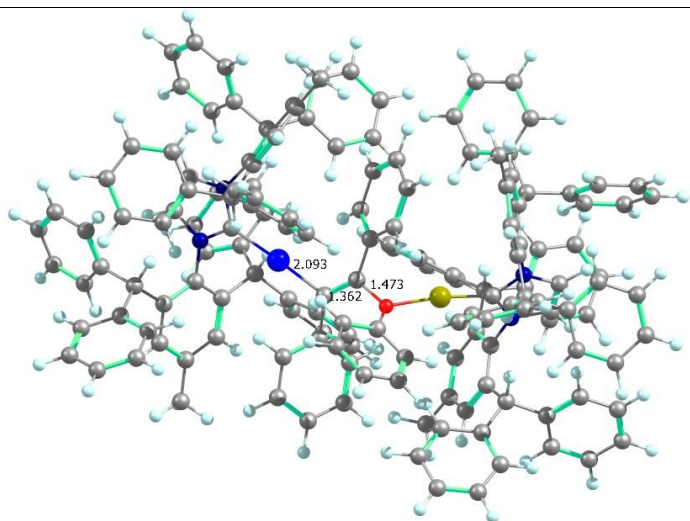
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 Thermal correction to Energy= 2.398807  
 Thermal correction to Enthalpy= 2.399751  
 Thermal correction to Gibbs Free Energy= 2.030261  
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	6	0.802528000	2.618731000	2.038145000
	1	-0.028175000	3.382482000	0.172027000
	1	1.562949000	1.572396000	3.792532000
	1	1.086131000	3.616647000	2.409228000
	1	-4.513909000	-0.506530000	2.258610000
	1	-3.881094000	0.153808000	-2.133164000
	1	-7.174220000	-1.644453000	0.937077000
	1	-6.896002000	-4.347132000	-5.077709000
	1	-7.331309000	-5.371586000	-3.705330000
	1	-5.638038000	-5.204657000	-4.179285000
	1	-2.007627000	4.442863000	5.086806000
	1	-1.021380000	5.017496000	3.739018000
	1	-0.647051000	3.470762000	4.512294000
	1	-4.225129000	3.120558000	-0.923891000
	6	-5.772307000	0.276277000	3.804614000
	6	-6.613175000	-0.849896000	3.820281000
	6	-6.221089000	1.480750000	4.360727000
	1	-6.268016000	-1.799482000	3.412551000
	1	-5.579498000	2.360949000	4.367470000
	6	-7.887901000	-0.766078000	4.383667000
	6	-7.501606000	1.560670000	4.918742000
	1	-8.531341000	-1.646587000	4.403568000
	1	-7.845426000	2.500703000	5.349635000
	6	-8.337083000	0.440951000	4.931059000
	1	-9.331218000	0.504033000	5.371436000
	6	-3.447976000	-0.636286000	4.095804000
	6	-3.535410000	-0.569742000	5.492221000
	6	-2.466189000	-1.442510000	3.497467000
	1	-4.305951000	0.040959000	5.964826000
	1	-2.398701000	-1.517073000	2.406789000
	6	-2.643309000	-1.300707000	6.283229000
	6	-1.574658000	-2.165134000	4.292531000
	1	-2.719819000	-1.252994000	7.369620000
	1	-0.808156000	-2.792024000	3.815056000
	6	-1.660213000	-2.096008000	5.686423000
	1	-0.967604000	-2.665839000	6.304585000
	6	-2.838495000	4.735848000	-0.799204000
	6	-2.702358000	6.117997000	-0.609221000
	6	-1.896888000	4.052576000	-1.586426000
	1	-3.433745000	6.665797000	-0.013213000
	1	-1.991771000	2.980855000	-1.749050000
	6	-1.638860000	6.806440000	-1.200592000
	6	-0.835949000	4.744444000	-2.176241000
	1	-1.545387000	7.882979000	-1.056431000
	1	-0.116763000	4.206842000	-2.798192000
	6	-0.703870000	6.123227000	-1.984033000
	1	0.116574000	6.664617000	-2.453108000
	6	-5.244868000	4.794225000	-0.062562000
	6	-5.568094000	5.474486000	1.119320000
	6	-6.100880000	4.891378000	-1.172047000
	1	-4.914412000	5.415200000	1.988573000
	1	-5.859022000	4.370771000	-2.099737000
	6	-6.735819000	6.240696000	1.191087000
	6	-7.264281000	5.660026000	-1.096100000
	1	-6.981007000	6.768060000	2.112747000
	1	-7.922301000	5.735033000	-1.961685000
	6	-7.585925000	6.335515000	0.086068000
	1	-8.493337000	6.935290000	0.143191000

	6	-5.061269000	0.943751000	-3.740456000
	6	-6.320131000	0.827432000	-4.343432000
	6	-4.401720000	2.184946000	-3.750574000
	1	-6.840709000	-0.130223000	-4.356757000
	1	-3.412368000	2.284496000	-3.306738000
	6	-6.917429000	1.942659000	-4.940581000
	6	-4.999746000	3.293743000	-4.352534000
	1	-7.897528000	1.845160000	-5.407659000
	1	-4.478601000	4.251485000	-4.365364000
	6	-6.261541000	3.176424000	-4.945871000
	1	-6.726708000	4.041597000	-5.416183000
	6	-3.233911000	-0.781625000	-3.929804000
	6	-3.187766000	-0.615641000	-5.318684000
	6	-2.203689000	-1.477193000	-3.274548000
	1	-3.983707000	-0.078776000	-5.836267000
	1	-2.244825000	-1.625863000	-2.189551000
	6	-2.114808000	-1.139531000	-6.048103000
	6	-1.140382000	-2.005874000	-4.008294000
	1	-2.080387000	-1.005512000	-7.129186000
	1	-0.350116000	-2.558719000	-3.498064000
	6	-1.092515000	-1.834611000	-5.396838000
	1	-0.261060000	-2.245005000	-5.967099000
	6	-8.061483000	-3.572012000	0.761040000
	6	-7.008187000	-4.232159000	1.416918000
	6	-9.315818000	-4.189472000	0.677317000
	1	-6.026655000	-3.768321000	1.481533000
	1	-10.145854000	-3.690958000	0.175442000
	6	-7.213203000	-5.491904000	1.983263000
	6	-9.516579000	-5.450746000	1.248042000
	1	-6.393563000	-5.999052000	2.491478000
	1	-10.496796000	-5.922983000	1.182993000
	6	-8.468642000	-6.104299000	1.901279000
	1	-8.627808000	-7.085535000	2.345997000
	6	-9.070890000	-1.397900000	-0.032234000
	6	-9.546417000	-0.609143000	1.028091000
	6	-9.782239000	-1.431892000	-1.239798000
	1	-9.007438000	-0.580694000	1.976126000
	1	-9.433330000	-2.048120000	-2.067895000
	6	-10.717442000	0.136968000	0.877540000
	6	-10.952494000	-0.680985000	-1.386250000
	1	-11.084476000	0.742686000	1.705725000
	1	-11.502458000	-0.714012000	-2.326482000
	6	-11.422245000	0.105109000	-0.330378000
	1	-12.336303000	0.685873000	-0.445211000
	6	4.676979000	2.540553000	-3.349801000
	6	4.544328000	3.815944000	-2.773061000
	6	5.752225000	2.283846000	-4.210009000
	1	3.706339000	4.034030000	-2.112124000
	1	5.867406000	1.305424000	-4.676670000
	6	5.469871000	4.819609000	-3.065024000
	6	6.684786000	3.288915000	-4.488518000
	1	5.351317000	5.811382000	-2.627706000
	1	7.519029000	3.080661000	-5.158364000
	6	6.545823000	4.557598000	-3.920578000
	1	7.266909000	5.341412000	-4.147339000
	6	2.288896000	1.820506000	-3.691189000
	6	2.186862000	2.729213000	-4.753257000
	6	1.130835000	1.178622000	-3.220464000
	1	3.076685000	3.228291000	-5.141005000
	1	1.201416000	0.454010000	-2.410384000
	6	0.941981000	3.001469000	-5.329501000
	6	-0.107888000	1.444126000	-3.807579000
	1	0.872364000	3.711496000	-6.153576000
	1	-0.998315000	0.918818000	-3.461894000
	6	-0.207266000	2.360031000	-4.860431000
	1	-1.174276000	2.562399000	-5.318785000
	6	6.353972000	-4.173817000	-2.273822000
	6	7.331690000	-4.897140000	-2.968336000
	6	5.251540000	-4.853382000	-1.728675000
	1	8.198963000	-4.391164000	-3.393514000
	1	4.478856000	-4.301725000	-1.180088000
	6	7.208679000	-6.283263000	-3.113870000
	6	5.130583000	-6.235497000	-1.878888000
	1	7.976691000	-6.839336000	-3.651035000
	1	4.271806000	-6.754468000	-1.453698000

