Electronic Supplementary Material (ESI) for Dalton Transactions

Computational Hammett Analysis of Redox Based Oxy-Insertion by Pt(II) Complexes

Travis M. Figg and Thomas R. Cundari*

Center for Catalytic Hydrocarbon Functionalization

Department of Chemistry and Center for Advanced Scientific Computing and Modeling

(CASCaM); University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017;

t@unt.edu

Table S-1. Calculated active site bond lengths for the various substituted catalytic components in the MCI ground state. Bond lengths given in Å.

Substituted Component	Pt-C_{ipso}	Pt-O	Pt-Py	C_{ipso}-O
Ph	2.03	2.09	3.02	3.00
p-NO_2-Ph	2.03	2.08	3.02	2.99
p-OMe-Ph	2.03	2.09	3.02	3.00
p-NMe_2-Ph	2.03	2.09	3.01	3.00
m-NO_2-Ph	2.03	2.08	3.01	2.98
m-OMe-Ph	2.03	2.08	3.00	2.99
m-NMe_2-Ph	2.03	2.09	3.00	2.98
m-$(NO_2)_2$-Ph	2.03	2.08	3.04	3.04
4-OMe-Py	2.03	2.08	3.00	2.98
4-NMe_2-Py	2.03	2.07	3.00	2.99
3-NO_2-Py	2.03	2.10	3.02	3.02
3-OMe-Py	2.03	2.08	3.01	3.00
3-NMe_2-Py	2.03	2.08	3.01	2.99
4,4'-NO_2-bpy	2.03	2.07	3.02	3.00
4,4'-OMe-bpy	2.03	2.09	3.01	3.01
4,4'-NMe_2-bpy	2.03	2.09	3.05	2.97
5,5'-NO_2-bpy	2.03	2.07	3.01	2.99
5,5'-OMe-bpy	2.03	2.09	3.01	3.00
5,5'-NMe_2-bpy	2.03	2.09	3.01	2.99

Table S-2. Calculated active site bond lengths for the various substituted catalytic components in the aryl migration transition state. Bond lengths given in Å.

Substituted Component	Pt-C_{ipso}	Pt-O	Pt-Py	C_{ipso}-O
Ph	2.16	1.92	2.07	2.28
p-NO_2-Ph	2.13	1.92	2.07	2.27
p-OMe-Ph	2.16	1.92	2.07	2.27
p-NMe_2-Ph	2.15	1.92	2.07	2.29
m-NO_2-Ph	2.13	1.92	2.07	2.28
m-OMe-Ph	2.16	1.92	2.07	2.27
m-NMe_2-Ph	2.17	1.92	2.07	2.28
m-$(NO_2)_2$-Ph	2.12	1.92	2.07	2.27
m-$(OMe)_2$-Ph	2.17	1.92	2.07	2.28
m-$(NMe_2)_2$-Ph	2.19	1.92	2.07	2.28
4-NO_2-Py	2.16	1.92	2.07	2.28
4-OMe-Py	2.15	1.92	2.07	2.27
4-NMe_2-Py	2.15	1.92	2.06	2.27
3-NO_2-Py	2.16	1.92	2.07	2.28
3-OMe-Py	2.16	1.92	2.07	2.28
3-NMe_2-Py	2.15	1.92	2.07	2.27
3,5-NO_2-Py	2.16	1.92	2.08	2.28
3,5-OMe-Py	2.15	1.92	2.07	2.28
3,5-NMe_2-Py	2.15	1.92	2.07	2.27
4,4'-NO_2-bpy	2.17	1.91	2.07	2.29
4,4'-OMe-bpy	2.15	1.93	2.07	2.26
4,4'-NMe_2-bpy	2.14	1.93	2.07	2.26
5,5'-NO_2-bpy	2.16	1.91	2.07	2.28
5,5'-OMe-bpy	2.15	1.92	2.07	2.27
5,5'-NMe_2-bpy	2.15	1.93	2.07	2.27

Table S-3. Cartesian Coordinates (Å) for B3LYP/CEP-31G(d) Optimized Stationary Points. Atomic Number (Z) is given in the first column.

MCI – $[(bpy)Pt^{II}(Ph)(OPy)]^+$

78	-0.237932000	-0.118498000	-0.085198000
6	-2.996210000	0.799589000	0.147350000
6	-1.490906000	2.614904000	0.231667000
6	-4.094620000	1.678825000	0.295230000
6	-2.542470000	3.542042000	0.382740000
1	-0.450499000	2.933673000	0.200368000
6	-3.871840000	3.066740000	0.414619000
1	-5.110977000	1.286445000	0.319487000
1	-2.308526000	4.603999000	0.471121000

1	-4.713331000	3.753516000	0.529946000
6	-3.152190000	-0.681306000	0.019218000
6	-2.003906000	-2.719191000	-0.219394000
6	-4.402392000	-1.347355000	0.012914000
6	-3.208302000	-3.456913000	-0.235922000
1	-1.027159000	-3.200863000	-0.309690000
6	-4.429019000	-2.753289000	-0.116134000
1	-5.336008000	-0.792006000	0.103349000
1	-3.181282000	-4.542721000	-0.340262000
1	-5.383351000	-3.285061000	-0.124325000
7	-1.983153000	-1.375494000	-0.094628000
7	-1.705324000	1.278957000	0.115648000
8	0.996252000	-1.787941000	-0.285224000
6	2.810643000	-2.060985000	1.175561000
6	3.163411000	-1.278917000	-1.047028000
6	4.193110000	-2.036913000	1.436256000
1	2.050345000	-2.367870000	1.894153000
6	4.555005000	-1.228631000	-0.837473000
1	2.669127000	-1.011615000	-1.979338000
6	5.081410000	-1.612760000	0.418121000
1	4.551652000	-2.343009000	2.420145000
1	5.198234000	-0.890031000	-1.650718000
1	6.158202000	-1.582597000	0.600055000
7	2.338160000	-1.692261000	-0.046916000
6	1.311787000	1.191281000	-0.104464000
6	1.720749000	1.817299000	-1.317732000
6	2.031927000	1.515083000	1.081045000
6	2.816416000	2.719511000	-1.350799000
1	1.180429000	1.612366000	-2.248083000
6	3.127286000	2.418542000	1.056349000
1	1.736007000	1.073709000	2.038799000
6	3.526819000	3.021612000	-0.162345000
1	3.104454000	3.188488000	-2.296606000
1	3.656852000	2.654344000	1.984464000
1	4.366505000	3.722225000	-0.183070000

MCI – [(bpy)Pt^{II}(*p*-NO_2-Ph)(OPy)]$^+$

78	-0.751690000	-0.207663000	-0.082652000
6	-3.081655000	1.528833000	0.158874000
6	-1.084718000	2.777284000	0.301783000
6	-3.850565000	2.705854000	0.315611000
6	-1.793533000	3.985108000	0.464358000
1	0.003482000	2.756397000	0.289483000
6	-3.205301000	3.950830000	0.470113000
1	-4.938996000	2.652749000	0.318809000
1	-1.239499000	4.917687000	0.580864000
1	-3.790297000	4.865079000	0.592057000
6	-3.691021000	0.174496000	-0.004019000
6	-3.232854000	-2.116118000	-0.281076000
6	-5.085948000	-0.067484000	-0.033254000
6	-4.607193000	-2.439381000	-0.321476000
1	-2.454505000	-2.876989000	-0.376535000
6	-5.548524000	-1.392106000	-0.193893000
1	-5.800419000	0.750008000	0.063554000
1	-4.919154000	-3.476988000	-0.450009000
1	-6.620952000	-1.598706000	-0.220135000
7	-2.795641000	-0.848430000	-0.126055000
7	-1.705252000	1.578994000	0.151231000
8	-0.111609000	-2.173667000	-0.343742000
6	1.463467000	-3.012303000	1.184423000
6	2.118494000	-2.448887000	-1.036692000
6	2.765712000	-3.449248000	1.489885000
1	0.625312000	-3.031115000	1.881451000
6	3.438922000	-2.868146000	-0.783104000
1	1.766989000	-2.054556000	-1.989091000
6	3.771662000	-3.375196000	0.495431000
1	2.974099000	-3.834897000	2.488966000
1	4.179596000	-2.790574000	-1.580264000
1	4.790265000	-3.705128000	0.712248000
7	1.176838000	-2.531770000	-0.057320000
6	1.133918000	0.533399000	-0.072074000
6	1.739713000	0.996577000	-1.279085000
6	1.911050000	0.592557000	1.123341000
6	3.069468000	1.478560000	-1.308818000
1	1.170940000	0.989609000	-2.213588000
6	3.243268000	1.069907000	1.123869000
1	1.477287000	0.271639000	2.075237000
6	3.805318000	1.499498000	-0.100920000
1	3.531252000	1.832122000	-2.231127000
1	3.836104000	1.115969000	2.037705000
7	5.205850000	1.986179000	-0.118305000
8	5.674992000	2.365119000	-1.212706000
8	5.835327000	1.980601000	0.961542000

