

Oxy-functionalization of Group 9 and 10 Transition Metal Methyl Ligands: Use of Pyridine-based Hemi-labile Ligands

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**Table S-1. B3LYP/CEP-31G(d) Optimized coordinates. Atomic number (Column 1). Cartesian coordinates (Columns 2 – 4) in Å.**

**Platinum – HLL Coordinates**

[(N-O)Pt <sup>II</sup> (Me)(THF)] <sup>+</sup>				[(N-O)Pt <sup>II</sup> (Me)(PyO)] <sup>+</sup>			
78	0.132237000	-0.230405000	-0.010619000	78	-0.158950000	-0.020226000	-0.307266000
6	0.512374000	-2.205373000	-0.355430000	6	0.417717000	-1.785776000	-1.154587000
1	-0.104951000	-2.574032000	-1.191464000	1	-0.314709000	-2.088226000	-1.921627000
1	1.573334000	-2.350221000	-0.618573000	1	1.396383000	-1.659469000	-1.645728000
1	0.295115000	-2.790233000	0.556353000	1	0.497558000	-2.580129000	-0.389836000
6	-1.813852000	2.052261000	-0.334150000	6	-2.429776000	1.906680000	0.161457000
1	-1.649481000	2.210712000	-1.418029000	1	-2.513698000	2.266938000	-0.882690000
1	-2.376677000	2.911719000	0.066836000	1	-3.012174000	2.579085000	0.813752000
8	-0.539138000	1.945419000	0.332571000	8	-1.043656000	1.914150000	0.560646000
6	0.311235000	3.096851000	0.098931000	6	-0.407180000	3.202572000	0.352407000
1	1.246975000	2.907763000	0.639079000	1	0.637855000	3.084126000	0.662565000
1	0.510518000	3.217326000	-0.980662000	1	-0.453169000	3.486947000	-0.713093000
1	-0.176780000	4.001747000	0.497487000	1	-0.907910000	3.963190000	0.974336000
7	-1.888685000	-0.403738000	-0.024689000	7	-2.103707000	-0.542195000	-0.010602000
6	-2.566175000	-1.572424000	0.139395000	6	-2.569014000	-1.819906000	0.028041000
6	-2.597445000	0.764284000	-0.113130000	6	-2.969222000	0.483907000	0.258353000

6	-3.972655000	-1.631745000	0.202765000	6	-3.912578000	-2.130969000	0.319033000
1	-1.962199000	-2.474343000	0.221633000	1	-1.842119000	-2.603552000	-0.180991000
6	-4.007425000	0.783528000	-0.041642000	6	-4.325308000	0.248173000	0.573727000
6	-4.712820000	-0.431876000	0.108106000	6	-4.813442000	-1.078034000	0.596541000
1	-4.460570000	-2.599211000	0.330651000	1	-4.229075000	-3.175123000	0.329765000
1	-4.535639000	1.737219000	-0.104269000	1	-4.980621000	1.093555000	0.793767000
1	-5.803901000	-0.438480000	0.160466000	1	-5.860441000	-1.281079000	0.832875000
8	2.200635000	0.149000000	0.068887000	8	1.725653000	0.778740000	-0.597581000
6	3.043667000	0.145660000	-1.158695000	7	2.838678000	0.199507000	-0.070014000
6	2.998957000	-0.298232000	1.235862000	6	2.794186000	-0.579230000	1.050886000
6	4.418045000	-0.388747000	-0.702381000	6	4.019172000	0.481718000	-0.696846000
1	3.084218000	1.189021000	-1.507391000	6	3.981184000	-1.113373000	1.590716000
6	4.451633000	-0.033463000	0.807381000	1	1.797646000	-0.738936000	1.464336000
1	2.651858000	0.287959000	2.097414000	6	5.231596000	-0.023743000	-0.192470000
1	4.475421000	-1.479605000	-0.842723000	1	3.929650000	1.109415000	-1.584143000
1	4.714480000	1.025471000	0.959732000	6	5.220635000	-0.836561000	0.967607000
1	2.798873000	-1.367723000	1.404965000	1	3.915574000	-1.732787000	2.486551000
1	5.237987000	0.077428000	-1.267759000	1	6.158264000	0.218535000	-0.714951000
1	2.543279000	-0.478159000	-1.910306000	1	6.150537000	-1.241900000	1.372472000
1	5.159251000	-0.656270000	1.373946000				
<b><sup>+</sup>OAT<sup>#</sup> Pt</b>							
	78	0.284822000	-0.459993000	0.083526000			
	6	0.408001000	-0.433539000	2.156277000			
	1	0.340890000	0.621196000	2.458346000			
	1	-0.448099000	-1.017684000	2.511059000			
	1	1.365745000	-0.887439000	2.441260000			
	6	2.095308000	2.152352000	0.014578000			
	1	2.141060000	2.493376000	1.066828000			
	1	2.381219000	2.991176000	-0.641688000			
	8	0.754377000	1.725286000	-0.300670000			
	6	-0.289412000	2.699057000	0.010760000			
	1	-1.244018000	2.204432000	-0.212512000			
	1	-0.237406000	2.980369000	1.076142000			
	1	-0.146665000	3.583474000	-0.630271000			
	7	2.410016000	-0.270442000	-0.137809000			
	6	3.164856000	-1.393008000	-0.273970000			
	6	3.006690000	0.952095000	-0.196824000			
	6	4.558444000	-1.339666000	-0.476941000			
	1	2.629620000	-2.343112000	-0.220592000			
	6	4.396529000	1.090232000	-0.409986000			
	6	5.186923000	-0.073640000	-0.547451000			
	1	5.122945000	-2.267478000	-0.580531000			
	1	4.842144000	2.085907000	-0.465530000			
	1	6.264117000	0.006223000	-0.711156000			
	8	-1.170444000	-1.481359000	0.140029000			
	7	-3.196582000	0.249473000	-0.180855000			
	6	-3.772135000	-0.137360000	-1.340747000			
	6	-4.007746000	0.460281000	0.879157000			
	6	-5.169564000	-0.307816000	-1.505766000			
	1	-3.092758000	-0.326194000	-2.180223000			
	6	-5.417154000	0.319883000	0.832067000			
	1	-3.518339000	0.755175000	1.815800000			
	6	-6.010216000	-0.072101000	-0.392068000			
	1	-5.573439000	-0.618692000	-2.471848000			
	1	-6.017931000	0.510032000	1.724360000			
	1	-7.093878000	-0.196544000	-0.473234000			

<b>[N~O)Pt<sup>IV</sup>(O)(Me)]<sup>+</sup></b>				<b>[(N~O)Pt<sup>IV</sup>(Py)(O)(Me)]<sup>+</sup></b>			
78	-0.929005000	-0.364143000	-0.154538000	78	0.088312000	-0.276279000	0.039652000
6	-1.214601000	-0.289150000	1.910276000	8	0.214768000	-2.103123000	-0.215240000

1	-1.445061000	0.755770000	2.158104000	6	0.083159000	0.441834000	2.002686000
1	-2.058863000	-0.957248000	2.110911000	1	0.261099000	1.529089000	1.998596000
1	-0.285304000	-0.640156000	2.376451000	1	-0.890222000	0.205751000	2.452777000
6	0.996659000	2.107642000	0.182073000	1	0.887068000	-0.083016000	2.534033000
1	0.889011000	2.405564000	1.242375000	6	-1.996769000	2.085386000	-0.084648000
1	1.429504000	2.949376000	-0.382582000	1	-2.523846000	2.805698000	-0.732728000
8	-0.301042000	1.777996000	-0.366054000	1	-1.990200000	2.488721000	0.946759000
6	-1.293824000	2.843917000	-0.224248000	8	-0.644341000	1.918047000	-0.549957000
1	-2.200584000	2.494086000	-0.731462000	6	0.071312000	3.172636000	-0.662829000
1	-1.492850000	3.038714000	0.842272000	1	1.038516000	2.943610000	-1.128028000
1	-0.907260000	3.748292000	-0.719071000	1	-0.492871000	3.861037000	-1.313768000
7	1.182973000	-0.319701000	-0.038656000	1	0.216620000	3.634502000	0.330561000
6	1.868655000	-1.492940000	-0.106366000	7	-1.986852000	-0.397892000	-0.032528000
6	1.855950000	0.860671000	0.061688000	6	-2.596791000	-1.612909000	-0.011067000
6	3.276714000	-1.530349000	-0.077294000	6	-2.723541000	0.742917000	-0.117309000
1	1.270117000	-2.402144000	-0.187664000	6	-3.999408000	-1.732606000	-0.080186000
6	3.267310000	0.902560000	0.085074000	1	-1.912610000	-2.463369000	0.041589000
6	3.989418000	-0.311313000	0.018987000	6	-4.132461000	0.695394000	-0.209035000
1	3.788495000	-2.492089000	-0.134338000	6	-4.782747000	-0.559857000	-0.181186000
1	3.781119000	1.863867000	0.153738000	1	-4.452834000	-2.724750000	-0.061658000
1	5.081700000	-0.304713000	0.036711000	1	-4.700793000	1.623652000	-0.299830000
8	-2.217229000	-1.573557000	-0.326700000	1	-5.871935000	-0.618273000	-0.245207000
				7	2.185451000	-0.204671000	-0.038579000
				6	2.869550000	0.914605000	0.323958000
				6	2.878002000	-1.289910000	-0.480459000
				6	4.273657000	1.003684000	0.248359000
				6	4.286613000	-1.280181000	-0.585594000
				6	5.001069000	-0.117324000	-0.219625000
				1	2.278426000	1.753568000	0.692504000
				1	2.262620000	-2.157175000	-0.725200000
				1	4.771424000	1.925489000	0.554145000
				1	4.796510000	-2.174595000	-0.947360000
				1	6.091240000	-0.083636000	-0.292098000
<b>+Methyl Migration<sup>‡</sup> Pt</b>				<b>Py</b>			
78	0.067973000	-0.193896000	-0.015536000	6	-1.150745000	-0.733908000	-0.000217000
8	0.245671000	-2.109723000	0.031291000	6	-1.215583000	0.684354000	-0.000119000
6	0.235569000	-1.215388000	1.984754000	6	0.000315000	1.408768000	0.000056000
1	0.202907000	-0.245098000	2.510537000	6	1.215891000	0.683825000	0.000207000
1	-0.632558000	-1.839961000	2.195928000	6	1.150417000	-0.734406000	0.000149000
1	1.186937000	-1.733105000	2.100663000	7	-0.000322000	-1.441058000	-0.000092000
6	-1.923316000	2.128059000	0.184970000	1	0.000524000	2.503340000	0.000213000
1	-2.429976000	2.964342000	-0.324027000	1	-2.075339000	-1.325386000	-0.000367000
1	-1.849452000	2.361910000	1.265013000	1	-2.183366000	1.192478000	-0.000224000
8	-0.589982000	1.970732000	-0.356734000	1	2.183921000	1.191480000	0.000365000
6	0.200675000	3.184230000	-0.265997000	1	2.074742000	-1.326301000	0.000202000
1	1.154141000	2.977889000	-0.767391000				
1	-0.323460000	4.000275000	-0.789735000				
1	0.367876000	3.459150000	0.790695000				
7	-1.986171000	-0.324227000	-0.054434000				
6	-2.616245000	-1.519789000	-0.193227000				
6	-2.702154000	0.834221000	-0.022427000				
6	-4.020458000	-1.601601000	-0.296958000				
1	-1.943878000	-2.381716000	-0.220378000				
6	-4.108852000	0.829203000	-0.138074000				
6	-4.780381000	-0.409520000	-0.269964000				
1	-4.493790000	-2.578686000	-0.405373000				
1	-4.660223000	1.771792000	-0.123752000				
1	-5.868985000	-0.438799000	-0.358815000				
7	2.127696000	-0.097621000	-0.105114000				
6	2.843050000	0.832965000	0.584340000				
6	2.788277000	-1.022114000	-0.857224000				
6	4.249356000	0.898152000	0.530159000				