	6	6.110097000	-6.955229000	-2.572461000
	1	6.017428000	-8.033995000	-2.686421000
	6	7.837650000	-2.124953000	-2.324960000
	6	8.716350000	-1.993715000	-1.238854000
	6	8.266144000	-1.752254000	-3.607519000
	1	8.399864000	-2.286112000	-0.237135000
	1	7.599083000	-1.860241000	-4.462036000
	6	10.004737000	-1.489692000	-1.433261000
	6	9.556170000	-1.248971000	-3.797468000
	1	10.679353000	-1.390674000	-0.582769000
	1	9.884717000	-0.964984000	-4.796649000
	6	10.427536000	-1.114515000	-2.712310000
	1	11.432656000	-0.724272000	-2.863409000
	6	4.009495000	4.574355000	1.368237000
	6	2.856668000	4.577716000	0.567403000
	6	4.269717000	5.673406000	2.200688000
	1	2.640365000	3.732341000	-0.084300000
	1	5.172060000	5.696176000	2.813338000
	6	1.977755000	5.664220000	0.600206000
	6	3.386850000	6.755875000	2.233761000
	1	1.089525000	5.664415000	-0.033212000
	1	3.600113000	7.608357000	2.878762000
	6	2.239327000	6.754763000	1.434316000
	1	1.558905000	7.604194000	1.454835000
	6	6.408898000	3.877506000	1.311175000
	6	7.136539000	3.954085000	2.507298000
	6	7.021123000	4.258540000	0.106815000
	1	6.678607000	3.665304000	3.452837000
	1	6.467504000	4.203544000	-0.831195000
	6	8.459556000	4.406257000	2.496988000
	6	8.342158000	4.711870000	0.101586000
	1	9.018082000	4.465694000	3.430751000
	1	8.808957000	5.009503000	-0.837036000
	6	9.065686000	4.786154000	1.296342000
	1	10.095092000	5.141352000	1.291024000
	6	7.388580000	-1.178825000	2.838420000
	6	8.095042000	-0.006666000	3.136839000
	6	8.089385000	-2.311835000	2.389288000
	1	7.575635000	0.876605000	3.506529000
	1	7.552573000	-3.238019000	2.182965000
	6	9.483842000	0.036964000	2.972322000
	6	9.476077000	-2.265611000	2.235459000
	1	10.025937000	0.953036000	3.204599000
	1	10.014395000	-3.151700000	1.898693000
	6	10.177199000	-1.088500000	2.520925000
	1	11.258646000	-1.054492000	2.401953000
	6	5.552397000	-2.260831000	4.126742000
	6	6.322142000	-2.295402000	5.300010000
	6	4.472636000	-3.142941000	3.981640000
	1	7.169980000	-1.620454000	5.417400000
	1	3.863809000	-3.136272000	3.075119000
	6	6.012486000	-3.204800000	6.314238000
	6	4.168340000	-4.052762000	4.998469000
	1	6.616629000	-3.231916000	7.220245000
	1	3.332598000	-4.741964000	4.867750000
	6	4.935499000	-4.085292000	6.166415000
	1	4.700477000	-4.797151000	6.955623000
	6	3.654534000	2.114197000	5.973661000
	1	3.082448000	3.050852000	5.959948000
	1	2.994742000	1.334169000	6.382056000
	1	4.467600000	2.249660000	6.706255000
	6	3.705329000	-2.354575000	-6.285553000
	1	3.354935000	-3.390566000	-6.161390000
	1	2.891814000	-1.796336000	-6.768705000
	1	4.540537000	-2.386804000	-7.003320000
	1	-7.905158000	0.828019000	-0.938768000
	1	-6.785169000	2.753311000	0.783058000



Zero-point correction= 2.253264 (Hartree/Particle)  
 Thermal correction to Energy= 2.400993  
 Thermal correction to Enthalpy= 2.401937  
 Thermal correction to Gibbs Free Energy= 2.030307  
 Sum of electronic and zero-point Energies= -1628.105829  
 Sum of electronic and thermal Energies= -1627.958100  
 Sum of electronic and thermal Enthalpies= -1627.957156  
 Sum of electronic and thermal Free Energies= -1628.328786

6	4.693239000	0.151818000	-0.077890000
7	5.747404000	-0.254167000	0.697764000
7	5.212957000	1.228084000	-0.747708000
6	6.875328000	0.538016000	0.528349000
6	6.535610000	1.484241000	-0.406562000
6	5.661529000	-1.383805000	1.610536000
6	4.457519000	2.013508000	-1.711484000
6	6.424418000	-2.545207000	1.356097000
6	6.328862000	-3.619438000	2.249797000
6	5.513534000	-3.543787000	3.385168000
6	4.780074000	-2.370864000	3.634148000
6	4.836303000	-1.285439000	2.759055000
6	7.351647000	-2.641279000	0.155511000
1	6.897888000	-4.531697000	2.051959000
6	5.417250000	-4.690754000	4.332969000
1	4.150982000	-2.319091000	4.526576000
6	4.037020000	-0.021225000	3.037617000
6	4.141167000	3.358017000	-1.415614000
6	3.460190000	4.116336000	-2.376422000
6	3.118680000	3.567278000	-3.618018000
6	3.442260000	2.228897000	-3.895093000
6	4.094609000	1.432508000	-2.951943000
6	4.527609000	3.993366000	-0.090025000
1	3.199020000	5.153121000	-2.153201000
6	2.414067000	4.385186000	-4.647168000
1	3.168337000	1.807720000	-4.866485000
6	4.393597000	-0.029807000	-3.249250000
79	2.796509000	-0.647622000	-0.168109000
6	-0.139396000	-0.991546000	-0.919881000
6	0.901429000	-1.533590000	-0.227606000
6	-4.605735000	-0.007324000	0.082655000
7	-5.543798000	0.710357000	-0.622709000
7	-5.206637000	-0.152456000	1.311375000
6	-6.673870000	0.995570000	0.130421000
6	-6.457191000	0.445295000	1.369375000
6	-5.341635000	1.205147000	-1.979238000
6	-4.597322000	-0.843247000	2.440854000
1	-7.520217000	1.565542000	-0.268857000
1	-7.075313000	0.434102000	2.273176000
6	-5.614300000	0.368053000	-3.088545000
6	-5.329701000	0.848813000	-4.369613000
6	-4.816715000	2.139843000	-4.565791000
6	-4.642718000	2.986484000	-3.462362000
6	-4.928283000	2.547766000	-2.166061000
6	-6.240905000	-1.003968000	-2.900999000
1	-5.516029000	0.215361000	-5.242085000
1	-4.290345000	4.008842000	-3.621088000
6	-4.876012000	3.516926000	-0.996733000
6	-3.818222000	-0.106620000	3.369895000
6	-3.200094000	-0.794574000	4.415906000
6	-3.368416000	-2.179465000	4.577166000
6	-4.202299000	-2.875844000	3.693994000
6	-4.837329000	-2.223416000	2.630180000
6	-3.691539000	1.404784000	3.270390000
1	-2.579060000	-0.248098000	5.131521000
1	-4.365617000	-3.947338000	3.838112000
6	-5.814999000	-2.991848000	1.754941000
1	-5.683841000	-1.521179000	-2.068594000
1	-4.480188000	2.958948000	-0.100421000
1	-3.689395000	1.688002000	2.179225000
1	-5.869761000	-2.504463000	0.740501000
29	-2.993386000	-0.737021000	-0.502777000
6	-1.479355000	-2.926927000	-1.798630000
6	-0.437454000	-3.350645000	-2.638205000
6	-2.669694000	-3.667378000	-1.694288000
6	-0.607942000	-4.527409000	-3.388081000
1	0.499516000	-2.776845000	-2.691075000
6	-2.823463000	-4.841937000	-2.447520000
1	-3.466929000	-3.327741000	-1.008763000
6	-1.794413000	-5.275487000	-3.302162000
1	0.208507000	-4.860314000	-4.047355000
1	-3.755542000	-5.421779000	-2.355563000
1	-1.913188000	-6.197491000	-3.889444000
8	-1.402565000	-1.738407000	-1.052277000
6	0.762124000	-2.823583000	0.499808000