MCI – [(bpy)Pt^{II}(*p*-OMe-Ph)(OPy)]$^+$

78	0.621317000	-0.212873000	0.086116000
6	3.023967000	1.421897000	-0.149352000
6	1.081188000	2.760591000	-0.195198000
6	3.841189000	2.569673000	-0.276575000
6	1.840368000	3.941599000	-0.325859000
1	-0.006578000	2.781222000	-0.157696000
6	3.248784000	3.846876000	-0.365582000
1	4.925899000	2.469183000	-0.306787000
1	1.326048000	4.901544000	-0.391575000
1	3.871202000	4.739075000	-0.463771000
6	3.576783000	0.036561000	-0.056589000
6	3.026367000	-2.240988000	0.137528000
6	4.960709000	-0.265509000	-0.074223000
6	4.385617000	-2.624740000	0.127880000
1	2.217410000	-2.970799000	0.222144000
6	5.368648000	-1.614058000	0.019157000
1	5.707592000	0.524238000	-0.156293000
1	4.655104000	-3.679291000	0.204783000
1	6.431351000	-1.867342000	0.008532000
7	2.640797000	-0.950752000	0.047244000
7	1.651641000	1.531388000	-0.106674000

8	-0.113330000	-2.154054000	0.289585000
6	-1.802441000	-2.917242000	-1.146318000
6	-2.330247000	-2.231954000	1.073321000
6	-3.143810000	-3.264902000	-1.391077000
1	-0.994504000	-3.018256000	-1.871340000
6	-3.687116000	-2.555258000	0.879485000
1	-1.916363000	-1.833825000	1.997862000
6	-4.103642000	-3.080552000	-0.366089000
1	-3.416593000	-3.667066000	-2.367906000
1	-4.389697000	-2.389550000	1.697236000
1	-5.151058000	-3.341212000	-0.534939000
7	-1.433826000	-2.423010000	0.067456000
6	-1.225377000	0.631299000	0.155112000
6	-1.766510000	1.110174000	1.386345000
6	-2.038362000	0.773862000	-0.999882000
6	-3.056196000	1.682145000	1.464795000
1	-1.174346000	1.047597000	2.305531000
6	-3.338866000	1.349803000	-0.950307000
1	-1.665399000	0.445659000	-1.976123000
6	-3.855159000	1.804302000	0.293007000
1	-3.455381000	2.048753000	2.413890000
1	-3.916421000	1.441760000	-1.871390000
6	-5.913464000	2.570012000	-0.688356000
1	-5.419263000	3.233610000	-1.421562000
1	-6.836030000	3.045872000	-0.329479000
1	-6.162539000	1.607268000	-1.172694000
8	-5.093919000	2.374142000	0.471794000

MCI – $[(bpy)Pt^{II}(m\text{-}NO_2\text{-}Ph)(OPy)]^+$

78	0.669855000	-0.205178000	0.214625000
6	3.165530000	1.232502000	-0.240099000
6	1.363142000	2.735615000	0.000590000
6	4.063301000	2.309672000	-0.427181000
6	2.205073000	3.851548000	-0.182671000
1	0.294812000	2.854163000	0.172224000
6	3.583927000	3.636198000	-0.398866000
1	5.122316000	2.116865000	-0.596913000
1	1.776423000	4.854380000	-0.154011000
1	4.268913000	4.474472000	-0.543990000
6	3.594467000	-0.198432000	-0.268475000
6	2.856957000	-2.426818000	-0.111606000
6	4.933471000	-0.620164000	-0.453859000
6	4.165693000	-2.927112000	-0.290111000
1	1.997625000	-3.086280000	0.031797000
6	5.221299000	-2.002761000	-0.464354000
1	5.737938000	0.103726000	-0.584064000
1	4.341844000	-4.003887000	-0.289408000
1	6.248384000	-2.347748000	-0.604205000
7	2.586998000	-1.104236000	-0.102429000
7	1.824174000	1.458843000	-0.023930000
8	-0.201633000	-2.085264000	0.414038000
6	-2.002730000	-2.368928000	-1.079071000
6	-2.370763000	-2.315856000	1.275058000
6	-3.372911000	-2.571328000	-1.320914000
1	-1.243429000	-2.293128000	-1.857462000
6	-3.751028000	-2.527712000	1.090265000
1	-1.884456000	-2.199602000	2.243455000
6	-4.263192000	-2.654418000	-0.223099000
1	-3.722781000	-2.653425000	-2.350647000
1	-4.398891000	-2.582248000	1.966296000
7	-1.543189000	-2.246045000	0.197414000
6	-1.079872000	0.760601000	0.567933000
6	-1.391520000	1.286122000	1.857877000
6	-2.061165000	0.905077000	-0.448839000
6	-2.630759000	1.925129000	2.129751000
1	-0.660406000	1.201728000	2.667862000
6	-3.300475000	1.524734000	-0.156357000
1	-1.888356000	0.558622000	-1.467792000
6	-3.610456000	2.052456000	1.117958000
1	-4.572527000	2.532390000	1.296719000
1	-5.331726000	-2.809397000	-0.389124000
1	-2.832759000	2.319272000	3.129158000
7	-4.322665000	1.604599000	-1.231688000
8	-4.096524000	0.984292000	-2.296828000
8	-5.355184000	2.267865000	-1.008432000

MCI – $[(bpy)Pt^{II}(m\text{-}OMe\text{-}Ph)(OPy)]^+$

78	-0.533924000	-0.233924000	-0.008586000
6	-3.013946000	1.287056000	0.190674000
6	-1.145178000	2.648654000	0.662334000
6	-3.887922000	2.378431000	0.405982000
6	-1.963199000	3.774122000	0.891462000
1	-0.061502000	2.703705000	0.749742000
6	-3.362716000	3.638805000	0.760615000
1	-4.964661000	2.247166000	0.301217000
1	-1.499786000	4.723563000	1.163682000
1	-4.029305000	4.487412000	0.929724000
6	-3.494647000	-0.077908000	-0.182972000
6	-2.832967000	-2.280978000	-0.668935000
6	-4.857860000	-0.409050000	-0.379722000
6	-4.167488000	-2.690696000	-0.884124000
1	-1.991148000	-2.970331000	-0.770960000
6	-5.197041000	-1.732914000	-0.734798000
1	-5.640710000	0.340637000	-0.264202000
1	-4.382809000	-3.724181000	-1.160092000
1	-6.242667000	-2.007480000	-0.892543000
7	-2.513329000	-1.014731000	-0.328508000
7	-1.650937000	1.435760000	0.319957000
8	0.300764000	-2.102865000	-0.395497000
6	1.836744000	-3.008678000	1.125975000
6	2.595048000	-2.036370000	-0.913125000
6	3.150532000	-3.364025000	1.482012000
1	0.953482000	-3.212773000	1.731531000
6	3.929521000	-2.361604000	-0.601933000
1	2.279066000	-1.527507000	-1.822139000
6	4.215723000	-3.035596000	0.608236000

1	3.321485000	-3.882665000	2.426492000
1	4.716035000	-2.083569000	-1.304698000
7	1.595547000	-2.369393000	-0.051724000
6	1.268705000	0.651852000	0.277596000
6	1.920445000	1.303188000	-0.799836000
6	1.915948000	0.638055000	1.548984000
6	3.195475000	1.920820000	-0.633058000
1	1.462004000	1.362349000	-1.791384000
6	3.179237000	1.255784000	1.716583000
1	1.437289000	0.163119000	2.410868000
6	3.835702000	1.899117000	0.635802000
1	3.661205000	1.246123000	2.698901000
1	4.805295000	2.371998000	0.795403000
1	5.244128000	-3.299563000	0.865633000
6	4.970977000	3.196481000	-1.643493000
8	3.716529000	2.508534000	-1.761942000
1	4.906327000	4.024749000	-0.914802000
1	5.781729000	2.506188000	-1.345935000
1	5.186764000	3.603068000	-2.640892000