6	4.196781000	-1.019121000	-0.968922000				
6	4.942642000	-0.044710000	-0.268223000				
1	2.268812000	1.525736000	1.202418000				
1	2.161633000	-1.767644000	-1.344365000				
1	4.776385000	1.661265000	1.105502000				
1	4.682393000	-1.773948000	-1.589594000				
1	6.033474000	-0.022158000	-0.334339000				
<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000
6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000
1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl Migration – Four Coordinate -Pt</b>				<b>Pt<sup>II</sup>-Methoxide</b>			
78	-0.852751000	-0.269905000	-0.193279000	78	0.031315000	-0.117444000	-0.045719000
6	-2.341521000	-0.763531000	1.590605000	6	-1.928340000	2.182682000	-0.202412000
1	-3.399921000	-0.745983000	1.329783000	1	-1.936870000	2.473908000	-1.269784000
1	-1.988440000	-1.690060000	2.043030000	1	-2.369407000	2.998313000	0.393157000
1	-1.998934000	0.149237000	2.099040000	8	-0.548037000	1.989556000	0.214891000
6	1.074141000	2.056805000	0.369891000	6	0.296794000	3.103602000	-0.199652000
1	0.869945000	2.252096000	1.439838000	1	1.293495000	2.919855000	0.216224000
1	1.570642000	2.935922000	-0.070683000	1	0.344292000	3.155295000	-1.300149000
8	-0.176306000	1.812340000	-0.323863000	1	-0.115794000	4.037325000	0.214294000
6	-1.151942000	2.892342000	-0.181100000	7	-2.008808000	-0.273399000	-0.072426000
1	-2.009840000	2.618362000	-0.806253000	6	-2.661554000	-1.463980000	-0.042456000
1	-1.450937000	2.995502000	0.875167000	6	-2.715022000	0.890453000	-0.029448000
1	-0.696294000	3.824135000	-0.550114000	6	-4.067057000	-1.536513000	0.047646000
7	1.201115000	-0.346254000	-0.006751000	1	-2.020163000	-2.344291000	-0.110337000
6	1.849085000	-1.535902000	-0.135135000	6	-4.122149000	0.898980000	0.083999000
6	1.908756000	0.800420000	0.203062000	6	-4.810926000	-0.336026000	0.122352000
6	3.252795000	-1.623352000	-0.049957000	1	-4.554233000	-2.512589000	0.064387000
1	1.224574000	-2.413007000	-0.310977000	1	-4.660275000	1.848211000	0.131682000
6	3.317273000	0.790125000	0.287406000	1	-5.899933000	-0.357638000	0.207192000
6	4.001023000	-0.441848000	0.164969000	7	2.087697000	0.031192000	-0.009778000
1	3.734146000	-2.596436000	-0.157295000	6	2.800991000	-0.557822000	-1.008673000
1	3.858184000	1.725645000	0.444728000	6	2.754272000	0.648832000	1.004575000
1	5.091000000	-0.476554000	0.228380000	6	4.212632000	-0.527746000	-1.039322000
8	-2.093067000	-1.581446000	-0.293647000	1	2.216735000	-1.070313000	-1.773014000
				6	4.161937000	0.717704000	1.051811000
				1	2.137896000	1.077073000	1.797951000
				6	4.908344000	0.121152000	0.006644000
				1	4.739758000	-1.010157000	-1.864217000
				1	4.648463000	1.217875000	1.891052000
				1	6.000806000	0.156045000	0.012565000
				8	0.270831000	-2.057474000	-0.361709000
				6	0.676085000	-2.816098000	0.782838000
				1	0.790457000	-3.861429000	0.440860000
				1	1.647087000	-2.481969000	1.198139000
				1	-0.075516000	-2.797381000	1.598667000
<b>Pt<sup>II</sup>-Methoxide- Four Coordinate</b>							
	78	-0.866483000	0.030400000	-0.132948000			
	6	1.375347000	1.924448000	0.493978000			
	1	1.201304000	2.075311000	1.575637000			

## Nickel – HLL Coordinates

[(N~O)Ni <sup>II</sup> (Me)(THF)] <sup>+</sup>				[(N~O)Ni <sup>II</sup> (Me)(PyO)] <sup>+</sup>			
6	1.121101000	-2.536564000	0.071290000	6	0.416105000	-1.626350000	-0.997065000
1	1.064613000	-3.046497000	-0.909943000	1	-0.279030000	-1.970684000	-1.781685000
1	2.184277000	-2.399731000	0.326850000	1	1.405723000	-1.486332000	-1.462419000
1	0.668133000	-3.184972000	0.842523000	1	0.497357000	-2.406711000	-0.215630000
6	-2.690382000	-0.952854000	0.311213000	6	-2.428947000	1.867618000	0.021441000
1	-2.851843000	-1.178375000	1.382286000	1	-2.540966000	2.291258000	-0.996266000
1	-3.604596000	-1.214886000	-0.246704000	1	-2.977650000	2.511653000	0.730282000
8	-1.588431000	-1.756373000	-0.184147000	8	-1.035443000	1.818685000	0.374334000
6	-1.897410000	-3.182750000	-0.149989000	6	-0.395008000	3.120338000	0.306092000
1	-1.100216000	-3.701131000	-0.689036000	1	0.650533000	2.967655000	0.592559000
1	-1.949748000	-3.533381000	0.893728000	1	-0.451524000	3.518600000	-0.721989000
1	-2.861328000	-3.339402000	-0.659096000	1	-0.895411000	3.806039000	1.010038000
7	-1.012703000	0.772613000	-0.037975000	7	-2.049319000	-0.551741000	-0.110059000
6	-0.619361000	2.060437000	-0.195833000	6	-2.491151000	-1.837257000	-0.085313000
6	-2.334157000	0.512006000	0.113441000	6	-2.963952000	0.444829000	0.064469000
6	-1.527057000	3.140437000	-0.202093000	6	-3.846383000	-2.180208000	0.095560000
1	0.453748000	2.217232000	-0.319261000	1	-1.735457000	-2.610221000	-0.213491000
6	-3.320936000	1.524971000	0.112542000	6	-4.340709000	0.190485000	0.257185000
6	-2.907007000	2.867125000	-0.043452000	6	-4.796038000	-1.146381000	0.264856000
1	-1.159129000	4.159522000	-0.332516000	1	-4.136946000	-3.231917000	0.104260000
1	-4.376272000	1.267581000	0.228477000	1	-5.031221000	1.024819000	0.399234000
1	-3.641510000	3.676015000	-0.048725000	1	-5.854934000	-1.373181000	0.409433000

1	2.018582000	2.731891000	0.110388000
8	0.102175000	1.949741000	-0.205995000
6	-0.681924000	3.160671000	0.049108000
1	-1.575328000	3.085680000	-0.582395000
1	-0.955861000	3.214616000	1.115117000
1	-0.080326000	4.033183000	-0.248868000
7	1.087227000	-0.441606000	-0.023436000
6	1.519928000	-1.710496000	-0.257483000
6	1.981545000	0.557607000	0.232470000
6	2.890458000	-2.035206000	-0.223813000
1	0.751572000	-2.452688000	-0.476389000
6	3.368702000	0.303916000	0.269592000
6	3.831438000	-1.013710000	0.046530000
1	3.198664000	-3.064369000	-0.413484000
1	4.063056000	1.123042000	0.467903000
1	4.900914000	-1.234463000	0.073010000
8	-2.131681000	-1.373684000	-0.227573000
6	-2.519916000	-2.202259000	0.881381000
1	-1.826834000	-3.061960000	0.955827000
1	-2.554864000	-1.655448000	1.837561000
1	-3.523193000	-2.592996000	0.637639000

8	1.754839000	0.172486000	-0.007414000	8	1.462316000	0.863571000	-0.254942000
6	2.537113000	0.323305000	1.233903000	7	2.640513000	0.239483000	-0.021212000
6	2.731970000	0.074046000	-1.109016000	6	2.790123000	-0.604710000	1.041418000
6	3.717408000	1.242272000	0.833423000	6	3.683578000	0.531935000	-0.850730000
1	2.870480000	-0.674442000	1.559990000	6	4.038878000	-1.196998000	1.309267000
6	3.849296000	1.073827000	-0.720424000	1	1.891410000	-0.768197000	1.635854000
1	3.093873000	-0.963989000	-1.162063000	6	4.955597000	-0.027841000	-0.622079000
1	3.500940000	2.288695000	1.093453000	1	3.445155000	1.213839000	-1.667651000
1	4.834093000	0.681925000	-1.012811000	6	5.142531000	-0.907525000	0.470982000
1	2.192001000	0.324343000	-2.031957000	1	4.129389000	-1.867712000	2.165111000
1	4.633885000	0.944700000	1.362899000	1	5.771231000	0.225972000	-1.300840000
1	1.858657000	0.749199000	1.985329000	1	6.120018000	-1.354993000	0.664182000
1	3.704199000	2.037866000	-1.229283000	28	-0.219599000	0.016795000	-0.251562000
28	0.152855000	-0.883036000	-0.027352000				

**+OAT<sup>‡</sup> - Ni**

	6	-0.186434000	-0.550987000	2.577419000
	1	0.820266000	-0.517949000	3.022316000
	1	-0.924412000	-0.062632000	3.223619000
	1	-0.485873000	-1.583964000	2.335127000
	6	2.133202000	1.665038000	-0.674817000
	1	2.649153000	2.231422000	0.126144000
	1	2.512115000	2.023480000	-1.647917000
	8	0.715883000	1.872118000	-0.576443000
	6	0.352377000	3.278223000	-0.488380000
	1	-0.730965000	3.307220000	-0.326387000
	1	0.865220000	3.749406000	0.367607000
	1	0.628697000	3.786483000	-1.427548000
	7	1.536880000	-0.536353000	0.258178000
	6	1.775467000	-1.860449000	0.447442000
	6	2.407567000	0.175036000	-0.513396000
	6	2.884552000	-2.530205000	-0.108185000
	1	1.056367000	-2.397851000	1.066219000
	6	3.541216000	-0.419079000	-1.114853000
	6	3.791647000	-1.793199000	-0.904484000
	1	3.023261000	-3.595488000	0.082606000
	1	4.208716000	0.188811000	-1.729462000
	1	4.662997000	-2.274818000	-1.354526000
	8	-1.419056000	1.404332000	1.233882000
	7	-1.877487000	-0.062258000	0.008522000
	6	-1.914955000	0.150146000	-1.331229000
	6	-2.832050000	-0.810049000	0.616497000
	6	-2.915190000	-0.436211000	-2.138638000
	1	-1.134361000	0.790103000	-1.743869000
	6	-3.858270000	-1.430321000	-0.124843000
	1	-2.774643000	-0.879965000	1.702160000
	6	-3.903639000	-1.242443000	-1.528219000
	1	-2.907233000	-0.250745000	-3.214276000
	1	-4.606106000	-2.028249000	0.399006000
	1	-4.695268000	-1.701027000	-2.125926000
	28	-0.064687000	0.429337000	0.922600000

<b>[N~O)Ni<sup>IV</sup>(O)(Me)]<sup>+</sup></b>			<b>[(N~O)Ni<sup>IV</sup>(Py)(O)(Me)]<sup>+</sup></b>				
6	-1.683540000	-1.016657000	1.581394000	8	0.169534000	-2.020764000	-0.297664000
1	-1.197028000	-0.189639000	2.119228000	6	0.147526000	-0.555308000	2.037046000
1	-2.777460000	-0.969718000	1.582295000	1	0.896799000	-1.319939000	2.259495000
1	-1.301856000	-2.004661000	1.852410000	1	0.448216000	0.450698000	2.363582000
6	0.107910000	1.996530000	0.100210000	1	-0.855882000	-0.843045000	2.367927000
1	-0.003989000	2.382428000	1.130729000	6	-1.563574000	1.962551000	0.491006000
1	0.316986000	2.842328000	-0.575680000	1	-1.962200000	2.920800000	0.124545000
8	-1.119338000	1.345620000	-0.309369000	1	-1.430276000	2.035941000	1.581891000