	6	1.749170000	-3.835790000	0.374779000
	6	-0.317152000	-3.068777000	1.390636000
	6	1.645861000	-5.046002000	1.077607000
	1	2.610132000	-3.655977000	-0.289441000
	6	-0.408918000	-4.269650000	2.110550000
	1	-1.081611000	-2.286871000	1.535607000
	6	0.567165000	-5.269924000	1.951300000
	1	2.423156000	-5.815831000	0.951514000
	1	-1.249355000	-4.424753000	2.806558000
	1	0.493560000	-6.212693000	2.513749000
	6	-0.283073000	0.323815000	-1.580848000
	6	0.418526000	1.465224000	-1.112009000
	6	-1.160678000	0.494018000	-2.687709000
	6	0.276519000	2.709574000	-1.741506000
	1	1.076473000	1.359119000	-0.235132000
	6	-1.310158000	1.746907000	-3.306968000
	1	-1.707581000	-0.371619000	-3.093427000
	6	-0.589808000	2.859861000	-2.841195000
	1	0.841309000	3.577184000	-1.359640000
	1	-1.997738000	1.849559000	-4.162038000
	1	-0.716371000	3.844111000	-3.317029000
	1	4.158968000	-0.625073000	-2.309430000
	1	3.617527000	0.345794000	2.048324000
	1	6.928465000	-2.002813000	-0.676977000
	1	5.705727000	-4.398320000	5.354000000
	1	6.056410000	-5.538772000	4.050440000
	1	4.386096000	-5.074233000	4.389939000
	1	3.006123000	4.460933000	-5.572818000
	1	2.208025000	5.411909000	-4.316629000
	1	1.448858000	3.933063000	-4.923475000
	1	4.610745000	3.177632000	0.689119000
	6	5.856071000	-0.267292000	-3.580703000
	6	6.393198000	-1.547812000	-3.366517000
	6	6.670033000	0.744139000	-4.107610000
	1	5.765329000	-2.349338000	-2.978613000
	1	6.264678000	1.738936000	-4.289672000
	6	7.730075000	-1.808747000	-3.674059000
	6	8.009744000	0.478782000	-4.409466000
	1	8.138258000	-2.807570000	-3.512500000
	1	8.637931000	1.269006000	-4.819644000
	6	8.542661000	-0.794997000	-4.193742000
	1	9.584019000	-1.001048000	-4.436314000
	6	3.473121000	-0.572771000	-4.330303000
	6	3.892922000	-0.736504000	-5.656193000
	6	2.154101000	-0.898022000	-3.970712000
	1	4.916628000	-0.493317000	-5.944358000
	1	1.826942000	-0.772842000	-2.933399000
	6	2.999175000	-1.219558000	-6.617570000
	6	1.262465000	-1.364512000	-4.938409000
	1	3.332622000	-1.352724000	-7.646466000
	1	0.234353000	-1.599405000	-4.663491000
	6	1.683555000	-1.529201000	-6.262896000
	1	0.988321000	-1.898667000	-7.014410000
	6	3.433899000	4.925807000	0.405034000
	6	3.565707000	6.319757000	0.381546000
	6	2.252428000	4.352798000	0.908470000
	1	4.478614000	6.782124000	0.003028000
	1	2.139578000	3.270971000	0.929625000
	6	2.529465000	7.130750000	0.856513000
	6	1.221203000	5.166022000	1.382015000
	1	2.642400000	8.214870000	0.840092000
	1	0.312375000	4.715784000	1.782095000
	6	1.356503000	6.558410000	1.355625000
	1	0.554066000	7.192332000	1.729560000
	6	5.888128000	4.664139000	-0.175384000
	6	6.310343000	5.351813000	-1.321655000
	6	6.743773000	4.587640000	0.935876000
	1	5.661607000	5.423570000	-2.193667000
	1	6.429589000	4.056226000	1.835681000
	6	7.571808000	5.954132000	-1.355589000
	6	8.001792000	5.192976000	0.898512000
	1	7.892671000	6.487101000	-2.250224000
	1	8.658433000	5.132246000	1.765985000
	6	8.419994000	5.877235000	-0.247553000
	1	9.400930000	6.349272000	-0.275167000