MCI – $[(bpy)Pt^{II}(m\text{-}NMe_2\text{-}Ph)(OPy)]^+$

78	-0.699554000	-0.258123000	-0.162723000
6	-3.118535000	1.351022000	0.084570000
6	-1.233239000	2.709622000	-0.328541000
6	-3.955021000	2.491126000	0.128223000
6	-2.013530000	3.883771000	-0.295199000
1	-0.159877000	2.740780000	-0.508173000
6	-3.402194000	3.774921000	-0.062501000
1	-5.023703000	2.379968000	0.310420000
1	-1.530313000	4.849554000	-0.450572000
1	-4.039494000	4.661415000	-0.029780000
6	-3.629856000	-0.040001000	0.280052000
6	-3.028395000	-2.310186000	0.384298000
6	-4.991827000	-0.356535000	0.507699000
6	-4.364056000	-2.708541000	0.613599000
1	-2.210584000	-3.032524000	0.322173000
6	-5.362121000	-1.708658000	0.676326000
1	-5.750855000	0.424639000	0.551115000
1	-4.604480000	-3.765845000	0.735865000
1	-6.407632000	-1.973104000	0.851245000
7	-2.678793000	-1.016535000	0.224406000
7	-1.766029000	1.473819000	-0.144505000
8	0.083371000	-2.188818000	-0.100484000
6	2.064913000	-2.728586000	1.021597000
6	2.092269000	-2.321125000	-1.325668000
6	3.442571000	-3.013921000	1.020192000
1	1.426801000	-2.755114000	1.905111000
6	3.474496000	-2.585427000	-1.381392000
1	1.480672000	-2.052763000	-2.184628000
6	4.162338000	-2.937217000	-0.197066000
1	3.928968000	-3.282905000	1.958952000
1	3.986134000	-2.509135000	-2.341609000
7	1.432041000	-2.400288000	-0.138204000
6	1.095382000	0.596186000	-0.569352000
6	1.456919000	0.910501000	-1.908714000
6	2.013113000	0.877458000	0.476231000
6	2.727457000	1.481997000	-2.174086000
1	0.761270000	0.732970000	-2.734530000
6	3.310276000	1.444887000	0.225058000
1	1.716008000	0.662017000	1.503737000
6	3.647230000	1.747582000	-1.136133000
1	4.606069000	2.200339000	-1.388055000
1	5.234093000	-3.147692000	-0.220645000
1	3.003746000	1.736833000	-3.202097000
7	4.219692000	1.674426000	1.269423000
6	3.713093000	1.692780000	2.647399000
6	5.408595000	2.493368000	0.994039000
1	2.915868000	2.449311000	2.801067000
1	4.542108000	1.918458000	3.333475000
1	3.308243000	0.707310000	2.934847000
1	6.037244000	2.022904000	0.219994000
1	6.014655000	2.566823000	1.908676000
1	5.155641000	3.519801000	0.658019000

MCI – $[(bpy)Pt^{II}(Ph)(4\text{-}NO_2\text{-}OPy)]^+$

78	0.800571000	-0.087800000	0.115593000
6	3.620448000	0.546485000	-0.252607000
6	2.292848000	2.495936000	-0.354112000
6	4.791199000	1.310090000	-0.470190000
6	3.421835000	3.310872000	-0.576194000
1	1.289745000	2.914990000	-0.300675000
6	4.697519000	2.708197000	-0.633881000
1	5.763987000	0.820958000	-0.514406000
1	3.287098000	4.386664000	-0.697686000
1	5.595868000	3.305981000	-0.803034000
6	3.638180000	-0.937701000	-0.078771000
6	2.311462000	-2.847568000	0.265526000
6	4.818650000	-1.720147000	-0.092889000
6	3.440030000	-3.696926000	0.264776000
1	1.298515000	-3.232866000	0.405476000
6	4.716778000	-3.117799000	0.081138000
1	5.796559000	-1.259562000	-0.232939000
1	3.313585000	-4.771560000	0.405117000
1	5.616009000	-3.738136000	0.074456000
7	2.412945000	-1.512119000	0.097676000
7	2.383856000	1.150288000	-0.193528000
8	-0.601878000	-1.619157000	0.416920000
6	-2.487226000	-1.755074000	-0.958528000
6	-2.648246000	-0.803632000	1.227023000
6	-3.860376000	-1.565451000	-1.184716000
1	-1.801485000	-2.197705000	-1.680654000
6	-4.026315000	-0.576576000	1.064474000
1	-2.089162000	-0.554108000	2.126253000
6	-4.616095000	-0.965009000	-0.155102000
1	-4.320636000	-1.866234000	-2.125241000
1	-4.612050000	-0.111781000	1.856502000

7	-1.923804000	-1.378608000	0.225266000
6	-0.613211000	1.367588000	0.161315000
6	-0.895489000	2.065201000	1.371691000
6	-1.370720000	1.714224000	-0.994325000
6	-1.910476000	3.056072000	1.433289000
1	-0.317998000	1.846327000	2.276128000
6	-2.385566000	2.706513000	-0.940816000
1	-1.165988000	1.223814000	-1.952221000
6	-2.663330000	3.377541000	0.276492000
1	-2.102593000	3.578169000	2.375430000
1	-2.946213000	2.958683000	-1.845955000
1	-3.440790000	4.145481000	0.318709000
7	-6.076089000	-0.734455000	-0.364866000
8	-6.702331000	-0.207893000	0.572545000
8	-6.548129000	-1.087136000	-1.461329000

MCI – $[(bpy)Pt^{II}(Ph)(4\text{-}OMe\text{-}OPy)]^{+}$

78	0.647285000	-0.085926000	0.139756000
6	3.463611000	0.580053000	-0.243212000
6	2.118313000	2.515797000	-0.336336000
6	4.627194000	1.354219000	-0.463475000
6	3.238701000	3.342118000	-0.560479000
1	1.110841000	2.924471000	-0.277709000
6	4.520019000	2.751608000	-0.624304000
1	5.604365000	0.874011000	-0.510976000
1	3.093905000	4.417062000	-0.678323000
1	5.412174000	3.358229000	-0.795055000
6	3.495356000	-0.904208000	-0.069237000
6	2.185527000	-2.823774000	0.289177000
6	4.681825000	-1.677763000	-0.091256000
6	3.320773000	-3.664230000	0.281741000
1	1.174933000	-3.212394000	0.438089000
6	4.591671000	-3.075740000	0.086239000
1	5.655042000	-1.209894000	-0.240155000
1	3.204103000	-4.739494000	0.426058000
1	5.495510000	-3.689354000	0.073481000
7	2.276528000	-1.488282000	0.117351000
7	2.221416000	1.170951000	-0.179752000
8	-0.715270000	-1.614156000	0.485152000
6	-2.464093000	-1.779846000	-1.093371000
6	-2.894908000	-0.947230000	1.088312000
6	-3.809266000	-1.658968000	-1.445234000
1	-1.690066000	-2.151174000	-1.765011000
6	-4.261890000	-0.794434000	0.805826000
1	-2.448698000	-0.698304000	2.049838000
6	-4.742396000	-1.153591000	-0.487433000
1	-4.147128000	-1.943734000	-2.442228000
1	-4.909920000	-0.396783000	1.584708000
7	-2.035441000	-1.431003000	0.155567000
6	-0.783121000	1.352373000	0.189320000
6	-1.110834000	2.003955000	1.413855000
6	-1.498442000	1.745349000	-0.978230000
6	-2.120860000	2.999732000	1.474989000
1	-0.571427000	1.744641000	2.330895000
6	-2.509733000	2.741133000	-0.925646000
1	-1.265580000	1.284723000	-1.944236000
6	-2.827223000	3.370985000	0.303658000
1	-2.344574000	3.487516000	2.428753000
1	-3.036421000	3.027637000	-1.841171000
1	-3.598266000	4.145917000	0.344980000
6	-7.013444000	-0.547840000	0.026534000
1	-7.090711000	-1.201124000	0.911973000
1	-7.959209000	-0.559645000	-0.528041000
1	-6.766932000	0.484480000	0.326565000
8	-6.020782000	-1.058892000	-0.896928000

MCI – $[(bpy)Pt^{II}(Ph)(4\text{-}NMe_2\text{-}OPy)]^{+}$

78	-0.849679000	-0.070902000	-0.157782000
6	-3.683438000	0.447971000	0.330187000
6	-2.431047000	2.443596000	0.437061000
6	-4.875898000	1.157989000	0.606042000
6	-3.582331000	3.208023000	0.717250000
1	-1.446541000	2.902477000	0.359516000
6	-4.831361000	2.554225000	0.802393000
1	-5.826885000	0.629317000	0.668475000
1	-3.485854000	4.285333000	0.860497000
1	-5.746062000	3.111782000	1.015871000
6	-3.648971000	-1.031079000	0.116040000
6	-2.259620000	-2.873583000	-0.335981000
6	-4.795518000	-1.862465000	0.151680000
6	-3.352262000	-3.768578000	-0.319066000
1	-1.236061000	-3.206330000	-0.526362000
6	-4.643429000	-3.248883000	-0.068501000
1	-5.785072000	-1.447211000	0.343068000
1	-3.188513000	-4.832418000	-0.498288000
1	-5.515726000	-3.906370000	-0.046420000
7	-2.409906000	-1.549498000	-0.122968000
7	-2.473668000	1.100052000	0.245950000
8	0.558870000	-1.523357000	-0.586654000
6	2.400530000	-1.651974000	0.893770000
6	2.690925000	-0.760469000	-1.279748000
6	3.757218000	-1.500674000	1.183009000
1	1.679209000	-2.062606000	1.600807000
6	4.057227000	-0.575536000	-1.063429000
1	2.190825000	-0.501302000	-2.211789000
6	4.652050000	-0.944568000	0.196968000
1	4.104583000	-1.810525000	2.166530000
1	4.642446000	-0.140350000	-1.870629000
7	1.888724000	-1.293278000	-0.316219000
6	0.505778000	1.437747000	-0.215132000
6	0.745397000	2.148175000	-1.427188000
6	1.246047000	1.832063000	0.936080000
6	1.693821000	3.202399000	-1.492571000
1	0.185729000	1.887027000	-2.331454000
6	2.194479000	2.887567000	0.880020000
1	1.081717000	1.324105000	1.892400000