28	0.092567000	-0.367476000	0.054813000
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<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000
6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000
1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl Migration – Four-Coordinate -Ni</b>				<b>Ni<sup>II</sup>-Methoxide</b>			
6	-1.915913000	-1.449621000	1.390044000	6	2.879252000	1.001364000	0.241130000
1	-1.327092000	-2.348423000	1.584032000	1	3.124755000	1.237475000	1.294943000
1	-1.653699000	-0.588758000	2.025549000	1	3.742274000	1.278697000	-0.388752000
1	-2.988354000	-1.633225000	1.310353000	8	1.720426000	1.745926000	-0.165630000
6	0.231859000	2.037524000	-0.009955000	6	1.891569000	3.193179000	-0.057026000
1	0.396214000	2.776409000	0.791634000	1	0.923444000	3.625614000	-0.325052000
1	0.255998000	2.555195000	-0.986678000	1	2.159751000	3.454455000	0.980185000
8	-1.064458000	1.410801000	0.173630000	1	2.685930000	3.498704000	-0.757060000
6	-2.201132000	2.293396000	-0.098880000	7	1.230750000	-0.783951000	-0.024173000
1	-3.105338000	1.716071000	0.130780000	6	0.885872000	-2.093804000	-0.146951000
1	-2.133170000	3.171233000	0.561922000	6	2.551358000	-0.474970000	0.088644000
1	-2.194464000	2.596822000	-1.158146000	6	1.830502000	-3.138891000	-0.152132000
7	0.776891000	-0.335545000	-0.123147000	1	-0.177635000	-2.309617000	-0.248237000
6	1.620709000	-1.402352000	-0.152132000	6	3.568274000	-1.457588000	0.084402000
6	1.269044000	0.924304000	0.028222000	6	3.203416000	-2.816227000	-0.031923000
6	3.015018000	-1.241911000	-0.026827000	1	1.492213000	-4.171313000	-0.253383000
1	1.159276000	-2.382249000	-0.284342000	1	4.615083000	-1.157053000	0.168836000
6	2.652838000	1.165039000	0.172982000	1	3.966155000	-3.598393000	-0.037077000
6	3.538740000	0.063058000	0.141593000	7	-1.597824000	-0.237109000	0.005182000
1	3.662591000	-2.119248000	-0.059895000	6	-2.279123000	-0.479155000	-1.146120000
1	3.021080000	2.185089000	0.302582000	6	-2.114990000	-0.675663000	1.182881000
1	4.614740000	0.219670000	0.247965000	6	-3.500325000	-1.187739000	-1.165920000
8	-1.854627000	-1.869677000	-0.759654000	1	-1.836290000	-0.085158000	-2.063277000
28	-1.109297000	-0.516621000	-0.270922000	6	-3.331840000	-1.388549000	1.255209000
				1	-1.541133000	-0.443483000	2.082791000
				6	-4.037553000	-1.652628000	0.057638000
				1	-4.009178000	-1.357268000	-2.116444000
				1	-3.706893000	-1.717563000	2.225923000
				1	-4.983249000	-2.200333000	0.078031000
				8	-0.814371000	2.346803000	-0.093097000
				6	-2.179226000	2.634690000	0.152313000
				1	-2.529399000	2.275755000	1.142633000
				1	-2.289158000	3.735754000	0.144461000
				1	-2.858707000	2.231819000	-0.627427000
				28	0.012143000	0.761549000	-0.045400000
<b>Ni<sup>II</sup>-Methoxide - Four Coordinate</b>							
	6	0.606087000	2.075312000	0.278563000			
	1	0.564120000	2.384500000	1.339207000			
	1	1.034734000	2.895976000	-0.319404000			
	8	-0.739572000	1.793900000	-0.191806000			
	6	-1.704447000	2.863066000	0.071422000			
	1	-2.651048000	2.550068000	-0.387799000			
	1	-1.824329000	3.001972000	1.158076000			

## Palladium – HLL Coordinates

[(N~O)Pd <sup>II</sup> (Me)(THF)] <sup>+</sup>				[(N~O)Pd <sup>II</sup> (Me)(PyO)] <sup>+</sup>			
6	0.501924000	-2.256163000	-0.337368000	6	0.403976000	-1.786633000	-1.124437000
1	-0.116476000	-2.594766000	-1.184050000	1	-0.312357000	-2.068775000	-1.912868000
1	1.567423000	-2.408563000	-0.569389000	1	1.405494000	-1.668682000	-1.566274000
1	0.238417000	-2.796708000	0.588050000	1	0.424608000	-2.551266000	-0.327683000
6	-1.787360000	2.004993000	-0.321778000	6	-2.490201000	1.886487000	0.091757000
1	-1.666375000	2.184343000	-1.409068000	1	-2.587992000	2.256586000	-0.948709000
1	-2.327502000	2.862960000	0.113787000	1	-3.073698000	2.550705000	0.752506000
8	-0.490372000	1.878485000	0.290614000	8	-1.104066000	1.901016000	0.478604000
6	0.343740000	3.042281000	0.071938000	6	-0.487578000	3.201916000	0.306336000
1	1.304630000	2.834650000	0.559284000	1	0.565304000	3.085275000	0.590700000
1	0.495066000	3.213629000	-1.009098000	1	-0.557380000	3.525633000	-0.747291000
1	-0.126664000	3.928365000	0.531033000	1	-0.983532000	3.936452000	0.963622000
7	-1.898361000	-0.457748000	-0.043777000	7	-2.169672000	-0.565435000	-0.092336000
6	-2.597140000	-1.611844000	0.109239000	6	-2.643959000	-1.836949000	-0.070427000
6	-2.582788000	0.722269000	-0.099330000	6	-3.028532000	0.460762000	0.177106000
6	-4.004060000	-1.648452000	0.198543000	6	-3.991662000	-2.147019000	0.207057000
1	-2.012958000	-2.530167000	0.162299000	1	-1.922067000	-2.625931000	-0.282018000
6	-3.992587000	0.771768000	-0.002682000	6	-4.391171000	0.233379000	0.479470000
6	-4.719754000	-0.431303000	0.139521000	6	-4.886965000	-1.089805000	0.487330000
1	-4.510391000	-2.607714000	0.316822000	1	-4.315891000	-3.188911000	0.205324000
1	-4.502999000	1.736575000	-0.039958000	1	-5.044027000	1.080422000	0.701036000
1	-5.809743000	-0.416187000	0.212030000	1	-5.937158000	-1.288089000	0.714096000
8	2.253635000	0.083350000	0.059275000	8	1.710545000	0.808050000	-0.551531000
6	3.111150000	0.064584000	-1.151601000	7	2.840119000	0.218597000	-0.097959000
6	3.042221000	-0.327065000	1.240164000	6	2.837557000	-0.597246000	0.998490000
6	4.490058000	-0.441882000	-0.672350000	6	4.000530000	0.514419000	-0.757131000

1	-1.344493000	3.787498000	-0.405357000
7	0.667157000	-0.340999000	-0.044873000
6	1.285091000	-1.544200000	-0.180314000
6	1.406852000	0.790241000	0.121663000
6	2.688709000	-1.662861000	-0.137419000
1	0.635578000	-2.406961000	-0.333534000
6	2.817292000	0.755262000	0.165713000
6	3.467785000	-0.494149000	0.040390000
1	3.148845000	-2.645748000	-0.248641000
1	3.384451000	1.679959000	0.292693000
1	4.558265000	-0.552463000	0.071686000
8	-2.031584000	-1.566919000	-0.340779000
6	-2.233866000	-2.607823000	0.611800000
1	-1.447473000	-3.382654000	0.510636000
1	-2.272469000	-2.242300000	1.654125000
1	-3.199085000	-3.087634000	0.366330000
28	-1.181749000	-0.087863000	-0.176933000

1	3.145753000	1.099490000	-1.527550000	6	4.039673000	-1.153848000	1.477425000
6	4.500181000	-0.056561000	0.829891000	1	1.858025000	-0.767821000	1.447088000
1	2.681534000	0.271242000	2.088885000	6	5.228609000	-0.012196000	-0.314296000
1	4.564109000	-1.534661000	-0.789950000	1	3.883160000	1.172203000	-1.619020000
1	4.749311000	1.008270000	0.963838000	6	5.257334000	-0.861665000	0.818294000
1	2.856502000	-1.396584000	1.433273000	1	4.003763000	-1.801617000	2.354763000
1	5.310129000	0.023426000	-1.238229000	1	6.136610000	0.244200000	-0.862311000
1	2.632985000	-0.583225000	-1.899537000	1	6.199472000	-1.283352000	1.175209000
1	5.206542000	-0.659693000	1.418981000	46	-0.182021000	-0.015681000	-0.334447000
46	0.166731000	-0.285236000	-0.026940000				

**\*OAT<sup>‡</sup> - Pd**

	6	0.329002000	-1.199196000	-2.364266000
	1	-0.629658000	-1.295388000	-2.894658000
	1	1.123976000	-0.831309000	-3.024671000
	1	0.614274000	-2.127376000	-1.845757000
	6	-2.126406000	1.762542000	0.591766000
	1	-2.549838000	2.256052000	-0.306171000
	1	-2.533512000	2.265513000	1.485582000
	8	-0.691036000	1.884069000	0.567408000
	6	-0.247225000	3.258111000	0.381276000
	1	0.842493000	3.219182000	0.267221000
	1	-0.695175000	3.682703000	-0.533419000
	1	-0.532295000	3.858088000	1.262070000
	7	-1.764279000	-0.578296000	-0.140067000
	6	-2.141371000	-1.879665000	-0.206235000
	6	-2.521908000	0.287436000	0.593513000
	6	-3.288516000	-2.382712000	0.443685000
	1	-1.504718000	-2.538495000	-0.799671000
	6	-3.675945000	-0.138252000	1.291917000
	6	-4.073656000	-1.492426000	1.211122000
	1	-3.545106000	-3.438966000	0.348098000
	1	-4.249607000	0.581292000	1.880184000
	1	-4.965225000	-1.841044000	1.737709000
	8	1.581065000	1.218856000	-1.433936000
	7	1.999115000	-0.151730000	0.156157000
	6	1.976295000	0.163447000	1.472672000
	6	3.019190000	-0.870019000	-0.366635000
	6	2.999527000	-0.268238000	2.348667000
	1	1.133833000	0.764733000	1.819725000
	6	4.071469000	-1.345336000	0.444934000
	1	3.000887000	-1.031403000	-1.444495000
	6	4.063981000	-1.038814000	1.827250000
	1	2.945606000	0.000380000	3.405317000
	1	4.878759000	-1.920963000	-0.011528000
	1	4.872725000	-1.383002000	2.476948000
	46	0.059171000	0.237511000	-0.935237000

<b>[N~O)Pd<sup>IV</sup>(O)(Me)]<sup>+</sup></b>				<b>[(N~O)Pd<sup>IV</sup>(Py)(O)(Me)]<sup>+</sup></b>			
6	1.312589000	-2.519954000	-0.355644000	8	0.223177000	-2.139120000	-0.196714000
1	0.658663000	-2.792964000	-1.199846000	6	0.117449000	0.010958000	2.064663000
1	2.370635000	-2.707183000	-0.573480000	1	0.808488000	0.844096000	2.248743000
1	1.006468000	-2.980186000	0.593751000	1	-0.913491000	0.235064000	2.363171000
6	-0.610669000	2.121534000	-0.273767000	1	0.476493000	-0.937409000	2.480106000
1	-0.641182000	2.451783000	-1.331827000	6	-1.985495000	2.049228000	0.016762000
1	-0.976948000	2.952061000	0.355271000	1	-2.501517000	2.791136000	-0.616597000
8	0.720356000	1.764956000	0.099459000	1	-2.003165000	2.419702000	1.061272000
6	1.686059000	2.852075000	0.026673000	8	-0.622830000	1.901876000	-0.421669000
1	2.638692000	2.432465000	0.372293000	6	0.058309000	3.173625000	-0.545308000
1	1.773543000	3.213699000	-1.012146000	1	1.032258000	2.970733000	-1.009045000
1	1.367973000	3.669182000	0.694765000	1	-0.520984000	3.844335000	-1.202062000

7	-0.978496000	-0.342841000	-0.036528000	1	0.190877000	3.646384000	0.444915000
6	-1.785818000	-1.429080000	0.137138000	7	-1.980167000	-0.433526000	-0.038108000
6	-1.525557000	0.909533000	-0.088267000	6	-2.591568000	-1.644705000	-0.080302000
6	-3.184417000	-1.317692000	0.228689000	6	-2.712991000	0.709675000	-0.078888000
1	-1.293315000	-2.399365000	0.201417000	6	-3.994965000	-1.760415000	-0.160013000
6	-2.925118000	1.094412000	0.003398000	1	-1.906464000	-2.496579000	-0.057061000
6	-3.767044000	-0.028588000	0.156764000	6	-4.123246000	0.671922000	-0.175218000
1	-3.788871000	-2.216496000	0.358765000	6	-4.775412000	-0.581988000	-0.208849000
1	-3.336351000	2.105361000	-0.039317000	1	-4.450982000	-2.751209000	-0.189366000
1	-4.849457000	0.099242000	0.233246000	1	-4.689711000	1.604787000	-0.222801000
8	2.523563000	-0.394087000	0.958009000	1	-5.864550000	-0.635082000	-0.279476000
46	1.103655000	-0.488872000	-0.127540000	7	2.213861000	-0.232524000	-0.048879000
				6	2.890004000	0.906226000	0.255810000
				6	2.911165000	-1.335432000	-0.428768000
				6	4.294868000	1.000218000	0.180513000
				6	4.321136000	-1.325611000	-0.531852000
				6	5.028192000	-0.141006000	-0.222664000
				1	2.294768000	1.763373000	0.577277000
				1	2.298076000	-2.216675000	-0.629672000
				1	4.787943000	1.939270000	0.438262000
				1	4.837210000	-2.235017000	-0.844532000
				1	6.118521000	-0.106035000	-0.296099000
				46	0.107455000	-0.315582000	0.017209000
<b>*Methyl Migration<sup>‡</sup> - Pd</b>				<b>Py</b>			
8	0.225608000	-2.136310000	-0.043775000	6	-1.150745000	-0.733908000	-0.000217000
6	0.202354000	-1.122002000	1.992839000	6	-1.215583000	0.684354000	-0.000119000
1	0.171842000	-0.133901000	2.481904000	6	0.000315000	1.408768000	0.000056000
1	-0.678505000	-1.735759000	2.181030000	6	1.215891000	0.683825000	0.000207000
1	1.146101000	-1.652598000	2.113232000	6	1.150417000	-0.734406000	0.000149000
6	-1.918107000	2.096572000	0.148236000	7	-0.000322000	-1.441058000	-0.000092000
1	-2.408842000	2.906524000	-0.417626000	1	0.000524000	2.503340000	0.000213000
1	-1.901505000	2.381101000	1.219093000	1	-2.075339000	-1.325386000	-0.000367000
8	-0.563088000	1.929373000	-0.322651000	1	-2.183366000	1.192478000	-0.000224000
6	0.187559000	3.168865000	-0.310363000	1	2.183921000	1.191480000	0.000365000
1	1.165732000	2.953541000	-0.758511000	1	2.074742000	-1.326301000	0.000202000
1	-0.336290000	3.924011000	-0.919956000				
1	0.309061000	3.540224000	0.723326000				
7	-1.981307000	-0.367537000	-0.051236000				
6	-2.616486000	-1.559738000	-0.175542000				
6	-2.689004000	0.792982000	-0.038433000				
6	-4.021104000	-1.638929000	-0.283980000				
1	-1.947187000	-2.424937000	-0.190364000				
6	-4.097427000	0.794000000	-0.156594000				
6	-4.774768000	-0.442217000	-0.273909000				
1	-4.498909000	-2.615005000	-0.381866000				
1	-4.644182000	1.739642000	-0.156085000				
1	-5.863430000	-0.466863000	-0.364621000				
7	2.162933000	-0.166141000	-0.087261000				
6	2.861271000	0.823892000	0.528455000				
6	2.835607000	-1.126884000	-0.776604000				
6	4.267236000	0.912904000	0.464551000				
6	4.244161000	-1.105652000	-0.897466000				
6	4.973980000	-0.070445000	-0.270257000				
1	2.278412000	1.549817000	1.100506000				
1	2.217148000	-1.916722000	-1.203138000				
1	4.782244000	1.724314000	0.981975000				
1	4.742050000	-1.891977000	-1.467457000				
1	6.063996000	-0.032422000	-0.343755000				
46	0.089111000	-0.252127000	-0.008748000				
<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000