	6	4.898467000	1.096037000	3.601941000
	6	6.120405000	0.843661000	4.239064000
	6	4.434718000	2.418397000	3.494532000
	1	6.490097000	-0.176869000	4.339527000
	1	3.478065000	2.627214000	3.018483000
	6	6.873226000	1.902735000	4.756862000
	6	5.186126000	3.471294000	4.020395000
	1	7.823383000	1.699286000	5.250358000
	1	4.815103000	4.493720000	3.943877000
	6	6.409605000	3.216612000	4.649782000
	1	6.993964000	4.038416000	5.060371000
	6	2.834880000	-0.290959000	3.927466000
	6	2.877357000	-0.087170000	5.312961000
	6	1.653154000	-0.752883000	3.325656000
	1	3.791640000	0.270580000	5.787651000
	1	1.619252000	-0.929008000	2.243586000
	6	1.742580000	-0.336659000	6.090612000
	6	0.523859000	-1.003481000	4.108324000
	1	1.778373000	-0.172287000	7.166861000
	1	-0.392241000	-1.361344000	3.638361000
	6	0.565441000	-0.793408000	5.491183000
	1	-0.317137000	-0.979363000	6.098967000
	6	7.401482000	-4.053270000	-0.405633000
	6	6.228117000	-4.585221000	-0.969870000
	6	8.571158000	-4.822638000	-0.400061000
	1	5.310036000	-4.001262000	-0.968501000
	1	9.492403000	-4.428825000	0.031174000
	6	6.231628000	-5.867181000	-1.521579000
	6	8.569975000	-6.106930000	-0.955642000
	1	5.320045000	-6.273862000	-1.957367000
	1	9.485659000	-6.697908000	-0.949217000
	6	7.403913000	-6.631850000	-1.517342000
	1	7.406061000	-7.630714000	-1.950208000
	6	8.727085000	-2.091855000	0.494581000
	6	9.407337000	-1.331426000	-0.470590000
	6	9.333441000	-2.328592000	1.736441000
	1	8.950816000	-1.144799000	-1.443976000
	1	8.824081000	-2.924376000	2.493212000
	6	10.674769000	-0.814294000	-0.193182000
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	1	11.066476000	-1.996062000	2.977468000
	6	11.274463000	-1.048651000	1.048519000
	1	12.263101000	-0.645973000	1.262880000
	6	-4.879036000	2.121004000	3.897357000
	6	-4.954020000	3.518699000	3.761122000
	6	-5.886988000	1.444178000	4.594977000
	1	-4.157581000	4.058995000	3.249098000
	1	-5.839154000	0.364553000	4.737353000
	6	-6.029540000	4.222442000	4.304977000
	6	-6.965412000	2.153995000	5.135238000
	1	-6.076535000	5.306584000	4.202376000
	1	-7.745044000	1.619302000	5.677946000
	6	-7.042138000	3.540872000	4.989918000
	1	-7.879983000	4.090932000	5.415552000
	6	-2.378791000	1.900251000	3.858762000
	6	-2.295808000	2.345705000	5.186437000
	6	-1.230852000	1.911027000	3.052249000
	1	-3.182531000	2.343930000	5.821798000
	1	-1.276967000	1.557349000	2.024551000
	6	-1.078499000	2.801896000	5.698804000
	6	-0.014890000	2.364882000	3.571374000
	1	-1.021412000	3.150326000	6.729819000
	1	0.877628000	2.358708000	2.947660000
	6	0.064637000	2.812270000	4.893627000
	1	1.014950000	3.160586000	5.296315000
	6	-5.392530000	-4.423830000	1.468178000
	6	-6.345478000	-5.447024000	1.363328000
	6	-4.040402000	-4.720193000	1.230526000
	1	-7.402567000	-5.238645000	1.533374000
	1	-3.281325000	-3.940386000	1.299830000
	6	-5.948835000	-6.748896000	1.042078000
	6	-3.648175000	-6.021544000	0.908528000
	1	-6.696873000	-7.538402000	0.969069000
	1	-2.594176000	-6.237687000	0.727368000



	6	-4.601106000	-7.040764000	0.815011000
	1	-4.294710000	-8.055743000	0.567144000
	6	-7.185135000	-2.890695000	2.409781000
	6	-8.217538000	-2.210543000	1.749049000
	6	-7.428268000	-3.463592000	3.667529000
	1	-8.048599000	-1.767051000	0.767405000
	1	-6.634612000	-4.003208000	4.183405000
	6	-9.479001000	-2.102281000	2.342239000
	6	-8.689655000	-3.351984000	4.256919000
	1	-10.277627000	-1.575112000	1.821180000
	1	-8.873840000	-3.800277000	5.233162000
	6	-9.717695000	-2.670330000	3.596665000
	1	-10.700880000	-2.586665000	4.057655000
	6	-3.936439000	4.689642000	-1.225148000
	6	-2.590684000	4.563543000	-0.846219000
	6	-4.385351000	5.897433000	-1.778996000
	1	-2.221646000	3.628217000	-0.428256000
	1	-5.429403000	6.014448000	-2.071719000
	6	-1.710615000	5.637040000	-1.008688000
	6	-3.500470000	6.966540000	-1.944561000
	1	-0.669531000	5.537138000	-0.699276000
	1	-3.858333000	7.903798000	-2.370492000
	6	-2.162749000	6.840562000	-1.558008000
	1	-1.477768000	7.678026000	-1.679646000
	6	-6.278033000	4.000443000	-0.651891000
	6	-7.272628000	4.148157000	-1.629515000
	6	-6.574099000	4.308185000	0.684780000
	1	-7.056470000	3.927804000	-2.674414000
	1	-5.807224000	4.211772000	1.452936000
	6	-8.549575000	4.589334000	-1.270147000
	6	-7.851744000	4.747520000	1.039572000
	1	-9.316807000	4.706364000	-2.035059000
	1	-8.072682000	4.982288000	2.080988000
	6	-8.843662000	4.887201000	0.063610000
	1	-9.838725000	5.232334000	0.340669000
	6	-7.698067000	-0.909188000	-2.474563000
	6	-8.466800000	0.241576000	-2.695416000
	6	-8.286483000	-2.026816000	-1.859761000
	1	-8.032948000	1.110033000	-3.190149000
	1	-7.707383000	-2.937500000	-1.709384000
	6	-9.805440000	0.278501000	-2.292233000
	6	-9.625468000	-1.986464000	-1.464378000
	1	-10.398380000	1.175844000	-2.467746000
	1	-10.078627000	-2.860141000	-0.995035000
	6	-10.387246000	-0.832138000	-1.675144000
	1	-11.431836000	-0.803366000	-1.368818000
	6	-6.103855000	-1.878813000	-4.138416000
	6	-7.116087000	-1.940622000	-5.107126000
	6	-4.936775000	-2.638894000	-4.309056000
	1	-8.028713000	-1.355726000	-4.986642000
	1	-4.137899000	-2.598000000	-3.569654000
	6	-6.964200000	-2.761172000	-6.228429000
	6	-4.789327000	-3.457553000	-5.431777000
	1	-7.757242000	-2.809933000	-6.974573000
	1	-3.881907000	-4.048774000	-5.553914000
	6	-5.802361000	-3.521356000	-6.393585000
	1	-5.688362000	-4.162320000	-7.266584000
	6	-4.500578000	2.613582000	-5.943326000
	1	-3.960056000	1.854530000	-6.528790000
	1	-5.422358000	2.843277000	-6.503065000
	1	-3.888106000	3.525708000	-5.955992000
	6	-2.667746000	-2.892458000	5.682391000
	1	-3.069529000	-3.898672000	5.868929000
	1	-1.595660000	-3.016275000	5.454243000
	1	-2.731357000	-2.346039000	6.635388000
	1	7.810469000	0.364554000	1.071595000
	1	7.112515000	2.306450000	-0.842976000