6	2.424449000	3.576140000	-0.337098000
1	1.851615000	3.732355000	-2.437040000
1	2.740611000	3.174398000	1.784169000
1	3.147664000	4.395857000	-0.381067000
7	5.985423000	-0.778751000	0.443393000
6	6.859526000	-0.196099000	-0.591210000
6	6.552339000	-1.179998000	1.743455000
1	6.874074000	-0.821068000	-1.501726000
1	7.883885000	-0.133314000	-0.203052000
1	6.530958000	0.822290000	-0.863366000
1	6.093888000	-0.613034000	2.573093000
1	7.630276000	-0.975412000	1.744431000
1	6.407755000	-2.259383000	1.927287000

MCI – $[(bpy)Pt^{II}(Ph)(3\text{-}NO_2\text{-}OPy)]^+$

78	-0.699643000	-0.111178000	0.087029000
6	-3.475272000	0.744842000	-0.139142000
6	-2.033060000	2.599390000	0.091276000
6	-4.598254000	1.602563000	-0.204321000
6	-3.111644000	3.505758000	0.034493000
1	-1.006504000	2.942621000	0.205724000
6	-4.421015000	2.999431000	-0.117652000
1	-5.598992000	1.186976000	-0.319476000
1	-2.913038000	4.575984000	0.107963000
1	-5.282046000	3.669657000	-0.166902000
6	-3.583413000	-0.743509000	-0.218727000
6	-2.377879000	-2.761560000	-0.178979000
6	-4.805981000	-1.439350000	-0.383382000
6	-3.552768000	-3.528488000	-0.341453000
1	-1.391900000	-3.225193000	-0.096112000
6	-4.788938000	-2.850015000	-0.445124000
1	-5.751501000	-0.903249000	-0.464943000
1	-3.491491000	-4.616978000	-0.385655000
1	-5.721552000	-3.404455000	-0.572887000
7	-2.398664000	-1.413334000	-0.119296000
7	-2.203852000	1.254687000	0.005397000
8	0.592985000	-1.760216000	0.161350000
6	2.391577000	-1.925290000	1.651244000
6	2.730787000	-1.106957000	-0.560057000
6	3.760803000	-1.800059000	1.951666000
1	1.638172000	-2.291710000	2.349007000
6	4.101239000	-0.956692000	-0.283498000
1	2.277815000	-0.879466000	-1.521039000
6	4.647141000	-1.296653000	0.971272000
7	1.917943000	-1.585247000	0.417870000
6	0.816718000	1.229848000	0.236344000
6	1.370140000	1.836585000	-0.928463000
6	1.390231000	1.569935000	1.495451000
6	2.470387000	2.729968000	-0.844815000
1	0.944466000	1.620174000	-1.913908000
6	2.486627000	2.467749000	1.587537000
1	0.976764000	1.147527000	2.417625000
6	3.035942000	3.045954000	0.415082000
1	3.879241000	3.738885000	0.483666000
1	5.714552000	-1.171278000	1.157572000
1	2.876102000	3.176476000	-1.757166000
1	2.901475000	2.718801000	2.568446000
1	4.115692000	-2.086089000	2.942355000
7	4.975485000	-0.431760000	-1.366583000
8	6.174651000	-0.262246000	-1.083686000
8	4.438403000	-0.207278000	-2.467264000

MCI – $[(bpy)Pt^{II}(Ph)(3\text{-}OMe\text{-}OPy)]^+$

78	-0.600579000	-0.105046000	0.011469000
6	-3.407984000	0.682365000	-0.062277000
6	-2.004746000	2.571810000	0.105763000
6	-4.555154000	1.510367000	-0.062409000
6	-3.107836000	3.450003000	0.112528000
1	-0.982280000	2.940123000	0.168608000
6	-4.410159000	2.910760000	0.025463000
1	-5.549273000	1.068798000	-0.128035000
1	-2.933401000	4.524639000	0.183610000
1	-5.289660000	3.558486000	0.026618000
6	-3.481941000	-0.808037000	-0.146102000
6	-2.223125000	-2.793701000	-0.181753000
6	-4.693026000	-1.535196000	-0.251954000
6	-3.384514000	-3.590463000	-0.288823000
1	-1.221054000	-3.228691000	-0.152139000
6	-4.641937000	-2.944473000	-0.324039000
1	-5.655296000	-1.023868000	-0.280774000
1	-3.297295000	-4.676751000	-0.343388000
1	-5.565027000	-3.522915000	-0.407192000
7	-2.276962000	-1.446970000	-0.112541000
7	-2.144127000	1.223680000	0.019357000
8	0.716989000	-1.717002000	-0.015702000
6	2.452987000	-1.801792000	1.559952000
6	2.885252000	-1.156763000	-0.693968000
6	3.816815000	-1.678896000	1.873236000
1	1.672378000	-2.101194000	2.257841000
6	4.274347000	-1.008521000	-0.427050000
1	2.450736000	-0.974829000	-1.674862000
6	4.747848000	-1.278523000	0.885776000
7	2.038249000	-1.540417000	0.287311000
6	0.880457000	1.280452000	0.083191000
6	1.368402000	1.883426000	-1.112224000
6	1.471052000	1.683388000	1.314939000
6	2.414882000	2.842044000	-1.082630000
1	0.929916000	1.614084000	-2.078876000
6	2.515820000	2.644703000	1.353020000
1	1.112499000	1.259743000	2.259042000
6	2.994413000	3.225761000	0.152331000
1	3.793390000	3.972481000	0.179752000
1	5.803390000	-1.183382000	1.141110000
1	2.767063000	3.288949000	-2.017249000
1	2.944065000	2.941960000	2.315238000
1	4.144884000	-1.894558000	2.891081000

6	6.441471000	-0.443580000	-1.293254000
1	6.636179000	0.340664000	-0.541801000
1	6.831639000	-0.128106000	-2.268430000
1	6.916495000	-1.393051000	-0.991549000
8	5.019976000	-0.622225000	-1.488097000

MCI – $[(bpy)Pt^{II}(Ph)(3\text{-}NMe_2\text{-}OPy)]^+$

78	-1.087337000	0.020166000	-0.141222000
6	-3.960063000	0.296411000	0.305856000
6	-2.810540000	2.233761000	1.003675000
6	-5.194999000	0.862779000	0.701048000
6	-4.007346000	2.852069000	1.420283000
1	-1.847798000	2.733028000	1.099686000
6	-5.225905000	2.155064000	1.265529000
1	-6.120546000	0.301465000	0.574496000
1	-3.968058000	3.853529000	1.851500000
6	-3.847986000	-1.070468000	-0.288370000
6	-2.353215000	-2.687547000	-1.113503000
6	-4.955972000	-1.914791000	-0.546952000
6	-3.403308000	-3.587003000	-1.402345000
1	-1.306271000	-2.927913000	-1.314958000
6	-4.728882000	-3.189029000	-1.111310000
1	-5.972724000	-1.593144000	-0.320979000
1	-3.181705000	-4.561187000	-1.841180000
7	-2.575801000	-1.470717000	-0.574042000
7	-2.779981000	0.990236000	0.458729000
8	0.389506000	-1.254600000	-0.832291000
6	2.198650000	-1.676631000	0.575541000
6	2.440136000	-0.274418000	-1.355319000
6	3.585175000	-1.540297000	0.904593000
1	1.470120000	-2.261280000	1.128186000
6	3.838703000	-0.089109000	-1.100958000
1	1.884927000	0.161746000	-2.178484000
6	4.393893000	-0.739821000	0.041538000
1	5.449752000	-0.618318000	0.263000000
7	1.712250000	-1.045935000	-0.520326000
6	0.189081000	1.546474000	0.254455000
6	0.330096000	2.625531000	-0.665879000
6	0.958679000	1.597359000	1.450893000
6	1.213117000	3.707128000	-0.408684000
1	-0.254297000	2.632800000	-1.592051000
6	1.841324000	2.677001000	1.717727000
1	0.868514000	0.797202000	2.192800000
6	1.974265000	3.736727000	0.786645000
1	1.294757000	4.524722000	-1.131884000
1	2.412949000	2.691922000	2.650904000
1	2.647603000	4.573872000	0.993289000
1	-6.173801000	2.600576000	1.575572000
1	-5.570374000	-3.853846000	-1.320160000
7	4.599323000	0.685483000	-1.951547000
7	4.099938000	-2.162447000	2.024942000
6	6.008142000	0.944718000	-1.629207000
6	3.947834000	1.430624000	-3.039475000
6	5.540355000	-2.084538000	2.300705000
6	3.247285000	-3.051839000	2.824657000
1	6.448144000	1.568928000	-2.417882000
1	6.119269000	1.475571000	-0.664197000
1	6.586143000	0.004393000	-1.582918000
1	5.864129000	-1.037526000	2.440932000
1	5.759015000	-2.630593000	3.227724000
1	6.141140000	-2.532244000	1.486123000
1	3.826091000	-3.437035000	3.674418000
1	2.373905000	-2.510846000	3.231650000
1	2.883229000	-3.915745000	2.236057000
1	4.708769000	1.999927000	-3.589469000
1	3.459193000	0.745765000	-3.755689000
1	3.192936000	2.140780000	-2.653985000