6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000
1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl Migration – Four Coordinate -Pd</b>				<b>Pd<sup>II</sup>-methoxide</b>			
6	-2.157315000	-1.343627000	1.482534000	6	2.858312000	1.004203000	0.396487000
1	-1.545959000	-2.217918000	1.709122000	1	2.851856000	1.218447000	1.482915000
1	-1.970996000	-0.460066000	2.110646000	1	3.819938000	1.342636000	-0.023831000
1	-3.210158000	-1.552836000	1.294320000	8	1.778093000	1.722043000	-0.240765000
6	0.775082000	2.084189000	-0.087360000	6	1.854432000	3.172372000	-0.092083000
1	1.153575000	2.869102000	0.587960000	1	0.937463000	3.564209000	-0.546049000
1	0.791090000	2.469075000	-1.125234000	1	1.903512000	3.439252000	0.977393000
8	-0.583990000	1.745756000	0.281393000	1	2.750538000	3.530892000	-0.623808000
6	-1.524776000	2.840915000	0.055389000	7	1.383754000	-0.925868000	-0.027038000
1	-2.499083000	2.499306000	0.426893000	6	1.166287000	-2.245667000	-0.250012000
1	-1.192312000	3.721152000	0.628193000	6	2.662710000	-0.488730000	-0.146366000
1	-1.582419000	3.076566000	-1.020352000	6	2.207820000	-3.196922000	-0.280682000
7	0.966232000	-0.364764000	-0.114665000	1	0.129488000	-2.542461000	-0.419622000
6	1.655926000	-1.536538000	-0.096635000	6	3.766757000	-1.371723000	0.118185000
6	1.620711000	0.822545000	0.011881000	6	3.536059000	-2.751132000	-0.087045000
6	3.058096000	-1.564830000	0.047680000	1	1.976506000	-4.247890000	-0.461387000
1	1.068416000	-2.449189000	-0.206656000	1	4.779133000	-0.983467000	0.249943000
6	3.023239000	0.870726000	0.176552000	1	4.371626000	-3.454664000	-0.110659000
6	3.753169000	-0.340229000	0.189594000	7	-1.803560000	-0.429293000	-0.012888000
1	3.577658000	-2.524206000	0.050661000	6	-2.771921000	-0.152770000	-0.927277000
1	3.524319000	1.834861000	0.287332000	6	-2.044601000	-1.360378000	0.948969000
1	4.838704000	-0.327488000	0.312069000	6	-4.015869000	-0.823366000	-0.925949000
8	-1.976697000	-1.835150000	-0.672351000	1	-2.538405000	0.631874000	-1.647962000
46	-1.096864000	-0.318886000	-0.256575000	6	-3.264438000	-2.065442000	1.028779000
				1	-1.246629000	-1.528486000	1.675848000
				6	-4.269134000	-1.796484000	0.068138000
				1	-4.758798000	-0.573558000	-1.685449000
				1	-3.413717000	-2.794919000	1.826911000
				1	-5.224606000	-2.326550000	0.098861000
				8	-1.123164000	2.258564000	-0.353846000
				6	-1.764566000	2.781248000	0.804624000
				1	-1.051886000	3.029345000	1.619583000
				1	-2.268093000	3.719642000	0.500733000
				1	-2.539662000	2.100075000	1.212793000
				46	-0.050221000	0.636644000	-0.103931000
<b>Pd<sup>II</sup>-Methoxide - Four Coordinate</b>							
	6	0.790530000	1.916259000	0.469893000			
	1	0.385382000	1.796234000	1.496960000			
	1	1.346057000	2.873366000	0.425009000			
	8	-0.282421000	1.909303000	-0.475457000			
	6	-1.286505000	2.881511000	-0.153685000			
	1	-2.067520000	2.795744000	-0.921725000			
	1	-1.727798000	2.681338000	0.841864000			
	1	-0.864214000	3.906362000	-0.168598000			
	7	1.185316000	-0.486335000	0.094297000			
	6	2.015401000	-1.540756000	-0.116759000			
	6	1.736752000	0.759221000	0.172504000			
	6	3.414983000	-1.414094000	-0.257361000			
	1	1.532212000	-2.519404000	-0.172489000			
	6	3.127667000	0.978155000	0.027949000			

## Cobalt – HLL Coordinates

[(N~O)Co <sup>I</sup> (Me)(THF)]				[(N~O)Co <sup>I</sup> (Me)(PyO)]			
6	0.524854000	-2.179730000	-0.484654000	6	-0.333161000	-1.645379000	1.276718000
1	-0.051915000	-2.558090000	-1.356230000	1	0.368511000	-1.886036000	2.104181000
1	1.594085000	-2.374499000	-0.729754000	1	-1.333824000	-1.539467000	1.749383000
1	0.290336000	-2.858220000	0.369523000	1	-0.387734000	-2.558778000	0.639027000
6	-1.610432000	1.977485000	-0.260421000	6	2.377136000	1.896515000	-0.035410000
1	-1.440054000	2.174519000	-1.339050000	1	2.434073000	2.257900000	1.012285000
1	-2.103459000	2.858248000	0.191070000	1	2.934007000	2.598284000	-0.683666000
8	-0.330557000	1.744308000	0.366346000	8	0.990835000	1.843841000	-0.428587000
6	0.580612000	2.830658000	0.146746000	6	0.324230000	3.102501000	-0.230959000
1	1.518450000	2.566806000	0.650453000	1	-0.713426000	2.963571000	-0.555117000
1	0.765973000	2.975024000	-0.935566000	1	0.340681000	3.389270000	0.837583000
1	0.168382000	3.762668000	0.577274000	1	0.817259000	3.885917000	-0.836899000
7	-1.715028000	-0.448699000	-0.106721000	7	2.026326000	-0.504049000	0.171924000
6	-2.445277000	-1.607674000	-0.003088000	6	2.513830000	-1.788418000	0.154011000
6	-2.439963000	0.724651000	-0.074685000	6	2.930776000	0.489875000	-0.141967000
6	-3.846825000	-1.638206000	0.127423000	6	3.843812000	-2.113506000	-0.173740000
1	-1.864756000	-2.527835000	-0.027895000	1	1.794443000	-2.562874000	0.414055000
6	-3.839258000	0.779498000	0.079131000	6	4.269718000	0.245135000	-0.503715000
6	-4.579480000	-0.425010000	0.174165000	6	4.758192000	-1.085482000	-0.518192000
1	-4.347980000	-2.606693000	0.200018000	1	4.148083000	-3.163108000	-0.162435000
1	-4.335775000	1.753431000	0.115788000	1	4.917086000	1.088450000	-0.760638000
1	-5.666072000	-0.415651000	0.286699000	1	5.793391000	-1.306473000	-0.788320000
8	2.096569000	0.141436000	0.132017000	8	-1.485625000	0.820990000	0.386740000
6	2.940421000	0.183005000	-1.060877000	7	-2.626588000	0.216154000	0.054576000
6	2.821946000	-0.523703000	1.225594000	6	-3.805724000	0.782978000	0.477970000
6	4.382203000	0.111827000	-0.518263000	6	-2.637693000	-0.923220000	-0.716448000
1	2.703423000	1.114702000	-1.596625000	6	-5.043748000	0.219521000	0.127466000
6	4.220309000	-0.881827000	0.660736000	1	-3.683200000	1.674533000	1.093799000
1	2.875743000	0.197652000	2.058796000	6	-3.856380000	-1.519410000	-1.087619000
1	5.095102000	-0.236609000	-1.281816000	1	-1.645650000	-1.286150000	-0.986550000
1	5.010155000	-0.782225000	1.421492000	6	-5.087054000	-0.954999000	-0.668147000
1	2.239672000	-1.400494000	1.535936000	1	-5.955460000	0.701547000	0.486273000
1	4.709075000	1.101223000	-0.155603000	1	-3.823164000	-2.421485000	-1.701834000
	6	3.988053000	-0.123555000	-0.185345000			
	1	4.024256000	-2.305301000	-0.421072000			
	1	3.520197000	1.996124000	0.084127000			
	1	5.065783000	0.021958000	-0.295504000			
	8	-2.845708000	-1.130318000	0.125340000			
	6	-3.794166000	-0.192625000	-0.311348000			
	1	-3.822535000	0.732753000	0.314126000			
	1	-3.641149000	0.119532000	-1.372154000			
	1	-4.809635000	-0.644081000	-0.255484000			
	46	-0.916729000	-0.736236000	0.102407000			

1	2.696013000	-0.678481000	-1.702143000	1	-6.039839000	-1.411284000	-0.945613000
1	4.226055000	-1.918111000	0.286751000	27	0.247086000	0.001338000	0.373109000
27	0.131111000	-0.303640000	-0.069623000				
<b>OAT<sup>2+</sup> - Co</b>							
	6	0.296800000	-1.926718000	-0.745098000			
	1	-0.337193000	-2.286678000	-1.583305000			
	1	1.341384000	-1.941893000	-1.107529000			
	1	0.221854000	-2.680654000	0.074255000			
	6	-2.288119000	1.910920000	-0.126689000			
	1	-2.103320000	2.173049000	-1.188633000			
	1	-2.918121000	2.699480000	0.327111000			
	8	-1.035674000	1.799734000	0.560889000			
	6	-0.229768000	2.985496000	0.435695000			
	1	0.696375000	2.792994000	0.989450000			
	1	0.018588000	3.177588000	-0.622711000			
	1	-0.772246000	3.848312000	0.868045000			
	7	-2.128952000	-0.523402000	-0.084112000			
	6	-2.700232000	-1.759997000	-0.007670000			
	6	-2.971120000	0.556328000	-0.031798000			
	6	-4.090365000	-1.968490000	0.111535000			
	1	-2.008164000	-2.600145000	-0.050368000			
	6	-4.371285000	0.438444000	0.092369000			
	6	-4.955748000	-0.849808000	0.157699000			
	1	-4.474092000	-2.989668000	0.166377000			
	1	-4.985182000	1.341549000	0.140424000			
	1	-6.037624000	-0.972007000	0.252248000			
	8	1.226451000	0.670341000	-0.595029000			
	7	2.746207000	0.325042000	0.053471000			
	6	2.938837000	-0.721021000	0.891463000			
	6	3.776250000	0.813213000	-0.676454000			
	6	4.207209000	-1.331724000	1.033109000			
	1	2.051851000	-1.055516000	1.434851000			
	6	5.075275000	0.272959000	-0.583237000			
	1	3.522227000	1.639722000	-1.346810000			
	6	5.299705000	-0.827423000	0.286835000			
	1	4.323826000	-2.174292000	1.719026000			
	1	5.883220000	0.704737000	-1.178964000			
	1	6.292745000	-1.276665000	0.374326000			
	27	-0.240288000	-0.160188000	-0.140990000			