**Table S2.** Benchmark (absolute energies in a.u.) for all DFT optimized complexes.

(a) SCF energy

Species	Egas phase BP86/SVP	Egas phase BP86- D3/SVP	Esolv, M06/TZVP	Esolv, M06- 2X/TZVP	Esolv, M06L/TZVP	Esolv, B3LYP- D3/TZVP	Esolv, B3LYP, D3BJ/TZVP	Esolv, M06/cc- pVTZ
[(iPr)Cu(OPh)]	-1663.379	-1663.498	-1663.726	-1664.210	-1664.624	-1664.935	-1665.019	-1663.732
[(iPr)Au(PhCCPh)]	-1834.024	-1834.169	-1834.379	-1834.843	-1835.532	-1835.868	-1835.974	-1834.394
[(iPr)Au(PhCCPh)<-(OPh)Cu(iPr)] ts	-3497.408	-3497.705	-3498.109	-3499.052	-3500.159	-3500.815	-3501.006	-3498.127
[(iPr)Au(OPh)]	-1601.796	-1601.918	-1602.086	-1602.443	-1603.058	-1603.350	-1603.435	-1602.094
[(iPr)Au(PhCCPh)]	-1834.024	-1834.169	-1834.379	-1834.843	-1835.532	-1835.868	-1835.974	-1834.394
[(iPr)Au(PhCCPh)<-(OPh)Au(iPr)] ts	-3435.824	-3436.123	-3436.467	-3437.282	-3438.591	-3439.227	-3439.420	-3436.487
[(iPr)Au(OPh)]	-1601.796	-1601.918	-1602.086	-1602.443	-1603.058	-1603.350	-1603.435	-1602.094
[(iPr)Cu(PhCCPh)]	-1895.605	-1895.746	-1896.018	-1896.611	-1897.099	-1897.452	-1897.557	-1896.031
[(iPr)Cu(PhCCPh)<-(OPh)Au(iPr)] ts	-3497.397	-3497.705	-3498.100	-3499.046	-3500.151	-3500.806	-3500.997	-3498.118
[(iPr)Cu(OPh)]	-1663.379	-1663.498	-1663.726	-1664.210	-1664.624	-1664.935	-1665.019	-1663.732
[(iPr)Cu(PhCCPh)]	-1895.605	-1895.746	-1896.018	-1896.611	-1897.099	-1897.452	-1897.557	-1896.031
[(iPr)Cu(PhCCPh)<-(OPh)Cu(iPr)] ts	-3558.981	-3559.278	-3559.741	-3560.816	-3561.718	-3562.392	-3562.583	-3559.757
[(iPr)Ag(OPh)]	-1612.977	-1613.094	-1613.314	-1613.694	-1614.287	-1614.563	-1614.650	-1613.320
[(iPr)Ag(PhCCPh)]	-1845.210	-1845.346	-1845.607	-1846.098	-1846.760	-1847.082	-1847.189	-1845.619
[(iPr)Ag(PhCCPh)<-(OPh)Ag(iPr)] ts	-3458.192	-3458.479	-3458.921	-3459.786	-3461.048	-3461.651	-3461.847	-3458.937
[(iPr)Ag(OPh)]	-1612.977	-1613.094	-1613.314	-1613.694	-1614.287	-1614.563	-1614.650	-1613.320
[(iPr)Au(PhCCPh)]	-1834.024	-1834.169	-1834.379	-1834.843	-1835.532	-1835.868	-1835.974	-1834.394
[(iPr)Au(PhCCPh)<-(OPh)Ag(iPr)] ts	-3447.010	-3447.302	-3447.697	-3448.536	-3449.823	-3450.441	-3450.636	-3447.716

(b) Gibbs Energy

Species	Ggas phase BP86/SV P	Ggas phase BP86- D3/SV P	Gsolv, M06/TZV P	Gsolv, M06- 2X/TZV P	Esolv, M06L/TZV P	Esolv, B3LYP- D3/TZV P	Esolv, B3LYP- D3BJ/TZV P	Esolv, M06/cc -pVTZ
[(iPr)Cu(OPh)]	-1662.813	-1662.928	-1663.160	-1663.644	-1664.059	-1664.369	-1664.453	-1663.166
[(iPr)Au(PhCCPh)]	-1833.371	-1833.510	-1833.726	-1834.190	-1834.879	-1835.216	-1835.321	-1833.741
[(iPr)Au(PhCCPh)<-(OPh)Cu(iPr)] ts	-3496.161	-3496.454	-3496.862	-3497.805	-3498.912	-3499.568	-3499.759	-3496.881
[(iPr)Au(OPh)]	-1601.229	-1601.349	-1601.520	-1601.877	-1602.492	-1602.784	-1602.869	-1601.528
[(iPr)Au(PhCCPh)]	-1833.371	-1833.510	-1833.726	-1834.190	-1834.879	-1835.216	-1835.321	-1833.741
[(iPr)Au(PhCCPh)<-(OPh)Au(iPr)] ts	-3434.574	-3434.872	-3435.218	-3436.032	-3437.342	-3437.977	-3438.170	-3435.238
[(iPr)Au(OPh)]	-1601.229	-1601.349	-1601.520	-1601.877	-1602.492	-1602.784	-1602.869	-1601.528
[(iPr)Cu(PhCCPh)]	-1894.952	-1895.079	-1895.365	-1895.958	-1896.446	-1896.799	-1896.904	-1895.378
[(iPr)Cu(PhCCPh)<-(OPh)Au(iPr)] ts	-3496.149	-3496.454	-3496.852	-3497.797	-3498.902	-3499.557	-3499.749	-3496.869
[(iPr)Cu(OPh)]	-1662.813	-1662.928	-1663.160	-1663.644	-1664.059	-1664.369	-1664.453	-1663.166
[(iPr)Cu(PhCCPh)]	-1894.952	-1895.079	-1895.365	-1895.958	-1896.446	-1896.799	-1896.904	-1895.378
[(iPr)Cu(PhCCPh)<-(OPh)Cu(iPr)] ts	-3557.734	-3558.023	-3558.494	-3559.569	-3560.471	-3561.145	-3561.336	-3558.510
[(iPr)Ag(OPh)]	-1612.414	-1612.528	-1612.751	-1613.131	-1613.724	-1613.999	-1614.086	-1612.756

[(iPr)Ag(PhCCPh)]	-1844.561	-1844.688	-1844.958	-1845.448	-1846.111	-1846.432	-1846.539	-1844.970
[(iPr)Ag(PhCCPh)-(OPh)Ag(iPr)] ts	-3456.948	-3457.231	-3457.677	-3458.542	-3459.804	-3460.407	-3460.603	-3457.693
[(iPr)Ag(OPh)]	-1612.414	-1612.528	-1612.751	-1613.131	-1613.724	-1613.999	-1614.086	-1612.756
[(iPr)Au(PhCCPh)]	-1833.371	-1833.510	-1833.726	-1834.190	-1834.879	-1835.216	-1835.321	-1833.741
[(iPr)Au(PhCCPh)-(OPh)Ag(iPr)] ts	-3445.768	-3446.054	-3446.455	-3447.294	-3448.581	-3449.199	-3449.394	-3446.474

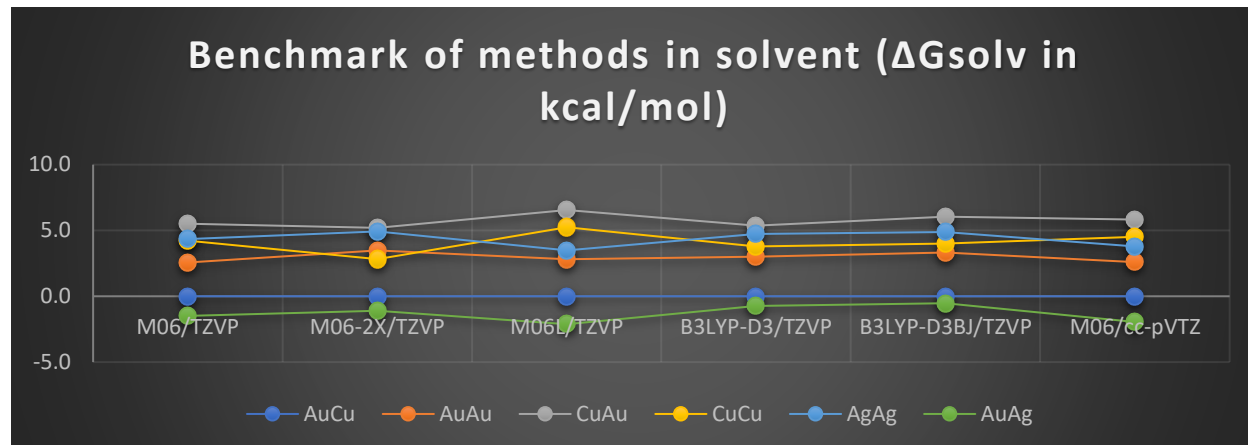
**Table S3.** Relative energies of the benchmark (absolute energies in a.u.) for all DFT optimized complexes.