MCI – $[(4,4'\text{-}NO_2\text{-}bpy)Pt^{II}(Ph)(OPy)]^+$

78	0.615310000	-0.166296000	-0.081246000
6	-2.146561000	0.758123000	0.037503000
6	-0.637914000	2.577729000	0.068579000
6	-3.251826000	1.633600000	0.113054000
6	-1.686290000	3.516899000	0.147005000
1	0.402825000	2.895617000	0.047246000
6	-3.000176000	3.015290000	0.166961000
1	-4.278855000	1.274309000	0.133146000
1	-1.483658000	4.586260000	0.189614000
6	-2.302080000	-0.726467000	-0.017218000
6	-1.150309000	-2.777788000	-0.116407000
6	-3.556685000	-1.380031000	-0.020176000
6	-2.351599000	-3.521184000	-0.125045000
1	-0.173810000	-3.265748000	-0.155307000
6	-3.551380000	-2.785582000	-0.074661000
1	-4.505765000	-0.848367000	0.015516000
1	-2.354646000	-4.609518000	-0.168992000
7	-1.133428000	-1.429509000	-0.063332000
7	-0.853763000	1.237185000	0.013385000
8	1.844959000	-1.833604000	-0.161211000
6	3.684709000	-2.046415000	1.277876000
6	4.003864000	-1.383224000	-0.989641000
6	5.072076000	-2.024126000	1.511665000
1	2.935759000	-2.311229000	2.024570000
6	5.399427000	-1.337758000	-0.807939000
1	3.496110000	-1.160450000	-1.926607000
6	5.944866000	-1.662301000	0.456654000
1	5.446153000	-2.284391000	2.502902000
1	6.031376000	-1.051100000	-1.649504000
1	7.025187000	-1.635570000	0.616880000
7	3.194563000	-1.733986000	0.046745000
6	2.159730000	1.146746000	-0.139669000
6	2.563073000	1.732670000	-1.373544000
6	2.870706000	1.512014000	1.038103000
6	3.651718000	2.642268000	-1.432763000
1	2.027885000	1.491013000	-2.297860000
6	3.957795000	2.424274000	0.984970000

1	2.576079000	1.100008000	2.009005000
6	4.354817000	2.989448000	-0.252458000
1	3.939284000	3.081379000	-2.392641000
1	4.482203000	2.696194000	1.905810000
1	5.188219000	3.696267000	-0.294109000
7	-4.153915000	3.960096000	0.249260000
7	-4.860055000	-3.511346000	-0.079589000
8	-5.890578000	-2.814417000	-0.036606000
8	-4.812175000	-4.752962000	-0.125752000
8	-5.293105000	3.457395000	0.264638000
8	-3.882864000	5.172868000	0.295829000

MCI – [(4,4'-OMe-bpy)Pt^{II}(Ph)(OPy)]$^{+}$

78	0.368160000	-0.164724000	-0.114713000
6	-2.375397000	0.829719000	0.070321000
6	-0.837987000	2.607535000	0.088112000
6	-3.450530000	1.727058000	0.173417000
6	-1.857347000	3.571637000	0.193313000
1	0.207322000	2.910467000	0.050739000
6	-3.206645000	3.127030000	0.236797000
1	-4.481735000	1.378017000	0.208413000
1	-1.580337000	4.623542000	0.236745000
6	-2.565469000	-0.654070000	0.001042000
6	-1.477198000	-2.720859000	-0.152968000
6	-3.826012000	-1.276464000	0.016016000
6	-2.691241000	-3.437383000	-0.146674000
1	-0.518512000	-3.241265000	-0.221639000
6	-3.902836000	-2.696096000	-0.058832000
1	-4.754576000	-0.710162000	0.080306000
1	-2.670321000	-4.524080000	-0.209853000
7	-1.406607000	-1.377058000	-0.080788000
7	-1.069011000	1.273377000	0.026232000
8	1.569571000	-1.871099000	-0.256333000
6	3.314276000	-2.123333000	1.291534000
6	3.775386000	-1.428188000	-0.939221000
6	4.684367000	-2.111245000	1.611494000
1	2.518519000	-2.390437000	1.987172000
6	5.157414000	-1.392173000	-0.671193000
1	3.326056000	-1.186010000	-1.900679000
6	5.623056000	-1.738283000	0.618817000
1	4.994666000	-2.386479000	2.620616000
1	5.840407000	-1.092224000	-1.466993000
1	6.691336000	-1.717580000	0.846528000
7	2.900174000	-1.792419000	0.037342000
6	1.945109000	1.109829000	-0.179184000
6	2.378533000	1.671239000	-1.416016000
6	2.664766000	1.475510000	0.995107000
6	3.494327000	2.546510000	-1.482686000
1	1.840557000	1.434223000	-2.340104000
6	3.780525000	2.352164000	0.937968000
1	2.352417000	1.086313000	1.970203000
6	4.203287000	2.888372000	-0.304010000
1	3.799959000	2.963671000	-2.447213000
1	4.308676000	2.619006000	1.858625000
1	5.059221000	3.567948000	-0.350524000
6	-4.102689000	5.351535000	0.402579000
6	-5.288910000	-4.660977000	-0.119852000
1	-5.109980000	5.778927000	0.475442000
1	-3.515958000	5.622445000	1.296680000
1	-3.605314000	5.720000000	-0.510558000
1	-6.368727000	-4.850294000	-0.089529000
1	-4.869582000	-5.041922000	-1.066612000
1	-4.800246000	-5.148664000	0.740833000
8	-5.146963000	-3.223733000	-0.040469000
8	-4.295726000	3.918746000	0.334834000

MCI – [(4,4'-NMe$_2$-bpy)Pt^{II}(Ph)(OPy)]$^{+}$

78	-0.716948000	-0.094572000	-0.163308000
6	2.093366000	0.709721000	0.029050000
6	0.693916000	2.588470000	-0.032518000
6	3.232085000	1.529931000	0.097917000
6	1.774946000	3.472430000	0.031538000
1	-0.324956000	2.967363000	-0.093032000
6	3.113844000	2.959909000	0.105221000
1	4.212622000	1.064191000	0.137308000
1	1.564564000	4.539901000	0.018703000
6	2.177710000	-0.788659000	-0.002488000
6	0.952746000	-2.767839000	-0.170121000
6	3.389893000	-1.499847000	0.064171000
6	2.104079000	-3.563384000	-0.115507000
1	-0.037537000	-3.220453000	-0.264657000
6	3.390893000	-2.934839000	0.008618000
1	4.326931000	-0.958054000	0.158054000
1	1.994534000	-4.644773000	-0.169218000
7	0.971084000	-1.416560000	-0.115572000
7	0.821041000	1.234375000	-0.027279000
8	-2.042633000	-1.684416000	-0.438474000
6	-4.287654000	-2.147897000	-0.794532000
6	-3.602410000	-1.240332000	1.297022000
6	-5.622111000	-2.232406000	-0.355484000
1	-3.939533000	-2.448037000	-1.783099000
6	-4.923141000	-1.296457000	1.781969000
1	-2.751916000	-0.867912000	1.865467000
6	-5.952093000	-1.798893000	0.951272000
1	-6.377390000	-2.622419000	-1.039461000
1	-5.124548000	-0.943988000	2.794536000
1	-6.982662000	-1.847920000	1.310039000
7	-3.317387000	-1.667201000	0.034045000
6	-2.221245000	1.269029000	-0.203196000
6	-2.562449000	2.055116000	0.935746000
6	-2.995795000	1.460223000	-1.384249000
6	-3.632582000	2.987917000	0.903491000
1	-1.990415000	1.946926000	1.864481000
6	-4.061459000	2.397005000	-1.429514000
1	-2.759568000	0.886976000	-2.286860000
6	-4.387440000	3.163607000	-0.282710000