<b>[N~O)Co<sup>III</sup>(O)(Me)]</b>				<b>[(N~O)Co<sup>III</sup>(Py)(O)(Me)]</b>			
6	-0.873414000	-2.852562000	0.044654000	8	0.147205000	-2.089149000	-0.113769000
1	-0.145685000	-3.113693000	0.833390000	6	0.037202000	0.169283000	2.026893000
1	-1.840828000	-3.328280000	0.266247000	1	0.207172000	1.263334000	2.136090000
1	-0.508811000	-3.231637000	-0.936967000	1	-0.930665000	-0.069035000	2.504100000
6	-0.215526000	1.855283000	0.528467000	1	0.830870000	-0.354983000	2.587497000
1	-0.833827000	1.427473000	1.338594000	6	-1.740767000	2.008079000	-0.119405000
1	0.142019000	2.858549000	0.833683000	1	-2.221383000	2.787234000	-0.740558000
8	-0.967756000	1.931489000	-0.685258000	1	-1.666186000	2.387417000	0.919361000
6	-2.285218000	2.466631000	-0.461236000	8	-0.428854000	1.714401000	-0.618267000
1	-2.769750000	2.522672000	-1.447320000	6	0.405950000	2.879018000	-0.664107000
1	-2.855747000	1.792463000	0.201242000	1	1.364201000	2.569042000	-1.100850000
1	-2.227406000	3.484472000	-0.025288000	1	-0.054754000	3.656123000	-1.302903000
7	0.730364000	-0.357213000	-0.053770000	1	0.571302000	3.292332000	0.349784000
6	1.780597000	-1.178026000	-0.312736000	7	-1.882559000	-0.432559000	-0.010526000
6	0.982698000	0.948679000	0.271425000	6	-2.563203000	-1.604380000	0.011566000
6	3.125910000	-0.753244000	-0.260926000	6	-2.566208000	0.727916000	-0.148500000
1	1.530709000	-2.209858000	-0.560496000	6	-3.970576000	-1.655918000	-0.095650000
6	2.303816000	1.444815000	0.354796000	1	-1.897118000	-2.471352000	0.099458000
6	3.396643000	0.587430000	0.088893000	6	-3.974011000	0.767178000	-0.288245000

1	3.924003000	-1.464049000	-0.482864000	6	-4.693275000	-0.449042000	-0.251428000
1	2.461383000	2.493980000	0.612363000	1	-4.478326000	-2.622269000	-0.063361000
1	4.423345000	0.958208000	0.146171000	1	-4.483475000	1.725265000	-0.420542000
8	-2.246719000	-0.528073000	0.915889000	1	-5.782596000	-0.453233000	-0.347805000
27	-1.110711000	-0.964118000	-0.139535000	7	2.058635000	-0.307428000	0.018433000
				6	2.798273000	0.682135000	0.576391000
				6	2.709909000	-1.275417000	-0.680206000
				6	4.203484000	0.772324000	0.448358000
				6	4.112870000	-1.267531000	-0.864107000
				6	4.879005000	-0.223463000	-0.295703000
				1	2.246948000	1.417042000	1.165406000
				1	2.047111000	-2.064464000	-1.044868000
				1	4.739952000	1.592955000	0.930075000
				1	4.581254000	-2.069338000	-1.439385000
				1	5.965492000	-0.189639000	-0.421164000
				27	0.079590000	-0.422209000	0.150202000
<b>Methyl Migration<sup>‡</sup> - Pd</b>				<b>Py</b>			
8	0.201107000	-2.046467000	0.140962000	6	-1.150745000	-0.733908000	-0.000217000
6	0.183822000	-1.215723000	1.888020000	6	-1.215583000	0.684354000	-0.000119000
1	0.107381000	-0.199557000	2.357643000	6	0.000315000	1.408768000	0.000056000
1	-0.661891000	-1.820880000	2.235118000	6	1.215891000	0.683825000	0.000207000
1	1.141327000	-1.666629000	2.170788000	6	1.150417000	-0.734406000	0.000149000
6	-1.725851000	2.049001000	0.188411000	7	-0.000322000	-1.441058000	-0.000092000
1	-2.171935000	2.923293000	-0.320581000	1	0.000524000	2.503340000	0.000213000
1	-1.645516000	2.276058000	1.272588000	1	-2.075339000	-1.325386000	-0.000367000
8	-0.411421000	1.787454000	-0.334951000	1	-2.183366000	1.192478000	-0.000224000
6	0.426147000	2.951762000	-0.316600000	1	2.183921000	1.191480000	0.000365000
1	1.375173000	2.673561000	-0.791039000	1	2.074742000	-1.326301000	0.000202000
1	-0.049923000	3.767096000	-0.892137000				
1	0.609405000	3.293963000	0.720856000				
7	-1.863781000	-0.359713000	-0.082690000				
6	-2.547866000	-1.527883000	-0.216959000				
6	-2.567386000	0.802257000	-0.035290000				
6	-3.954823000	-1.569213000	-0.320087000				
1	-1.888810000	-2.402317000	-0.226309000				
6	-3.973990000	0.855412000	-0.153448000				
6	-4.688716000	-0.357734000	-0.295297000				
1	-4.456953000	-2.533650000	-0.425036000				
1	-4.489580000	1.819348000	-0.129162000				
1	-5.778096000	-0.355112000	-0.387694000				
7	1.995053000	-0.153357000	-0.111803000				
6	2.752978000	0.700075000	0.623431000				
6	2.642612000	-1.048812000	-0.909406000				
6	4.164013000	0.742819000	0.566092000				
6	4.051735000	-1.076911000	-1.037790000				
6	4.832598000	-0.161409000	-0.294639000				
1	2.204063000	1.355034000	1.305297000				
1	1.990756000	-1.751340000	-1.426560000				
1	4.711328000	1.452939000	1.190456000				
1	4.513760000	-1.809647000	-1.703322000				
1	5.923882000	-0.160040000	-0.371806000				
27	0.065096000	-0.298532000	0.007987000				
<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000
6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000

1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl migration – Four Coordinate Co</b>				<b>Co<sup>I</sup>-Methoxide</b>			
6	-2.193350000	-1.605219000	1.166563000	6	2.811333000	0.997556000	0.445995000
1	-1.712157000	-2.576834000	1.329243000	1	2.762166000	1.179874000	1.540121000
1	-1.855593000	-0.880172000	1.938516000	1	3.807345000	1.307728000	0.080108000
1	-3.285506000	-1.684270000	1.196351000	8	1.778048000	1.762623000	-0.196855000
6	0.389644000	2.018139000	-0.113895000	6	1.888799000	3.183124000	0.047669000
1	0.702479000	2.878202000	0.504328000	1	0.982204000	3.626536000	-0.376660000
1	0.301228000	2.343695000	-1.170560000	1	1.923543000	3.381956000	1.134790000
8	-0.894634000	1.522752000	0.327561000	1	2.809311000	3.556321000	-0.438347000
6	-1.982251000	2.426996000	0.036246000	7	1.195963000	-0.749249000	-0.043420000
1	-2.891385000	1.959646000	0.435569000	6	0.901898000	-2.069592000	-0.293433000
1	-1.802572000	3.396963000	0.533800000	6	2.534432000	-0.458451000	-0.129850000
1	-2.083996000	2.567393000	-1.054736000	6	1.867012000	-3.091776000	-0.357436000
7	0.748237000	-0.367653000	-0.158860000	1	-0.150578000	-2.298332000	-0.461569000
6	1.545488000	-1.477230000	-0.152628000	6	3.562515000	-1.417055000	0.053395000
6	1.354988000	0.851708000	-0.005767000	6	3.238653000	-2.777302000	-0.181080000
6	2.944223000	-1.411827000	0.007330000	1	1.539481000	-4.114825000	-0.558580000
1	1.023719000	-2.426618000	-0.288286000	1	4.600386000	-1.097780000	0.184156000
6	2.743223000	1.003380000	0.182141000	1	4.014250000	-3.544319000	-0.236818000
6	3.565911000	-0.150418000	0.184196000	7	-1.594438000	-0.264135000	0.018688000
1	3.525995000	-2.336010000	-0.002030000	6	-2.484813000	-0.214454000	-1.009677000
1	3.167471000	2.002069000	0.315720000	6	-1.932197000	-1.001844000	1.111371000
1	4.646689000	-0.067347000	0.320429000	6	-3.720059000	-0.899727000	-0.994804000
8	-2.198815000	-1.624584000	-0.718928000	1	-2.182568000	0.400426000	-1.858989000
27	-1.127174000	-0.434136000	-0.282981000	6	-3.148685000	-1.712992000	1.220045000
				1	-1.194922000	-1.011188000	1.917323000
				6	-4.065394000	-1.666598000	0.143217000
				1	-4.387549000	-0.822842000	-1.856001000
				1	-3.360938000	-2.281523000	2.128300000
				1	-5.015810000	-2.205821000	0.190342000
				8	-0.817126000	2.378044000	-0.162635000
				6	-2.136610000	2.724066000	0.157089000
				1	-2.529215000	2.202831000	1.061762000
				1	-2.203633000	3.815831000	0.364653000
				1	-2.864680000	2.523875000	-0.667093000
				27	0.024143000	0.732588000	-0.071543000
<b>Co<sup>I</sup>-Methoxide - Four Coordinate</b>							
	6	-0.901287000	2.006152000	-0.100936000			
	1	-0.900847000	2.359023000	-1.151617000			
	1	-1.422775000	2.750523000	0.526907000			
	8	0.470040000	1.860136000	0.339768000			
	6	1.287247000	3.009814000	0.037149000			
	1	2.284103000	2.801180000	0.447983000			
	1	1.355184000	3.160822000	-1.055534000			
	1	0.861380000	3.907617000	0.520252000			
	7	-0.628701000	-0.397246000	-0.096256000			
	6	-1.123971000	-1.674676000	-0.110194000			
	6	-1.535969000	0.630182000	-0.006027000			
	6	-2.499796000	-1.962104000	-0.023686000			
	1	-0.373344000	-2.462387000	-0.197343000			
	6	-2.925076000	0.425062000	0.109182000			
	6	-3.430694000	-0.898502000	0.096872000			
	1	-2.827211000	-3.003968000	-0.043951000			
	1	-3.594030000	1.285676000	0.196934000			
	1	-4.502945000	-1.090617000	0.178426000			
	8	2.378288000	-1.231718000	-0.441269000			
	6	2.856763000	-2.261931000	0.401419000			
	1	2.807399000	-2.021249000	1.485197000			

## Rhodium – HLL Coordinates

[(N~O)Rh <sup>I</sup> (Me)(THF)]				[(N~O)Rh <sup>I</sup> (Me)(PyO)]			
6	0.536999000	-2.215732000	-0.545084000	6	0.496503000	-1.734589000	-1.266871000
1	-0.089378000	-2.569364000	-1.389848000	1	-0.300283000	-2.453113000	-1.543971000
1	1.595318000	-2.366762000	-0.851527000	1	1.035730000	-1.501275000	-2.211114000
1	0.354886000	-2.891841000	0.320584000	1	1.202588000	-2.261081000	-0.584767000
6	-1.785861000	1.983817000	-0.337352000	6	-2.579032000	1.749768000	-0.214844000
1	-1.505660000	2.062068000	-1.407388000	1	-2.544428000	1.861427000	-1.317484000
1	-2.385926000	2.868950000	-0.053350000	1	-3.293407000	2.485229000	0.201049000
8	-0.577455000	1.927524000	0.448760000	8	-1.256735000	1.987914000	0.313060000
6	0.296154000	3.031263000	0.177844000	6	-0.703314000	3.228525000	-0.153262000
1	1.193001000	2.881503000	0.794287000	1	0.314243000	3.291588000	0.254188000
1	0.581714000	3.052910000	-0.891655000	1	-0.651893000	3.239834000	-1.258075000
1	-0.191108000	3.987759000	0.451116000	1	-1.312546000	4.081440000	0.205085000
7	-1.841764000	-0.457183000	-0.098484000	7	-2.042499000	-0.638072000	-0.055674000
6	-2.538813000	-1.625402000	0.049618000	6	-2.409063000	-1.925788000	0.232357000
6	-2.576936000	0.707636000	-0.109506000	6	-2.998802000	0.335516000	0.144648000
6	-3.940983000	-1.682315000	0.186422000	6	-3.688854000	-2.285512000	0.703267000
1	-1.935214000	-2.532345000	0.056182000	1	-1.636725000	-2.678479000	0.077564000
6	-3.979054000	0.732993000	0.043845000	6	-4.292350000	0.055839000	0.631535000
6	-4.691895000	-0.482434000	0.186866000	6	-4.665342000	-1.282204000	0.911100000
1	-4.423065000	-2.656514000	0.298122000	1	-3.901076000	-3.338090000	0.906464000
1	-4.498859000	1.694799000	0.045755000	1	-4.994294000	0.880159000	0.783411000
1	-5.778534000	-0.489416000	0.301028000	1	-5.664250000	-1.525013000	1.281351000
8	2.284337000	0.138450000	0.142313000	8	1.683708000	1.002971000	-0.481437000
6	3.111879000	0.214026000	-1.054405000	7	2.767630000	0.359614000	-0.027685000
6	3.027449000	-0.551682000	1.203335000	6	3.219160000	0.625833000	1.241802000
6	4.553776000	0.263021000	-0.510400000	6	3.464274000	-0.492434000	-0.847763000
1	2.798057000	1.111232000	-1.607747000	6	4.396706000	0.034886000	1.729172000
6	4.473686000	-0.744848000	0.666698000	1	2.584598000	1.303620000	1.813064000
1	2.981706000	0.098197000	2.092417000	6	4.644297000	-1.116069000	-0.399163000
1	5.297532000	-0.022260000	-1.271079000	1	3.031917000	-0.628394000	-1.836563000
1	5.231214000	-0.558522000	1.443772000	6	5.130705000	-0.858415000	0.905368000
1	2.519315000	-1.500838000	1.422630000	1	4.719607000	0.272438000	2.744785000
1	4.791012000	1.276607000	-0.145870000	1	5.165628000	-1.791528000	-1.080348000
1	2.935394000	-0.677502000	-1.679942000	1	6.044928000	-1.333628000	1.268119000
1	4.608885000	-1.773060000	0.293808000	45	-0.186252000	0.002330000	-0.432807000
45	0.138636000	-0.269004000	-0.044617000				
OAT <sup>z</sup> - Rh							
	6	0.344007000	-1.892442000	-1.087068000			
	1	-0.360108000	-2.172893000	-1.894995000			
	1	1.354235000	-1.802835000	-1.526349000			
	1	2.285647000	-3.205248000	0.238639000			
	1	3.917005000	-2.482566000	0.154702000			
	27	1.161534000	0.004096000	-0.082869000			