(a) SCF

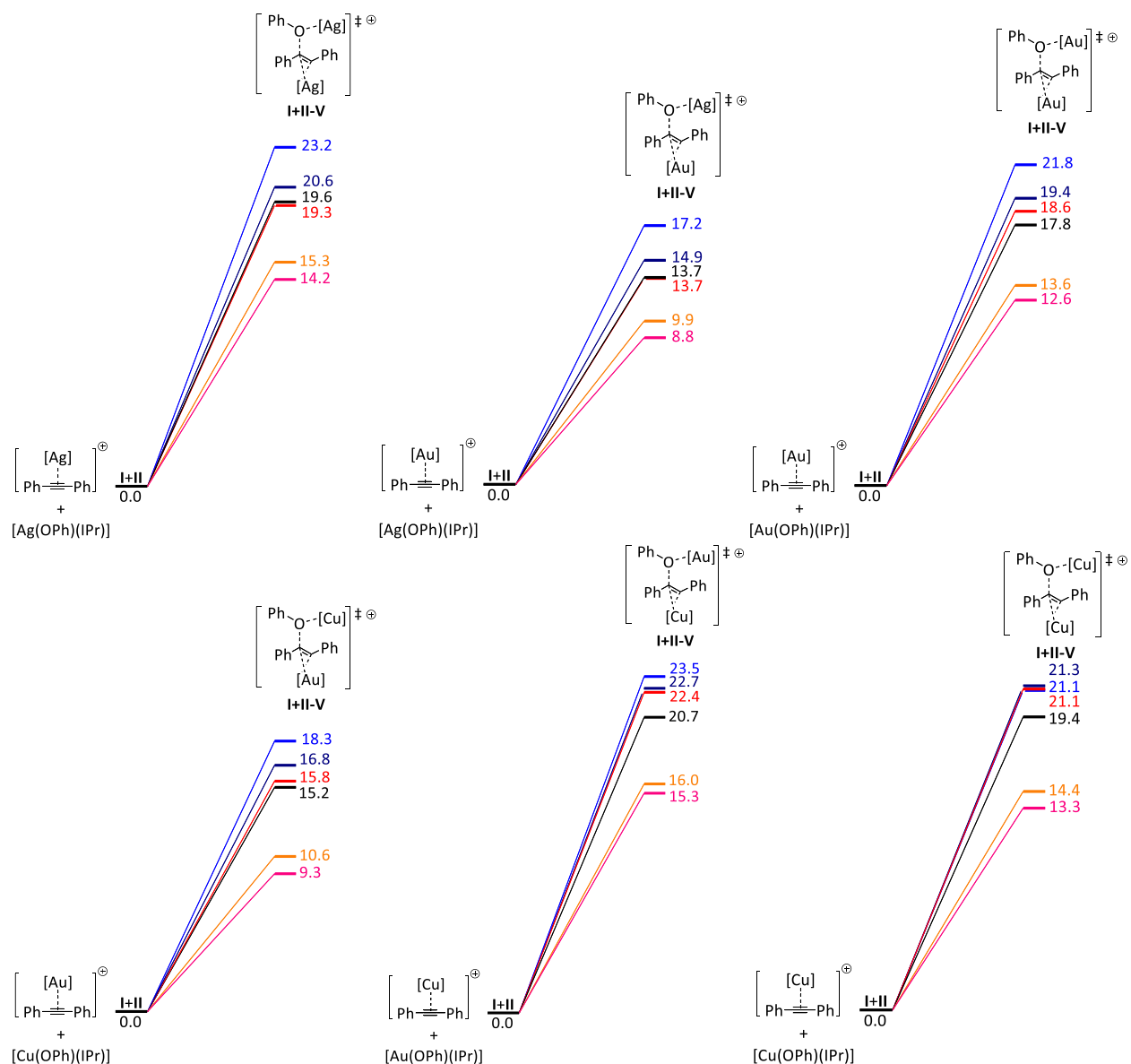
Species	$\Delta E_{\text{gas}}$	$\Delta E_{\text{gas}}$ BP86- BD3/svp	$\Delta E_{\text{solv}}$ , M06/TZVP	$\Delta E_{\text{solv}}$ , M06- 2x/TZVP	$\Delta E_{\text{solv}}$ , M06L/TZVP	$\Delta E_{\text{solv}}$ , B3LYP, GD3/TZVP	$\Delta E_{\text{solv}}$ , B3LYP, GD3BJ/TZVP	$\Delta E_{\text{solv}}$ , M06/cc- pVTZ
[(iPr)Au(PhCCPh)<-(OPh)Cu(iPr)] ts	-3.1	-23.6	-2.5	0.6	-1.9	-7.5	-8.4	-0.9
[(iPr)Au(PhCCPh)<-(OPh)Au(iPr)] ts	-2.5	-22.7	-1.3	2.5	-0.6	-5.6	-6.6	0.2
[(iPr)Cu(PhCCPh)<-(OPh)Au(iPr)] ts	2.5	-26.1	2.5	5.2	4.1	-2.3	-3.0	4.3
[(iPr)Cu(PhCCPh)<-(OPh)Cu(iPr)] ts	1.9	-21.4	1.9	3.3	3.1	-3.3	-4.4	3.6
[(iPr)Ag(PhCCPh)<-(OPh)Ag(iPr)] ts	-3.1	-24.6	0.0	3.6	-0.3	-4.2	-5.4	1.0
[(iPr)Au(PhCCPh)<-(OPh)Ag(iPr)] ts	-5.6	-24.0	-2.5	1.1	-2.4	-6.2	-7.3	-1.2

(b) Gibbs Energy

Species	$\Delta E_{\text{gas}}$	$\Delta E_{\text{gas}}$ BP86- BD3/svp	$\Delta E_{\text{solv}}$ , M06/TZVP	$\Delta E_{\text{solv}}$ , M06- 2x/TZVP	$\Delta E_{\text{solv}}$ , M06L/TZVP	$\Delta E_{\text{solv}}$ , B3LYP, GD3/TZVP	$\Delta E_{\text{solv}}$ , B3LYP, GD3BJ/TZVP	$\Delta E_{\text{solv}}$ , M06/cc- pVTZ
[(iPr)Au(PhCCPh)<-(OPh)Cu(iPr)] ts	15.0	15.2	18.3	15.8	10.6	9.3	16.8	15.0
[(iPr)Au(PhCCPh)<-(OPh)Au(iPr)] ts	0.2	16.6	17.8	21.8	18.6	13.6	12.6	19.4
[(iPr)Cu(PhCCPh)<-(OPh)Au(iPr)] ts	4.3	20.5	20.7	23.5	22.4	16.0	15.3	22.7
[(iPr)Cu(PhCCPh)<-(OPh)Cu(iPr)] ts	3.6	19.5	19.4	21.1	21.1	14.4	13.3	21.3
[(iPr)Ag(PhCCPh)<-(OPh)Ag(iPr)] ts	1.0	17.1	19.6	23.2	19.3	15.3	14.2	20.6
[(iPr)Au(PhCCPh)<-(OPh)Ag(iPr)] ts	-1.2	10.8	13.7	17.2	13.7	9.9	8.8	14.9