1	-3.869497000	3.574352000	1.796875000
1	-4.628226000	2.529580000	-2.356352000
1	-5.207924000	3.886472000	-0.314896000
7	4.207910000	3.782708000	0.171658000
7	4.552516000	-3.663188000	0.068856000
6	4.026322000	5.244542000	0.161059000
6	5.561795000	3.211056000	0.223605000
6	5.848992000	-2.978852000	0.180272000
6	4.502098000	-5.132674000	-0.009269000
1	5.008235000	5.730247000	0.228150000
1	3.537556000	5.582744000	-0.770047000
1	3.418688000	5.578527000	1.020620000
1	6.296162000	4.024976000	0.272934000
1	5.696682000	2.576037000	1.118044000
1	5.780122000	2.607786000	-0.676624000
1	6.034437000	-2.319878000	-0.687869000
1	5.907509000	-2.373808000	1.103354000
1	6.650947000	-3.727136000	0.215282000
1	5.522346000	-5.532262000	0.054253000
1	3.914551000	-5.559239000	0.823198000
1	4.059310000	-5.470490000	-0.963457000

MCI – [(5,5'-NO_2-bpy)Pt^{II}(Ph)(OPy)]$^+$

78	0.019492000	-0.210361000	-0.092471000
6	-1.089604000	2.491040000	0.084602000
6	1.270797000	2.526408000	0.090492000
6	-1.142113000	3.902966000	0.173018000
6	1.258367000	3.931461000	0.180534000
1	2.204077000	1.968270000	0.054633000
6	0.049779000	4.652505000	0.222316000
1	-2.100325000	4.419630000	0.205027000
6	-2.316779000	1.639232000	0.035390000
6	-3.106421000	-0.573544000	-0.079278000
6	-3.636447000	2.157469000	0.060352000
6	-4.439513000	-0.113145000	-0.054507000
1	-2.864084000	-1.635624000	-0.138612000
6	-4.727550000	1.265340000	0.014096000
1	-3.823881000	3.229272000	0.113580000
7	-2.080310000	0.295483000	-0.034372000
7	0.115849000	1.820125000	0.042096000
8	-0.434120000	-2.223527000	-0.251159000
6	0.532270000	-3.732483000	1.264984000
6	1.338205000	-3.592641000	-0.974509000
6	1.437075000	-4.769007000	1.558580000
1	-0.185178000	-3.318145000	1.973613000
6	2.268297000	-4.621868000	-0.732229000
1	1.217293000	-3.080516000	-1.927584000
6	2.321136000	-5.221003000	0.548407000
1	3.033455000	-6.023047000	0.755335000
7	0.504929000	-3.182733000	0.019832000
6	2.020236000	-0.519635000	-0.180041000
6	2.707435000	-0.438143000	-1.424214000
6	2.777256000	-0.821424000	0.986461000
6	4.106429000	-0.666110000	-1.504068000
1	2.159994000	-0.189895000	-2.339458000
6	4.177294000	-1.046905000	0.911940000
1	2.286608000	-0.871190000	1.964263000
6	4.845711000	-0.973674000	-0.335209000
1	5.925360000	-1.137581000	-0.392741000
1	0.052905000	5.740673000	0.290159000
1	-5.761150000	1.612750000	0.030175000
1	1.439106000	-5.202407000	2.559766000
1	2.930868000	-4.934354000	-1.540352000
1	4.740042000	-1.266130000	1.824109000
1	4.613402000	-0.591096000	-2.470574000
7	-5.546045000	-1.104378000	-0.100410000
7	2.557661000	4.655971000	0.228765000
8	-5.225834000	-2.308076000	-0.136521000
8	-6.705733000	-0.652862000	-0.096916000
8	2.501654000	5.897213000	0.303207000
8	3.593456000	3.966653000	0.191056000

MCI – [(5,5'-OMe-bpy)Pt^{II}(Ph)(OPy)]$^+$

78	0.094574000	-0.156010000	-0.097116000
6	-2.349788000	1.415127000	0.092785000
6	-0.438757000	2.804258000	0.105295000
6	-3.184377000	2.550778000	0.186082000
6	-1.228654000	3.984290000	0.201876000
1	0.646696000	2.879850000	0.070588000
6	-2.640159000	3.850254000	0.241206000
1	-4.267138000	2.428861000	0.216705000
6	-2.861798000	0.019742000	0.036717000
6	-2.241220000	-2.247614000	-0.097518000
6	-4.231007000	-0.334394000	0.061914000
6	-3.598134000	-2.681636000	-0.076292000
1	-1.427437000	-2.973425000	-0.164514000
6	-4.613435000	-1.691617000	0.005517000
1	-5.005088000	0.431066000	0.123822000
7	-1.902642000	-0.951654000	-0.042592000
7	-0.978400000	1.569755000	0.051022000
8	0.879634000	-2.082204000	-0.266957000
6	2.535296000	-2.742876000	1.258675000
6	3.120490000	-2.151989000	-0.973564000
6	3.874789000	-3.048562000	1.561675000
1	1.706504000	-2.827829000	1.961833000
6	4.476600000	-2.436398000	-0.722131000
1	2.727890000	-1.804511000	-1.927497000
6	4.863450000	-2.891856000	0.559870000
1	5.910203000	-3.119234000	0.774608000
7	2.196044000	-2.313830000	0.011820000
6	1.919577000	0.727886000	-0.176453000
6	2.455656000	1.183055000	-1.415846000
6	2.715651000	0.904982000	0.991317000
6	3.743120000	1.776260000	-1.491350000
1	1.866246000	1.086048000	-2.333791000
6	4.003505000	1.499339000	0.924581000

1	2.330807000	0.591732000	1.967803000
6	4.524557000	1.933721000	-0.319688000
1	5.513407000	2.398405000	-0.372822000
1	-3.301285000	4.713848000	0.312736000
1	-5.671039000	-1.955351000	0.024766000
1	4.124307000	-3.397063000	2.564984000
1	5.201937000	-2.294361000	-1.524281000
1	4.589064000	1.629928000	1.839831000
1	4.125879000	2.121284000	-2.456767000
6	-5.143794000	-4.519297000	-0.129636000
6	-1.271538000	6.380853000	0.332676000
1	-5.659388000	-4.236769000	0.804891000
1	-5.059157000	-5.611338000	-0.189051000
1	-5.703353000	-4.141880000	-1.003260000
1	-1.923297000	6.509144000	-0.549221000
1	-0.516789000	7.176460000	0.353068000
1	-1.871299000	6.413580000	1.259030000
8	-3.787650000	-4.024184000	-0.137042000
8	-0.529441000	5.145713000	0.245699000