1	0.365825000	-2.715334000	-0.338715000
6	-2.479524000	1.898074000	-0.126668000
1	-2.266020000	2.089730000	-1.198269000
1	-3.181613000	2.671497000	0.239359000
8	-1.251181000	1.942625000	0.614963000
6	-0.517105000	3.156148000	0.383690000
1	0.419513000	3.064432000	0.948067000
1	-0.279897000	3.270374000	-0.689583000
1	-1.099844000	4.028165000	0.740391000
7	-2.228214000	-0.544768000	-0.069977000
6	-2.749663000	-1.799159000	0.051548000
6	-3.093497000	0.514290000	0.032765000
6	-4.119981000	-2.050901000	0.275456000
1	-2.033344000	-2.616524000	-0.042364000
6	-4.476362000	0.346800000	0.257607000
6	-5.013263000	-0.958630000	0.377074000
1	-4.466845000	-3.083010000	0.362806000
1	-5.115517000	1.229218000	0.342510000
1	-6.081173000	-1.112684000	0.550515000
8	1.355031000	0.808615000	-0.572013000
7	3.002834000	0.237943000	-0.033295000
6	3.129019000	-0.787079000	0.824084000
6	4.075151000	0.796228000	-0.616676000
6	4.400258000	-1.317467000	1.156981000
1	2.185780000	-1.169655000	1.231191000
6	5.386979000	0.338958000	-0.342732000
1	3.866583000	1.615065000	-1.313484000
6	5.548712000	-0.741111000	0.561436000
1	4.477217000	-2.153273000	1.856266000
1	6.244060000	0.811874000	-0.828103000
1	6.546456000	-1.125383000	0.793118000
45	-0.209708000	-0.126959000	-0.207512000

[N~O)Rh <sup>III</sup> (O)(Me)]				[(N~O)Rh <sup>III</sup> (Py)(O)(Me)]			
6	-1.344727000	-2.266707000	1.069024000	8	0.266636000	-2.149772000	-0.140355000
1	-0.720879000	-2.089977000	1.961408000	6	0.137545000	0.496095000	1.959987000
1	-2.390638000	-2.454063000	1.359379000	1	0.308846000	1.593170000	1.926562000
1	-0.963872000	-3.152262000	0.516267000	1	-0.817437000	0.304538000	2.481171000
6	0.500613000	1.815182000	0.767437000	1	0.952653000	0.035692000	2.543335000
1	-0.441920000	1.458250000	1.219671000	6	-2.069457000	2.004024000	-0.011308000
1	1.040016000	2.443287000	1.505684000	1	-2.710373000	2.760892000	-0.502426000
8	0.243475000	2.558795000	-0.427878000	1	-1.943704000	2.296644000	1.050576000
6	-0.845168000	3.482179000	-0.257662000	8	-0.788364000	1.950221000	-0.648440000
1	-0.956221000	4.011990000	-1.215718000	6	-0.118020000	3.215228000	-0.624731000
1	-1.775800000	2.937965000	-0.018673000	1	0.827912000	3.081471000	-1.168520000
1	-0.620209000	4.219809000	0.540419000	1	-0.725236000	3.989328000	-1.133086000
7	0.777847000	-0.487939000	-0.126937000	1	0.088659000	3.542585000	0.413461000
6	1.561094000	-1.522478000	-0.542268000	7	-1.957509000	-0.466001000	-0.016288000
6	1.377582000	0.632193000	0.379430000	6	-2.532185000	-1.696250000	-0.024958000
6	2.967559000	-1.500571000	-0.473278000	6	-2.746185000	0.636841000	-0.087876000
1	1.036707000	-2.393196000	-0.944295000	6	-3.931285000	-1.872118000	-0.098746000
6	2.787203000	0.719104000	0.484395000	1	-1.795459000	-2.509016000	0.017169000
6	3.601322000	-0.352163000	0.056699000	6	-4.155165000	0.545205000	-0.188688000
1	3.535876000	-2.363649000	-0.825144000	6	-4.763011000	-0.731174000	-0.184893000
1	3.225199000	1.633474000	0.889524000	1	-4.347114000	-2.881969000	-0.094349000
1	4.690095000	-0.292803000	0.129652000	1	-4.753788000	1.456484000	-0.265945000
8	-2.442601000	0.545884000	0.112292000	1	-5.849927000	-0.829363000	-0.253621000
45	-1.269848000	-0.698247000	-0.235724000	7	2.238272000	-0.231878000	-0.036599000
				6	2.943075000	0.890368000	0.252944000
				6	2.925655000	-1.343560000	-0.412807000
				6	4.351296000	0.968124000	0.164268000

	6	4.335581000	-1.359408000	-0.525711000			
	6	5.067880000	-0.183643000	-0.238785000			
	1	2.357972000	1.756283000	0.572535000			
	1	2.275199000	-2.208759000	-0.588939000			
	1	4.858284000	1.903938000	0.410362000			
	1	4.836255000	-2.280278000	-0.833587000			
	1	6.158674000	-0.164576000	-0.322702000			
	45	0.129172000	-0.328531000	0.056809000			
<b>Methyl Migration<sup>‡</sup> - Rh</b>					<b>Py</b>		
8	0.267835000	-2.129918000	0.102949000	6	-1.150745000	-0.733908000	-0.000217000
6	0.254242000	-1.342832000	1.909066000	6	-1.215583000	0.684354000	-0.000119000
1	0.205732000	-0.367238000	2.451786000	6	0.000315000	1.408768000	0.000056000
1	-0.601636000	-1.963486000	2.194518000	6	1.215891000	0.683825000	0.000207000
1	1.207743000	-1.835659000	2.120733000	6	1.150417000	-0.734406000	0.000149000
6	-1.952047000	2.062986000	0.244629000	7	-0.000322000	-1.441058000	-0.000092000
1	-2.517050000	2.928946000	-0.148020000	1	0.000524000	2.503340000	0.000213000
1	-1.815053000	2.194900000	1.338302000	1	-2.075339000	-1.325386000	-0.000367000
8	-0.655909000	1.995395000	-0.379891000	1	-2.183366000	1.192478000	-0.000224000
6	0.109343000	3.187866000	-0.158225000	1	2.183921000	1.191480000	0.000365000
1	1.051215000	3.067754000	-0.710045000	1	2.074742000	-1.326301000	0.000202000
1	-0.433953000	4.071459000	-0.544296000				
1	0.318521000	3.326172000	0.920842000				
7	-1.955557000	-0.364315000	-0.064830000				
6	-2.574319000	-1.564752000	-0.223604000				
6	-2.708816000	0.768937000	-0.024122000				
6	-3.976332000	-1.673230000	-0.352843000				
1	-1.873462000	-2.407446000	-0.237223000				
6	-4.113815000	0.747791000	-0.171548000				
6	-4.765633000	-0.498540000	-0.333026000				
1	-4.429136000	-2.659608000	-0.475961000				
1	-4.678218000	1.683776000	-0.153437000				
1	-5.852020000	-0.547288000	-0.445323000				
7	2.158586000	-0.104270000	-0.103448000				
6	2.906934000	0.895960000	0.430658000				
6	2.812383000	-1.127692000	-0.724427000				
6	4.315419000	0.949058000	0.343327000				
6	4.221050000	-1.155050000	-0.864160000				
6	4.992199000	-0.098085000	-0.329360000				
1	2.350844000	1.673678000	0.960565000				
1	2.159152000	-1.928680000	-1.073492000				
1	4.854982000	1.783588000	0.797231000				
1	4.689116000	-1.995810000	-1.381341000				
1	6.082050000	-0.091091000	-0.425221000				
45	0.085353000	-0.210938000	-0.006096000				

<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000
6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000
1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl Migration – Four Coordinate Rh</b>				<b>Rh<sup>I</sup>-methoxide</b>			

6	-2.365339000	-1.506796000	1.274280000	6	-2.913639000	-0.859274000	0.435869000
1	-1.840809000	-2.451521000	1.446066000	1	-2.856760000	-1.022513000	1.531766000
1	-2.136496000	-0.762301000	2.059396000	1	-3.927095000	-1.131587000	0.088446000
1	-3.446568000	-1.633418000	1.168679000	8	-1.930651000	-1.696411000	-0.205238000
6	0.907686000	2.038132000	-0.163438000	6	-2.046174000	-3.095607000	0.148420000
1	1.421617000	2.873949000	0.344725000	1	-1.142442000	-3.574034000	-0.247430000
1	0.785942000	2.286634000	-1.238197000	1	-2.070343000	-3.207965000	1.247803000
8	-0.395832000	1.821973000	0.413845000	1	-2.969359000	-3.505050000	-0.301351000
6	-1.298311000	2.917964000	0.159962000	7	-1.264888000	0.904240000	-0.007247000
1	-2.243278000	2.668193000	0.659186000	6	-0.959740000	2.221754000	-0.222666000
1	-0.881333000	3.850943000	0.582483000	6	-2.602673000	0.593859000	0.110687000
1	-1.469471000	3.032413000	-0.925739000	6	-1.925339000	3.242299000	-0.323974000
7	0.913771000	-0.390200000	-0.133508000	1	0.102771000	2.448104000	-0.327757000
6	1.550341000	-1.598446000	-0.093717000	6	-3.630094000	1.551970000	-0.010573000
6	1.680417000	0.740768000	-0.021003000	6	-3.299919000	2.913376000	-0.221731000
6	2.945887000	-1.721408000	0.063514000	1	-1.596124000	4.270173000	-0.494255000
1	0.903649000	-2.470643000	-0.200320000	1	-4.672446000	1.231471000	0.069596000
6	3.078148000	0.699977000	0.161847000	1	-4.077256000	3.675713000	-0.310901000
6	3.735280000	-0.553829000	0.199949000	7	1.729058000	0.340221000	0.053617000
1	3.392635000	-2.717700000	0.081572000	6	2.569804000	0.379295000	-1.020191000
1	3.635533000	1.634733000	0.262785000	6	2.104826000	1.024764000	1.171534000
1	4.817992000	-0.615455000	0.332181000	6	3.782944000	1.102663000	-1.025337000
8	-2.251279000	-1.570111000	-0.687533000	1	2.241832000	-0.191000000	-1.890461000
45	-1.101413000	-0.246167000	-0.243047000	6	3.304236000	1.767946000	1.257793000
				1	1.413066000	0.960909000	2.013560000
				6	4.165224000	1.815212000	0.136328000
				1	4.404827000	1.096596000	-1.923361000
				1	3.545852000	2.288138000	2.187493000
				1	5.100104000	2.381893000	0.167058000
				8	0.844835000	-2.507319000	-0.160180000
				6	2.210153000	-2.781865000	0.003301000
				1	2.637071000	-2.363810000	0.945675000
				1	2.365926000	-3.883067000	0.039429000
				1	2.846342000	-2.405067000	-0.834302000
				45	-0.010362000	-0.697970000	-0.044423000
<b>Rh<sup>I</sup>-Methoxide - Four- Coordinate</b>							
	6	1.036881000	1.937940000	0.540671000			
	1	0.745175000	1.982646000	1.609146000			
	1	1.728437000	2.770207000	0.317195000			
	8	-0.157771000	2.053370000	-0.268491000			
	6	-0.932241000	3.222437000	0.063851000			
	1	-1.782113000	3.241372000	-0.631313000			
	1	-1.299100000	3.160633000	1.104625000			
	1	-0.317492000	4.131961000	-0.070836000			
	7	0.774000000	-0.411427000	-0.022298000			
	6	1.262527000	-1.662156000	-0.275000000			
	6	1.670627000	0.594418000	0.230535000			
	6	2.642047000	-1.953267000	-0.265084000			
	1	0.507449000	-2.420005000	-0.489827000			
	6	3.065252000	0.384599000	0.236932000			
	6	3.570542000	-0.916074000	-0.003928000			
	1	2.970863000	-2.974787000	-0.467946000			
	1	3.736314000	1.225156000	0.431945000			
	1	4.645960000	-1.108669000	0.002362000			
	8	-2.134165000	-1.613244000	-0.268765000			
	6	-2.275627000	-2.420912000	0.885791000			
	1	-1.300719000	-2.853562000	1.211319000			
	1	-2.709957000	-1.883960000	1.755952000			
	1	-2.946167000	-3.272867000	0.643968000			
	45	-1.140027000	0.049754000	-0.209890000			