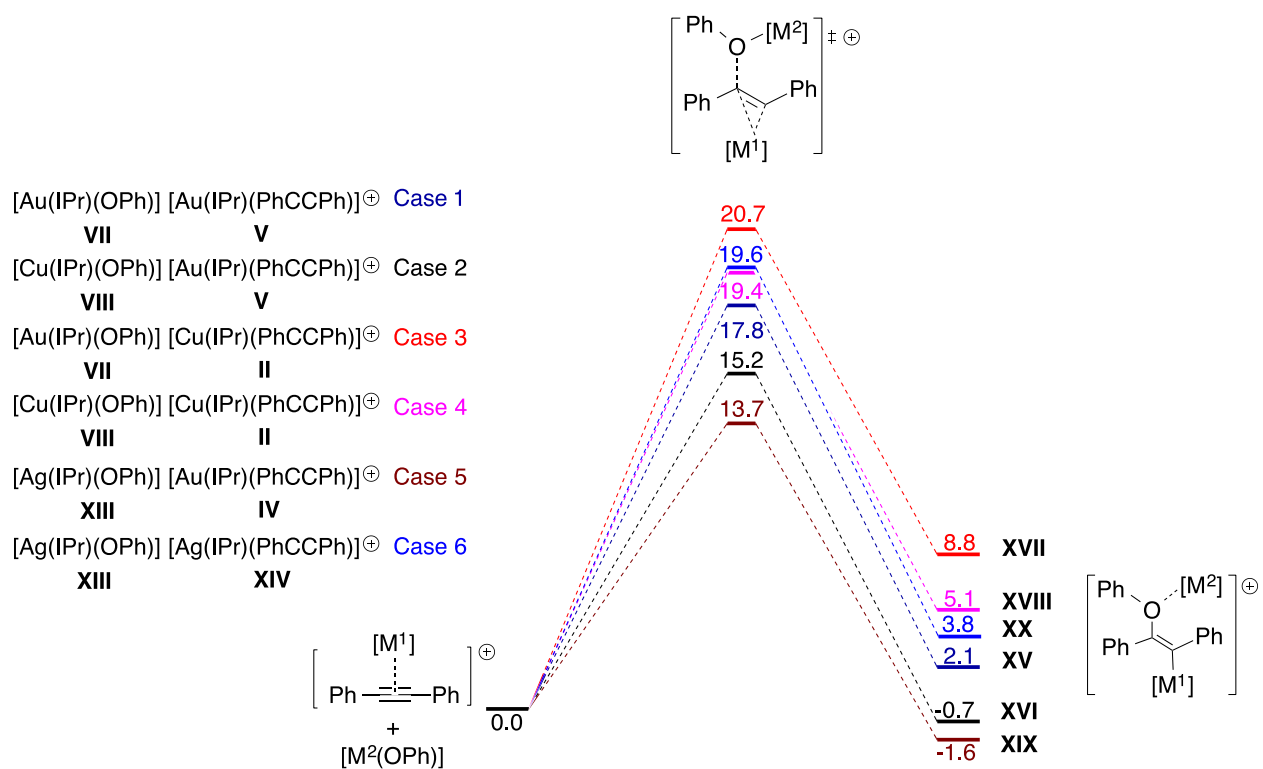


**Figure S1.** Relative energies of the benchmark (energies in kcal/mol).

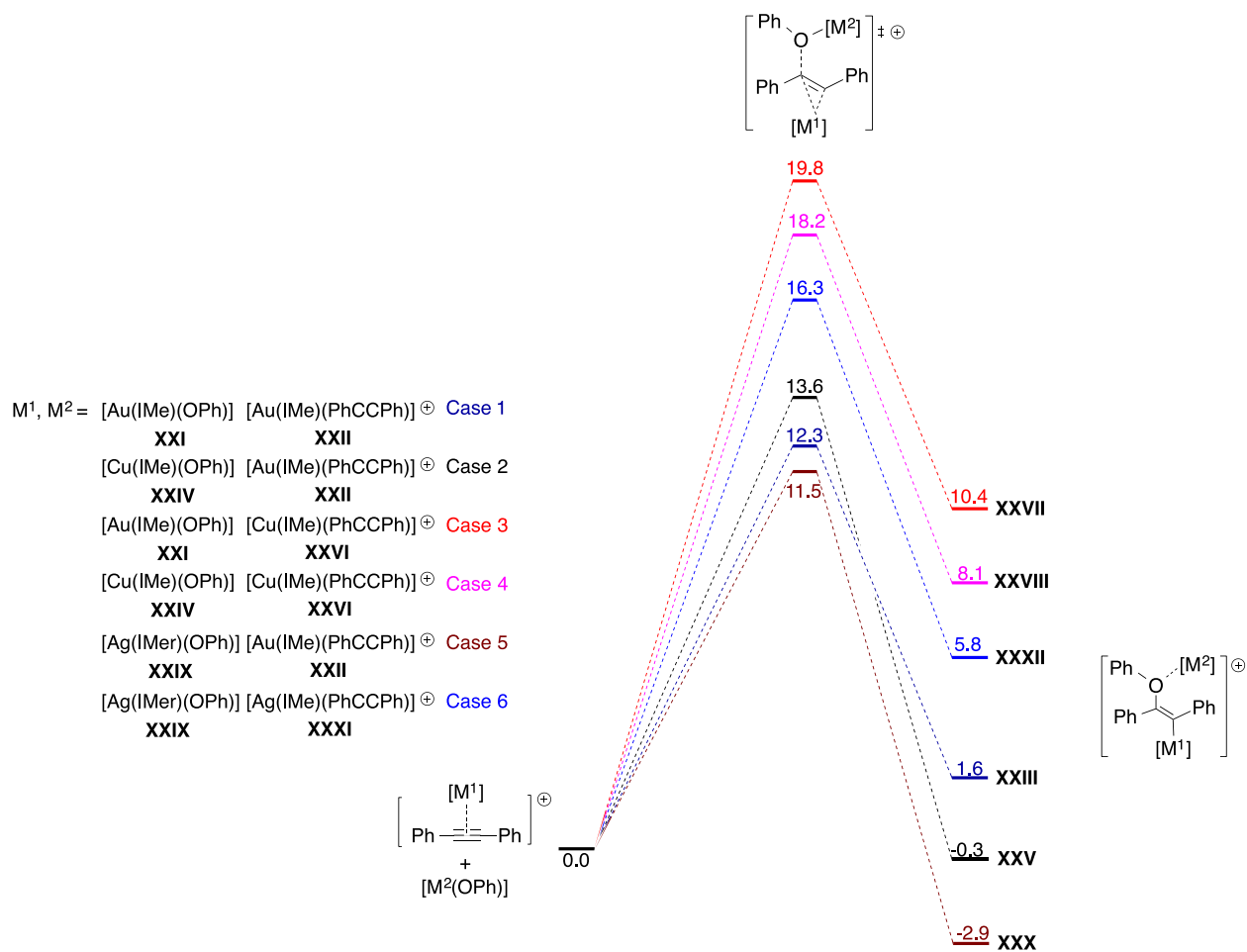


	AgAg	AuAg	AuAu	AuCu	CuAu	CuCu	M06/TZVP~sdd//BP86/SVP~sdd
M06/cc-pVTZ	20.6	14.9	19.4	16.8	22.7	21.3	M06-2X/TZVP~sdd//BP86/SVP~sdd
M06-2X/cc-pVTZ	23.2	17.2	21.8	18.3	23.5	21.1	M06L/TZVP~sdd//BP86/SVP~sdd
M06L/TZVP	19.6	13.7	18.6	15.8	22.4	21.1	B3LYP-GD3/TZVP~sdd//BP86/SVP~sdd
M06/TZVP	19.3	13.7	17.8	15.2	20.7	19.4	B3LYP-GD3bj/TZVP~sdd//BP86/SVP~sdd
B3LYP-D3	15.3	9.9	13.6	10.6	16.0	14.4	M06/cc-pVTZ~sdd//BP86/SVP~sdd
B3LYP-D3BJ	14.2	8.8	12.6	9.3	15.3	13.3	

Figure S2. C-O bond formation step with the different computational methods (in kcal/mol).