MCI – $[(5,5'\text{-}NMe_2\text{-bpy})Pt^{II}(Ph)(OPy)]^+$

78	0.033011000	0.219047000	-0.124330000
6	0.445926000	-2.640786000	0.135977000
6	-1.864024000	-2.113184000	0.081027000
6	0.124748000	-4.015804000	0.257599000
6	-2.266383000	-3.482715000	0.208608000
1	-2.593387000	-1.313338000	0.001560000
6	-1.208231000	-4.446663000	0.293342000
1	0.923312000	-4.755174000	0.324192000
6	1.829238000	-2.114147000	0.089583000
6	3.142785000	-0.159518000	-0.089664000
6	3.002338000	-2.909877000	0.149553000
6	4.381461000	-0.882888000	-0.039858000
1	3.111092000	0.925419000	-0.187292000
6	4.267899000	-2.308357000	0.086037000
1	2.935054000	-3.994651000	0.240667000
7	1.941963000	-0.760106000	-0.025382000
7	-0.571140000	-1.719363000	0.048297000
8	0.959423000	2.089582000	-0.307219000
6	0.362326000	3.644291000	1.348658000
6	-0.452381000	3.877325000	-0.876729000
6	-0.288739000	4.826873000	1.744172000
1	0.961400000	3.016494000	2.008456000
6	-1.128510000	5.064444000	-0.533708000
1	-0.452856000	3.430015000	-1.869265000
6	-1.047505000	5.550472000	0.791909000
1	-1.564400000	6.469384000	1.078135000
7	0.271700000	3.208740000	0.061485000
6	-1.830399000	1.016756000	-0.249617000
6	-2.477083000	1.164798000	-1.511998000
6	-2.540280000	1.461550000	0.903386000
6	-3.768337000	1.744678000	-1.622659000
1	-1.977984000	0.816939000	-2.422642000
6	-3.833058000	2.041377000	0.803295000
1	-2.092204000	1.347875000	1.896541000
6	-4.452069000	2.189256000	-0.463210000
1	-5.449607000	2.631178000	-0.543792000
1	-1.421260000	-5.511146000	0.385334000
1	5.155769000	-2.938521000	0.129694000
1	-0.197827000	5.160698000	2.778936000
1	-1.706919000	5.581350000	-1.300547000
1	-4.353043000	2.368418000	1.709229000
1	-4.237937000	1.840201000	-2.606714000
7	5.598957000	-0.238018000	-0.107465000
7	-3.598779000	-3.833445000	0.247677000
6	6.839605000	-1.025232000	-0.099821000
6	5.647737000	1.216730000	-0.303492000
6	-3.971625000	-5.253078000	0.312794000
6	-4.636478000	-2.801496000	0.103010000
1	6.933037000	-1.619180000	0.827380000
1	7.698923000	-0.343895000	-0.151487000
1	6.893646000	-1.713715000	-0.964140000
1	6.696268000	1.540192000	-0.343777000
1	5.157174000	1.519160000	-1.247809000
1	5.159145000	1.752652000	0.531083000
1	-3.601926000	-5.814589000	-0.565896000
1	-5.065946000	-5.336766000	0.335990000
1	-3.575013000	-5.731894000	1.226527000
1	-4.565384000	-2.044554000	0.904537000
1	-5.624921000	-3.274630000	0.170964000
1	-4.567126000	-2.283762000	-0.871830000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(Py)]^+$

6	2.691495000	0.301491000	-0.349850000
6	2.171479000	-1.631359000	-1.624715000
6	4.076570000	0.035720000	-0.466246000
6	3.537592000	-1.948139000	-1.778725000
1	1.354094000	-2.204232000	-2.069419000
6	4.502835000	-1.103731000	-1.183374000
1	4.810287000	0.696836000	-0.005456000
1	3.824008000	-2.832299000	-2.349849000
1	5.568898000	-1.323823000	-1.276033000
6	2.122433000	1.488497000	0.356154000
6	0.164721000	2.596070000	1.031242000
6	2.925658000	2.527202000	0.889002000
6	0.894157000	3.671892000	1.580162000
1	-0.926065000	2.586238000	1.061327000
6	2.306061000	3.631543000	1.510625000
1	4.011959000	2.485785000	0.810057000
1	0.365662000	4.506536000	2.043350000
1	2.910732000	4.442650000	1.922497000
7	0.757173000	1.533704000	0.442399000
7	1.782040000	-0.541613000	-0.924668000
78	-0.213151000	-0.116954000	-0.656135000
8	-0.638030000	-1.109882000	-2.161146000
7	-2.248514000	0.383870000	-0.556086000
6	-2.865655000	0.670960000	0.622532000

6	-2.967728000	0.416247000	-1.711297000
6	-4.227494000	1.028262000	0.691271000
1	-2.256550000	0.586662000	1.522721000
6	-4.335706000	0.768286000	-1.724785000
1	-2.420101000	0.128098000	-2.608466000
6	-4.979779000	1.082846000	-0.506913000
1	-4.677418000	1.242148000	1.662333000
1	-4.869745000	0.785590000	-2.676313000
1	-6.037890000	1.356843000	-0.488485000
6	-0.312019000	-1.187790000	1.127009000
6	0.406186000	-0.902174000	2.310270000
6	-1.148539000	-2.332020000	1.053902000
6	0.273902000	-1.758655000	3.436348000
1	1.062027000	-0.035206000	2.392453000
6	-1.270578000	-3.181068000	2.183746000
1	-1.689055000	-2.571697000	0.137677000
6	-0.563705000	-2.896820000	3.377510000
1	0.828772000	-1.527188000	4.350093000
1	-1.914928000	-4.062281000	2.119173000
1	-0.660922000	-3.554435000	4.245303000

Oxo - $[(bpy)Pt^{IV}(p\text{-}NO_2\text{-}Ph)(O)(Py)]^+$

6	2.164430000	-1.952987000	-0.073428000
6	1.528176000	-1.707618000	-2.347209000
6	2.739566000	-3.216815000	-0.345943000
6	2.085868000	-2.959598000	-2.681821000
1	1.064398000	-1.032067000	-3.069664000
6	2.694194000	-3.727096000	-1.662227000
1	3.209135000	-3.797333000	0.447923000
1	2.038548000	-3.311274000	-3.713332000
1	3.128688000	-4.704425000	-1.884627000
6	2.175455000	-1.299253000	1.269870000
6	1.488101000	0.555367000	2.537964000
6	2.864204000	-1.839022000	2.384169000
6	2.153812000	0.086126000	3.690235000
1	0.939575000	1.498638000	2.553760000
6	2.851945000	-1.140982000	3.610200000
1	3.411964000	-2.777245000	2.297356000
1	2.120268000	0.668695000	4.612131000
1	3.381153000	-1.542083000	4.477470000
7	1.491306000	-0.117206000	1.365536000
7	1.570191000	-1.240969000	-1.078268000
78	0.706771000	0.561704000	-0.582545000
8	0.862992000	1.123694000	-2.336789000
7	-0.011846000	2.490225000	-0.150714000
6	-0.851558000	2.732570000	0.893458000
6	0.383430000	3.525811000	-0.941335000
6	-1.312981000	4.027232000	1.204858000
1	-1.173295000	1.866727000	1.472722000
6	-0.033829000	4.852170000	-0.692039000
1	1.017732000	3.253057000	-1.784537000
6	-0.893629000	5.112941000	0.398507000
1	-1.991176000	4.166373000	2.048562000
1	0.313616000	5.649710000	-1.350882000
1	-1.233287000	6.129640000	0.612472000
6	-1.113008000	-0.313645000	-0.104969000
6	-1.338228000	-1.272982000	0.911556000
6	-2.175791000	0.078027000	-0.964791000
6	-2.625316000	-1.837118000	1.087258000
1	-0.542982000	-1.598045000	1.581506000
6	-3.464980000	-0.479880000	-0.799644000
1	-2.008658000	0.800320000	-1.764001000
6	-3.667806000	-1.427768000	0.228422000
1	-2.819910000	-2.572870000	1.867814000
1	-4.291793000	-0.194046000	-1.450187000
7	-5.020872000	-2.015964000	0.411194000
8	-5.164328000	-2.856278000	1.323292000
8	-5.924404000	-1.630184000	-0.357599000

Oxo - $[(bpy)Pt^{IV}(p\text{-OMe-Ph})(O)(Py)]^+$

6	-2.748059000	0.855057000	-0.087360000
6	-1.955967000	1.138916000	-2.306191000
6	-3.822133000	1.743625000	-0.330986000
6	-3.006046000	2.030212000	-2.611456000
1	-1.195710000	0.815719000	-3.021511000
6	-3.948779000	2.340564000	-1.604491000
1	-4.543036000	1.973350000	0.453515000
1	-3.072436000	2.461802000	-3.611099000
1	-4.770042000	3.032819000	-1.804078000
6	-2.524348000	0.145433000	1.207854000
6	-1.126909000	-1.305142000	2.414436000
6	-3.435371000	0.212587000	2.291119000
6	-1.986352000	-1.294711000	3.533332000
1	-0.208407000	-1.894351000	2.418969000
6	-3.163692000	-0.513686000	3.469476000
1	-4.345067000	0.808026000	2.215064000
1	-1.733251000	-1.880444000	4.418407000
1	-3.857413000	-0.475794000	4.312372000
7	-1.382002000	-0.603922000	1.287816000
7	-1.846232000	0.583810000	-1.077902000
78	-0.279154000	-0.668438000	-0.624479000
8	-0.049243000	-1.051698000	-2.422772000
7	1.232100000	-2.075340000	-0.251282000
6	2.044259000	-1.991353000	0.837609000
6	1.399762000	-3.099817000	-1.131747000
6	3.044471000	-2.948131000	1.105657000
1	1.898446000	-1.126948000	1.485652000
6	2.378254000	-4.098660000	-0.931115000
1	0.746732000	-3.075004000	-2.004057000
6	3.214271000	-4.027876000	0.205890000
1	3.673638000	-2.832851000	1.989976000
1	2.471790000	-4.904192000	-1.661405000
1	3.979943000	-4.787314000	0.384954000
6	0.906484000	0.898132000	0.062672000
6	0.623694000	1.742256000	1.164092000
6	2.057691000	1.141378000	-0.724456000