## Iridium – HLL Coordinates

[(N~O)Ir <sup>I</sup> (Me)(THF)]				[(N~O)Ir <sup>I</sup> (Me)(PyO)]			
6	0.542362000	-2.165853000	-0.535238000	6	0.391458000	-1.694211000	-1.365106000
1	-0.077602000	-2.534468000	-1.378553000	1	-0.360750000	-1.966754000	-2.133655000
1	1.600063000	-2.300123000	-0.853532000	1	1.349232000	-1.543768000	-1.905392000
1	0.386530000	-2.858663000	0.322828000	1	0.528093000	-2.581856000	-0.707089000
6	-1.823813000	2.037647000	-0.323464000	6	-2.436893000	1.885972000	0.170456000
1	-1.539240000	2.134213000	-1.389784000	1	-2.431462000	2.198741000	-0.892450000
1	-2.429211000	2.913701000	-0.024392000	1	-3.077296000	2.578330000	0.748307000
8	-0.612776000	1.977524000	0.464721000	8	-1.080439000	1.933626000	0.668192000
6	0.262581000	3.082664000	0.198736000	6	-0.450305000	3.199067000	0.405515000
1	1.156717000	2.931222000	0.818326000	1	0.575331000	3.122982000	0.789253000
1	0.549778000	3.105679000	-0.869572000	1	-0.421433000	3.402026000	-0.680747000
1	-0.227586000	4.036089000	0.474971000	1	-0.992512000	4.010234000	0.928325000
7	-1.837505000	-0.403815000	-0.067783000	7	-2.034520000	-0.529834000	-0.033675000
6	-2.525568000	-1.586551000	0.076991000	6	-2.494372000	-1.825223000	0.012175000
6	-2.599297000	0.752954000	-0.106804000	6	-2.946435000	0.461581000	0.290231000
6	-3.926950000	-1.658965000	0.183758000	6	-3.811900000	-2.167628000	0.369418000
1	-1.909009000	-2.482916000	0.107281000	1	-1.761572000	-2.586785000	-0.249260000
6	-4.001999000	0.751408000	0.021910000	6	-4.270499000	0.185609000	0.683021000
6	-4.700500000	-0.472771000	0.160663000	6	-4.735407000	-1.152042000	0.719657000
1	-4.393553000	-2.640955000	0.293848000	1	-4.096175000	-3.222737000	0.376564000
1	-4.535552000	1.705622000	0.006751000	1	-4.928024000	1.017896000	0.948389000
1	-5.788503000	-0.496869000	0.254376000	1	-5.761206000	-1.387114000	1.012312000
8	2.247860000	0.165317000	0.148815000	8	1.751151000	0.807032000	-0.592470000
6	3.069824000	0.283794000	-1.053415000	7	2.829436000	0.208106000	-0.065013000
6	3.008171000	-0.530494000	1.199274000	6	4.064747000	0.660582000	-0.457231000
6	4.510586000	0.337688000	-0.509906000	6	2.707634000	-0.797219000	0.864070000
1	2.738034000	1.190088000	-1.578866000	6	5.236598000	0.106505000	0.083778000
6	4.448924000	-0.697590000	0.644332000	1	4.040155000	1.454691000	-1.204329000
1	2.959732000	0.111341000	2.093015000	6	3.859429000	-1.382252000	1.425336000
1	5.255452000	0.080124000	-1.279146000	1	1.665265000	-1.055908000	1.084755000
1	5.211509000	-0.522788000	1.418984000	6	5.147293000	-0.936841000	1.042266000
1	2.508429000	-1.484761000	1.411304000	1	6.200444000	0.491395000	-0.255209000
1	4.736060000	1.345637000	-0.123128000	1	3.727166000	-2.179783000	2.159275000
1	2.899152000	-0.593058000	-1.699224000	1	6.047713000	-1.382361000	1.471417000
1	4.589049000	-1.715743000	0.246580000	77	-0.166249000	0.009016000	-0.348921000
77	0.110463000	-0.221337000	-0.031518000				
OAT <sup>‡</sup> - Ir							
	6	0.441079000	-1.793383000	-1.097263000			
	1	-0.255759000	-2.106529000	-1.899576000			
	1	1.436812000	-1.655853000	-1.561023000			
	1	0.526584000	-2.630891000	-0.369616000			
	6	-2.484386000	1.887559000	-0.080337000			
	1	-2.277807000	2.105935000	-1.146976000			
	1	-3.200539000	2.634227000	0.310944000			
	8	-1.243702000	1.956049000	0.652557000			

6	-0.550474000	3.197712000	0.441451000
1	0.400592000	3.118619000	0.983292000
1	-0.344022000	3.350450000	-0.633310000
1	-1.150883000	4.039179000	0.837632000
7	-2.123793000	-0.539616000	-0.032748000
6	-2.602761000	-1.821214000	0.092783000
6	-3.045638000	0.484950000	0.070551000
6	-3.959813000	-2.121050000	0.315744000
1	-1.855973000	-2.609945000	0.003643000
6	-4.415657000	0.255568000	0.300937000
6	-4.903435000	-1.069680000	0.420574000
1	-4.260847000	-3.167858000	0.401916000
1	-5.088484000	1.112681000	0.388735000
1	-5.963235000	-1.267971000	0.595706000
8	1.444387000	0.881074000	-0.454349000
7	2.975580000	0.232821000	-0.000097000
6	3.071976000	-0.800723000	0.853821000
6	4.056694000	0.790147000	-0.571352000
6	4.334537000	-1.346370000	1.188680000
1	2.115264000	-1.163226000	1.245331000
6	5.356588000	0.312528000	-0.286716000
1	3.855635000	1.617183000	-1.259473000
6	5.495577000	-0.779470000	0.608081000
1	4.394887000	-2.188726000	1.881420000
1	6.223919000	0.778848000	-0.759576000
1	6.485960000	-1.178391000	0.845043000
77	-0.173712000	-0.058657000	-0.191709000

[N-O]Ir <sup>III</sup> (O)(Me)				[(N-O)Ir <sup>III</sup> (Py)(O)(Me)]			
6	-1.096994000	-1.686707000	1.480032000	8	0.251798000	-2.105174000	-0.182566000
1	-0.462133000	-1.330612000	2.310409000	6	0.098281000	0.700714000	1.918067000
1	-2.129635000	-1.839486000	1.830516000	1	0.209090000	1.803698000	1.831688000
1	-0.706540000	-2.667913000	1.127925000	1	-0.835387000	0.499172000	2.475572000
6	1.021392000	1.857326000	0.789739000	1	0.935935000	0.330239000	2.534754000
1	0.092112000	1.601633000	1.329939000	6	-2.075934000	2.058024000	-0.104347000
1	1.679842000	2.440363000	1.465452000	1	-2.703415000	2.783897000	-0.655093000
8	0.732526000	2.606428000	-0.393683000	1	-1.980269000	2.409501000	0.942029000
6	-0.272681000	3.607105000	-0.165525000	8	-0.777768000	1.972512000	-0.703200000
1	-0.396104000	4.147596000	-1.115728000	6	-0.093639000	3.232402000	-0.719564000
1	-1.231481000	3.138099000	0.119220000	1	0.865504000	3.059570000	-1.227017000
1	0.047118000	4.322360000	0.620165000	1	-0.679218000	3.983037000	-1.283931000
7	0.982166000	-0.462579000	-0.105748000	1	0.085766000	3.607118000	0.306531000
6	1.622235000	-1.585911000	-0.551459000	7	-1.953570000	-0.415856000	-0.010009000
6	1.736288000	0.582099000	0.367194000	6	-2.535692000	-1.647780000	0.030281000
6	3.021184000	-1.731697000	-0.529091000	6	-2.746755000	0.686497000	-0.126040000
1	0.981654000	-2.377903000	-0.946680000	6	-3.933318000	-1.821721000	-0.037873000
6	3.147717000	0.500140000	0.403081000	1	-1.806534000	-2.463402000	0.094150000
6	3.812064000	-0.664373000	-0.041285000	6	-4.153804000	0.587786000	-0.223160000
1	3.465810000	-2.658217000	-0.897611000	6	-4.765755000	-0.685533000	-0.167923000
1	3.707627000	1.360566000	0.775178000	1	-4.348088000	-2.831023000	0.005902000
1	4.902116000	-0.733709000	-0.017430000	1	-4.750432000	1.496629000	-0.335334000
8	-2.306386000	0.767938000	-0.213645000	1	-5.852709000	-0.784622000	-0.230040000
77	-1.067297000	-0.447111000	-0.149592000	7	2.189505000	-0.198625000	-0.020543000
				6	2.907383000	0.883981000	0.384100000
				6	2.873106000	-1.265411000	-0.527147000
				6	4.313605000	0.961716000	0.289433000
				6	4.280266000	-1.271596000	-0.654557000
				6	5.023023000	-0.139233000	-0.246887000
				1	2.330631000	1.711714000	0.798569000
				1	2.225796000	-2.106374000	-0.792135000
				1	4.825513000	1.863673000	0.632250000

	1	4.771109000	-2.154104000	-1.071105000
	1	6.112460000	-0.113592000	-0.342719000
	77	0.103972000	-0.278072000	0.061424000
<b>Methyl Migration* - Ir</b>				
8	0.285882000	-2.101576000	0.146385000	
6	0.292696000	-1.360593000	1.932224000	
1	0.231521000	-0.396013000	2.488040000	
1	-0.545138000	-2.001597000	2.226564000	
1	1.261598000	-1.832003000	2.122742000	
6	-1.945845000	2.102585000	0.231824000	
1	-2.496624000	2.973106000	-0.169300000	
1	-1.797481000	2.239471000	1.322773000	
8	-0.650155000	2.008965000	-0.398001000	
6	0.157905000	3.169478000	-0.146909000	
1	1.099290000	3.023078000	-0.691969000	
1	-0.352656000	4.076192000	-0.522097000	
1	0.359460000	3.274841000	0.936305000	
7	-1.956339000	-0.323421000	-0.063018000	
6	-2.587562000	-1.525119000	-0.211311000	
6	-2.712774000	0.815756000	-0.027202000	
6	-3.988808000	-1.625076000	-0.330913000	
1	-1.899131000	-2.375559000	-0.225819000	
6	-4.115572000	0.795979000	-0.172946000	
6	-4.776026000	-0.448263000	-0.320060000	
1	-4.444342000	-2.611612000	-0.442255000	
1	-4.674334000	1.735357000	-0.161405000	
1	-5.862654000	-0.493840000	-0.427844000	
7	2.110856000	-0.059624000	-0.115900000	
6	2.872694000	0.858477000	0.544701000	
6	2.760727000	-1.012981000	-0.851755000	
6	4.279287000	0.903444000	0.462640000	
6	4.167883000	-1.036238000	-0.990443000	
6	4.949733000	-0.059676000	-0.333190000	
1	2.320372000	1.566316000	1.165568000	
1	2.109866000	-1.757560000	-1.306443000	
1	4.825641000	1.669878000	1.017259000	
1	4.627206000	-1.815601000	-1.602808000	
1	6.039419000	-0.051746000	-0.426871000	
77	0.063695000	-0.172301000	-0.009832000	