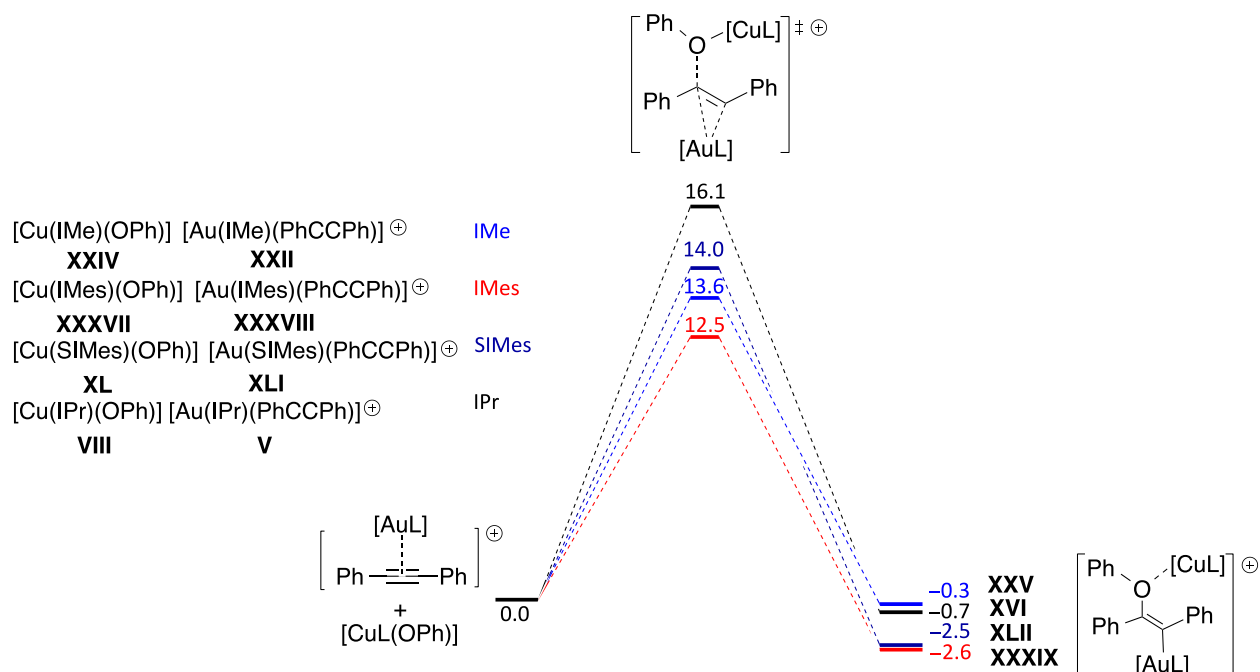


**Figure S3.** Influence of the metal-IPr catalyst in the rds (detailed labels for reactant and product catalysts; Gibbs free energies in solvent are given in kcal/mol).



**Figure S4.** Influence of the metal-IMe catalyst in the rds using IMe instead of IPr (detailed labels for reactant and product catalysts; Gibbs free energies in solvent are given in kcal/mol).





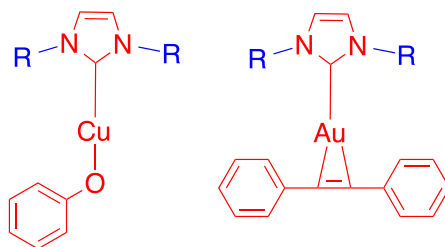
**Figure S5.** Rate determining step for the dual systems:  $[\text{Cu}(\text{IMes})(\text{OPh})][\text{Au}(\text{IMes})(\text{PhCChPh})]^{\oplus}$ ,  $[\text{Cu}(\text{SIMes})(\text{OPh})][\text{Au}(\text{SIMes})(\text{PhCChPh})]^{\oplus}$ ,  $[\text{Cu}(\text{IMes})(\text{OPh})][\text{Au}(\text{IMes})(\text{PhCChPh})]^{\oplus}$ , and comparing with our initial  $[\text{Cu}(\text{IPr})(\text{OPh})][\text{Au}(\text{IPr})(\text{PhCChPh})]^{\oplus}$ , (detailed labels for reactant and product catalysts; Gibbs free energies in solvent are given in kcal/mol).

## IPr\* (with QM/MM)

Method for optimization

— PM6

— BP86/SVP ~ SDD



Method for single-point calculation in solvent phase (SMD, phenol)

— PM6

— M06/TZVP ~ SDD

R= IPr or IPr\*  
Methodology ONIOM double-layer.

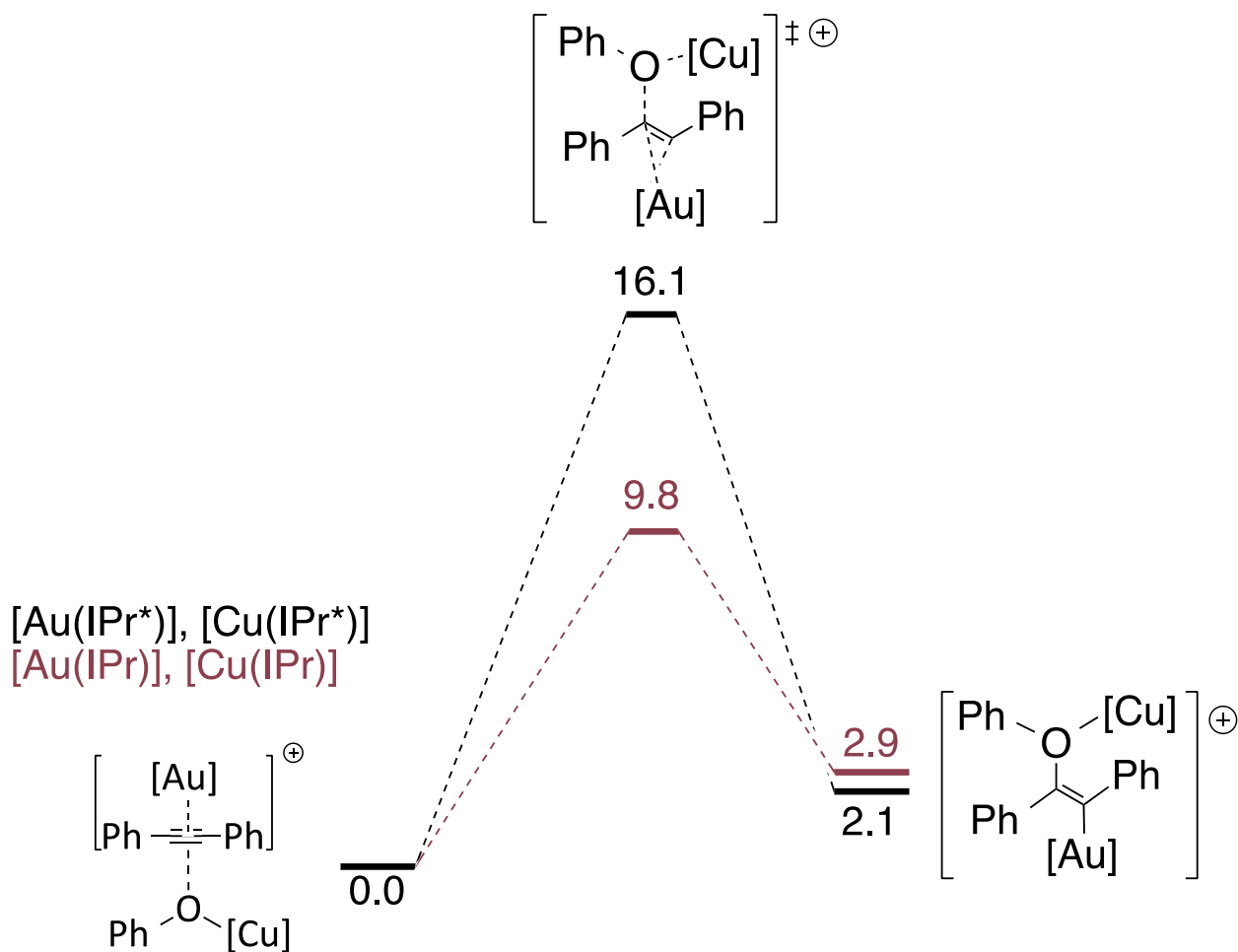


Figure S6. rds for IPr and IPr\* systems.