<b>PyO</b>				<b>THF</b>			
6	0.291298000	-1.189525000	-0.000188000	6	-1.174217000	-0.433075000	-0.135694000
6	-1.116124000	-1.212065000	-0.000123000	8	0.000004000	-1.265896000	0.000000000
6	-1.849993000	0.000002000	0.000094000	6	1.174218000	-0.433069000	0.135694000
6	-1.116116000	1.212068000	0.000219000	6	0.738482000	1.006589000	-0.234389000
6	0.291303000	1.189526000	0.000145000	6	-0.738487000	1.006586000	0.234388000
7	0.995081000	-0.000002000	-0.000042000	1	-1.535852000	-0.481407000	-1.182448000
1	-2.942045000	0.000007000	0.000143000	1	-1.964554000	-0.830701000	0.524467000
1	0.923470000	-2.078191000	-0.000346000	1	1.535853000	-0.481398000	1.182449000
1	-1.618286000	-2.182215000	-0.000239000	1	1.964559000	-0.830692000	-0.524465000
1	-1.618275000	2.182219000	0.000377000	1	1.355573000	1.774980000	0.258325000
1	0.923481000	2.078188000	0.000237000	1	0.794515000	1.159614000	-1.325777000
8	2.295484000	-0.000004000	-0.000096000	1	-0.794520000	1.159609000	1.325777000
				1	-1.355583000	1.774974000	-0.258324000
<b>Methyl Migration – Four Coordinate -Ir</b>				<b>Ir<sup>I</sup>-Methoxide</b>			
6	-2.462725000	-1.202942000	1.337906000	6	-2.918555000	-0.728433000	0.439298000
1	-2.183449000	-2.246666000	1.500812000	1	-2.867079000	-0.897027000	1.533407000
1	-2.077913000	-0.544304000	2.131984000	1	-3.925595000	-1.002454000	0.078570000
1	-3.535634000	-1.054042000	1.185592000	8	-1.928940000	-1.579323000	-0.194427000
6	1.227938000	2.043713000	-0.138358000	6	-2.040504000	-2.974209000	0.191250000

1	1.747652000	2.875636000	0.368680000	1	-1.160265000	-3.470116000	-0.232832000
1	1.100352000	2.286872000	-1.213138000	1	-2.019638000	-3.062689000	1.291743000
8	-0.081127000	1.840983000	0.441976000	1	-2.984703000	-3.377874000	-0.215091000
6	-0.983816000	2.935325000	0.165931000	7	-1.238483000	1.002048000	-0.001850000
1	-1.928923000	2.696692000	0.668561000	6	-0.914268000	2.326348000	-0.197138000
1	-0.557424000	3.869965000	0.573491000	6	-2.591185000	0.717134000	0.111525000
1	-1.151240000	3.025391000	-0.921473000	6	-1.866991000	3.355653000	-0.292856000
7	1.139719000	-0.370965000	-0.059360000	1	0.151004000	2.541171000	-0.288250000
6	1.743318000	-1.604480000	-0.026083000	6	-3.598819000	1.691787000	-0.012084000
6	1.963092000	0.732741000	0.018566000	6	-3.249843000	3.051200000	-0.209497000
6	3.134590000	-1.771360000	0.095750000	1	-1.518732000	4.380191000	-0.445745000
1	1.064368000	-2.454172000	-0.105426000	1	-4.645828000	1.384477000	0.061330000
6	3.359765000	0.639506000	0.170111000	1	-4.013937000	3.826215000	-0.298620000
6	3.975320000	-0.635351000	0.205950000	7	1.704535000	0.428326000	0.066472000
1	3.541861000	-2.784626000	0.110431000	6	2.469115000	0.616861000	-1.053943000
1	3.950504000	1.556296000	0.244272000	6	2.164361000	0.961455000	1.239814000
1	5.057393000	-0.736701000	0.313236000	6	3.679288000	1.340910000	-1.045097000
8	-2.250226000	-1.268652000	-0.581781000	1	2.073315000	0.167889000	-1.964721000
77	-0.858437000	-0.198638000	-0.185736000	6	3.366072000	1.696528000	1.331352000
				1	1.533791000	0.779364000	2.110097000
				6	4.146921000	1.898686000	0.169059000
				1	4.234784000	1.456356000	-1.978595000
				1	3.671819000	2.093894000	2.301858000
				1	5.081797000	2.464211000	0.207451000
				8	0.840512000	-2.401157000	-0.135802000
				6	2.227176000	-2.638337000	-0.177032000
				1	2.772812000	-2.196691000	0.687903000
				1	2.410084000	-3.733267000	-0.154535000
				1	2.711683000	-2.250702000	-1.103200000
				77	-0.016842000	-0.586561000	-0.030769000

**Ir<sup>I</sup>-Methoxide – Four Coordinate**

6	1.395390000	1.880301000	0.547576000
1	1.099786000	1.964803000	1.611749000
1	2.079317000	2.706450000	0.285064000
8	0.197657000	1.943349000	-0.267543000
6	-0.608507000	3.109895000	0.013142000
1	-1.451705000	3.078062000	-0.687496000
1	-0.979347000	3.076898000	1.052268000
1	-0.002303000	4.018331000	-0.156988000
7	1.068483000	-0.443851000	-0.025998000
6	1.529890000	-1.717007000	-0.257869000
6	2.004765000	0.527026000	0.263623000
6	2.894588000	-2.052331000	-0.202254000
1	0.758265000	-2.452444000	-0.487124000
6	3.387427000	0.263575000	0.314938000
6	3.856531000	-1.052139000	0.088343000
1	3.188516000	-3.086746000	-0.392665000
1	4.078256000	1.081250000	0.536475000
1	4.922745000	-1.284960000	0.130401000
8	-2.318732000	-1.195118000	-0.195729000
6	-2.879658000	-1.868066000	0.934999000
1	-2.424107000	-2.874564000	1.032536000
1	-2.737201000	-1.319313000	1.882940000
1	-3.964183000	-1.999797000	0.752275000
77	-0.838459000	-0.004343000	-0.154367000

**Table S-2. Computed Stationary Points. Stoichiometry - charge (if any) and multiplicity (other than singlet) noted.  $\nu_i$  = number of imaginary frequencies; a.u. = atomic units.**

File Name	Stoichiometry	G(a.u.)	$\nu_i$	Comment
THF	C4H8O	-43.2848	0	THF
Py	C5H5N	-41.0765	0	pyridine
PyO	C5H5NO	-56.9906	0	Py-N-oxide
4CN_Ni.out	C8H12NNiO2(1+,3)	-263.4316	0	triplet (N~O)Ni(OMe)
4CN_Ni	C8H12NNiO2(1+)	-263.4027	0	(N~O)Ni(OMe)
OxoA_Ni.out	C8H12NNiO2(1+,3)	-263.3481	0	(N~O)Ni(Me)O triplet
co4_ts_Ni.out	C8H12NNiO2(1+,3)	-263.3470	1	4 coord Me migration TS triplet
PyOxoA_Ni	C8H12NNiO2(1+)	-263.3151	0	(N~O)Ni(Me)O
co4_ts_Ni	C8H12NNiO2(1+)	-263.3130	1	4 coord Me migration TS Ni
4CN_Co	C8H12CoNO2	-239.2502	0	(N~O)Co(OMe)
OxoA_Co	C8H12CoNO2	-239.2203	0	(N~O)Co(Me)O
co_ts_Co	C8H12CoNO2	-239.1920	1	4 coord Me migration TS Co
productFromCO_Pd	C8H12NO2Pd(1+)	-221.2123	0	(N~O)Pd(OMe)
co_ts_Pd	C8H12NO2Pd(1+)	-221.1085	1	4 coord Me migration TS Pd
PyOxoA_Pd	C8H12NO2Pd(1+)	-221.1076	0	(N~O)Pd(Me)O
productFromCO	C8H12NO2Pt(1+)	-213.6399	0	(N~O)Pt(OMe)
op_oxo	C8H12NO2Pt(1+)	-213.5828	0	(N~O)Pt(Me)O
co_ts_031511	C8H12NO2Pt(1+)	-213.5558	1	4 coord Me migration TS Pt
7_product_4	C8H12NO2Rh	-204.1791	0	(N~O)Rh(OMe)
5_Oxo_4	C8H12NO2Rh	-204.1475	0	(N~O)Rh(Me)O
6_co_4	C8H12NO2Rh	-204.1048	1	4 coord Me migration Rh
productFromCO_ir	C8H12IrNO2	-198.9119	0	(N~O)Ir(OMe)
PyOxoA_ir	C8H12IrNO2	-198.9081	0	(N~O)Ir(Me)O
newA_co_ts_ir	C8H12IrNO2	-198.8493	0	4 coord Me migration TS Ir
adduct_Ni	C12H20NNiO2(1+)	-290.7324	0	THF complex of Ni
precursor_Ni	C12H20NNiO2(1+,3)	-290.7301	0	triplet THF complex of Ni
adduct_CoA_tight	C12H20CoNO2	-266.5323	1	THF complex of Co
reactantA_mci_Pd	C12H20NO2Pd(1+)	-248.5685	0	THF complex of Pd
reactant_mciA	C12H20NO2Pt(1+)	-241.0063	0	THF complex of Pt
2_precuser	C12H20NO2Rh	-231.4901	0	THF complex of Rh
reactant_mciA_ir	C12H20IrNO2	-226.2270	0	THF complex of Ir
5CN_Ni.out	C13H17N2NiO2(1+,3)	-304.5300	0	(N~O)Ni(Py)(OMe) triplet
5CN_Ni	C13H17N2NiO2(1+)	-304.5205	0	(N~O)Ni(Py)(OMe) singlet
mci_a_Ni	C13H17N2NiO2(1+)	-304.4585	0	(N~O)Ni(PyO)(Me) singlet
adduct_a_ni.out	C13H17N2NiO2(1+,3)	-304.4575	0	(N~O)Ni(PyO)(Me) triplet
Oxo5_Ni.out	C13H17N2NiO2(1+,3)	-304.4292	0	triplet oxo intermediate Ni
co5_ts_Ni.out	C13H17N2NiO2(1+,3)	-304.4282	1	migration TS triplet Ni
PyOxo5_Ni	C13H17N2NiO2(1+)	-304.4133	0	singlet oxo intermediate Ni
co5_ts_Ni	C13H17N2NiO2(1+)	-304.4121	1	migration TS Ni
no_ts4_Ni	C13H17N2NiO2(1+)	-304.3858	1	OAT TS Ni
5CN_Co	C13H17CoN2O2	-280.3426	0	(N~O)Co(Py)(OMe)
Oxo5_Co	C13H17CoN2O2	-280.3005	0	singlet oxo intermediate Co
co_ts5_Co	C13H17CoN2O2	-280.2601	1	migration TS Co
mciA_Co	C13H17CoN2O2	-280.2515	0	(N~O)Co(PyO)(Me) singlet
oat_ts_Co	C13H17CoN2O2	-280.2300	1	OAT TS Co
product_Pd	C13H17N2O2Pd(1+)	-262.3335	0	(N~O)Pd(Py)(OMe)
bisPyInterMa_Pd	C13H17N2O2Pd(1+)	-262.2919	0	(N~O)Pt(PyO)(Me) singlet

PyOxo5_Pd	C13H17N2O2Pd(1+)	-262.2322	0	singlet oxo intermediate Pd
co_ts5cn_Pd	C13H17N2O2Pd(1+)	-262.2250	1	migration TS Pd
no_ts_Pd	C13H17N2O2Pd(1+)	-262.1966	1	OAT TS Pd
productA	C13H17N2O2Pt(1+)	-254.7748	0	(N~O)Pt(Py)(OMe)
bisPyInterMa	C13H17N2O2Pt(1+)	-254.7318	0	(N~O)Pt(PyO)(Me) singlet
PyOxo5	C13H17N2O2Pt(1+)	-254.6913	0	singlet oxo intermediate Pt
co_ts5cn	C13H17N2O2Pt(1+)	-254.6710	1	migration TS Pt
no_tsa3	C13H17N2O2Pt(1+)	-254.6533	1	OAT TS Pt
7_product_5	C13H17N2O2Rh	-245.2803	0	(N~O)Ir(Py)(OMe)
5_Oxo_5	C13H17N2O2Rh	-245.2336	0	singlet oxo intermediate Rh
3_MCI	C13H17N2O2Rh	-245.2037	0	(N~O)Rh(PyO)(Me) singlet
6_co_5	C13H17N2O2Rh	-245.1910	1	migration TS Rh
4_OAT	C13H17N2O2Rh	-245.1798	1	OAT TS Rh
product_ir	C13H17IrN2O2	-240.0167	0	(N~O)Ir(Py)(OMe)
PyOxo5_ir	C13H17IrN2O2	-239.9876	0	singlet oxo intermediate Ir
bisPyInterMa_ir	C13H17IrN2O2	-239.9472	0	(N~O)Ir(PyO)(Me) singlet
no_ts4_ir	C13H17IrN2O2	-239.9297	1	OAT TS Ir
co_ts5cn	C13H17IrN2O2	-239.9283	1	migration TS Ir