6	1.493854000	2.807852000	1.486073000
1	-0.256270000	1.597748000	1.791041000
6	2.935418000	2.211787000	-0.409177000
1	2.283400000	0.517724000	-1.590313000
6	2.656500000	3.052140000	0.703209000
1	1.284888000	3.459198000	2.337945000
1	3.811584000	2.371891000	-1.038443000
6	4.601642000	4.417137000	0.330246000
1	5.317759000	3.575531000	0.340357000
1	4.337518000	4.669938000	-0.712409000
1	5.057527000	5.290604000	0.814565000
8	3.428430000	4.109533000	1.101688000

Oxo - [(bpy)Pt^{IV}(*p*-NMe$_2$-Ph)(O)(Py)]$^+$

6	1.884698000	-2.245561000	-0.110786000
6	1.281977000	-1.863781000	-2.373681000
6	2.248552000	-3.580792000	-0.407121000
6	1.630586000	-3.182756000	-2.732657000
1	0.925129000	-1.107108000	-3.076960000
6	2.115811000	-4.054618000	-1.730686000
1	2.623311000	-4.241465000	0.374472000
1	1.521294000	-3.505455000	-3.768960000
1	2.388892000	-5.084482000	-1.972316000
6	2.004993000	-1.624573000	1.242308000
6	1.627662000	0.292617000	2.542818000
6	2.598118000	-2.288837000	2.344631000
6	2.208684000	-0.297813000	3.685018000
1	1.237429000	1.310935000	2.576184000
6	2.700474000	-1.619860000	3.582118000
1	2.985266000	-3.302283000	2.239480000
1	2.269257000	0.266387000	4.616978000
1	3.158900000	-2.115804000	4.440647000
7	1.523047000	-0.348922000	1.358329000
7	1.408919000	-1.430558000	-1.098913000
78	0.850441000	0.477473000	-0.576988000
8	1.041854000	1.027849000	-2.336931000
7	0.432218000	2.480481000	-0.117074000
6	-0.369791000	2.828522000	0.925801000
6	0.978938000	3.455454000	-0.893529000
6	-0.635496000	4.173758000	1.253692000
1	-0.821576000	2.008288000	1.483845000
6	0.761565000	4.825767000	-0.627618000
1	1.567110000	3.100432000	-1.739723000
6	-0.055156000	5.195806000	0.464708000
1	-1.290384000	4.400811000	2.096762000
1	1.225508000	5.572306000	-1.274436000
1	-0.240553000	6.248834000	0.692552000
6	-1.087892000	-0.107296000	-0.094126000
6	-1.468602000	-1.033994000	0.900195000
6	-2.086531000	0.445053000	-0.936012000
6	-2.828351000	-1.387179000	1.077511000
1	-0.738405000	-1.503668000	1.560750000
6	-3.444412000	0.095535000	-0.766168000
1	-1.820009000	1.137258000	-1.735709000
6	-3.859490000	-0.822730000	0.256151000
1	-3.070593000	-2.104949000	1.861428000
1	-4.172375000	0.541737000	-1.443601000
7	-5.202367000	-1.140375000	0.447952000
6	-5.552143000	-2.251667000	1.340270000
6	-6.187194000	-0.715193000	-0.554985000
1	-5.112879000	-3.215029000	1.010577000
1	-6.645023000	-2.362305000	1.368136000
1	-5.213464000	-2.052144000	2.371884000
1	-6.215109000	0.384867000	-0.639130000
1	-5.978730000	-1.135305000	-1.559438000
1	-7.186951000	-1.047105000	-0.242105000

Oxo - [(bpy)Pt^{IV}(*m*-NO$_2$-Ph)(O)(Py)]$^+$

6	-1.906674000	-1.918954000	0.076429000
6	-1.165531000	-2.160573000	-2.165651000
6	-3.131598000	-2.555294000	-0.234775000
6	-2.363675000	-2.806445000	-2.536114000
1	-0.326570000	-1.990977000	-2.844671000
6	-3.364142000	-2.997888000	-1.555486000
1	-3.893251000	-2.698843000	0.531224000
1	-2.497492000	-3.143368000	-3.564954000
1	-4.308310000	-3.484880000	-1.810042000
6	-1.536408000	-1.438612000	1.441440000
6	0.081949000	-0.345913000	2.746642000
6	-2.345706000	-1.660221000	2.582678000
6	-0.664315000	-0.532081000	3.929466000
1	1.047773000	0.160958000	2.768458000
6	-1.908208000	-1.198273000	3.841666000
1	-3.294630000	-2.189054000	2.496641000
1	-0.277371000	-0.161151000	4.879738000
1	-2.521572000	-1.359410000	4.730905000
7	-0.341664000	-0.777447000	1.538198000
7	-0.965898000	-1.731864000	-0.898284000
78	0.754768000	-0.726798000	-0.375891000
8	1.643360000	-1.476495000	-1.813518000
7	2.599731000	0.123910000	0.166880000
6	2.682133000	1.282934000	0.876619000
6	3.744456000	-0.517102000	-0.197178000
6	3.915685000	1.837640000	1.272998000
1	1.740133000	1.779520000	1.110346000
6	5.018412000	-0.026125000	0.165468000
1	3.604939000	-1.412772000	-0.802220000
6	5.110886000	1.168283000	0.914815000
1	3.927384000	2.772382000	1.836249000
1	5.907270000	-0.578342000	-0.144137000
1	6.084065000	1.570695000	1.207870000
6	-0.098587000	1.130998000	-0.739081000
6	-1.238434000	1.648760000	-0.092926000
6	0.509213000	1.862738000	-1.796682000
6	-1.743634000	2.903761000	-0.512422000
1	-1.756343000	1.141315000	0.716125000

6	-0.021237000	3.116802000	-2.193620000
1	1.379826000	1.461725000	-2.317010000
6	-1.159717000	3.658011000	-1.552241000
1	-1.585482000	4.618856000	-1.840665000
1	0.454485000	3.666287000	-3.009561000
7	-2.946196000	3.437336000	0.184524000
8	-3.443636000	2.739556000	1.096725000
8	-3.383195000	4.544321000	-0.182741000

Oxo - [(bpy)Pt^{IV}(*m*-OMe-Ph)(O)(Py)]$^{+}$

6	-2.360944000	-1.311750000	0.021791000
6	-1.671764000	-1.611938000	-2.228998000
6	-3.692484000	-1.653684000	-0.314330000
6	-2.979367000	-1.962564000	-2.626261000
1	-0.808779000	-1.600980000	-2.899037000
6	-4.004919000	-1.977454000	-1.653095000
1	-4.472843000	-1.664300000	0.446445000
1	-3.175474000	-2.215012000	-3.669224000
1	-5.029677000	-2.238409000	-1.927501000
6	-1.905285000	-0.975674000	1.404389000
6	-0.106317000	-0.283974000	2.746230000
6	-2.745882000	-1.083189000	2.540270000
6	-0.877393000	-0.371006000	3.924799000
1	0.940493000	0.022038000	2.783185000
6	-2.227932000	-0.776673000	3.816100000
1	-3.778992000	-1.415222000	2.437132000
1	-0.426268000	-0.129277000	4.888415000
1	-2.860749000	-0.861180000	4.702451000
7	-0.602202000	-0.572802000	1.522657000
7	-1.393887000	-1.295549000	-0.943778000
78	0.505776000	-0.746499000	-0.380908000
8	1.206378000	-1.653043000	-1.835649000
7	2.489679000	-0.371711000	0.194184000
6	2.835747000	0.726404000	0.920019000
6	3.454940000	-1.256574000	-0.177180000
6	4.162147000	0.970904000	1.329552000
1	2.035200000	1.428785000	1.151931000
6	4.806216000	-1.082059000	0.195935000
1	3.113279000	-2.084485000	-0.798200000
6	5.170225000	0.046451000	0.964605000
1	4.388377000	1.870224000	1.905060000
1	5.543863000	-1.821042000	-0.121353000
1	6.208749000	0.206542000	1.266008000
6	0.153007000	1.275805000	-0.739056000
6	-0.850599000	2.051841000	-0.109750000
6	0.981320000	1.816466000	-1.748666000
6	-1.016244000	3.413298000	-0.500246000
1	-1.491251000	1.631946000	0.661426000
6	0.800728000	3.177748000	-2.118484000
1	1.734169000	1.208806000	-2.249715000
6	-0.182096000	3.977150000	-1.504595000
1	-0.327974000	5.022198000	-1.785594000
1	1.434615000	3.605409000	-2.900178000
6	-2.858259000	3.748730000	1.017662000
1	-3.518839000	4.584352000	1.284019000
1	-3.463854000	2.920374000	0.604057000
1	-2.324167000	3.403594000	1.923225000
8	-1.948200000	4.263476000	0.039737000

Oxo - [(bpy)Pt^{IV}(*m*-NMe$_2$-Ph)(O)(Py)]$^{+}$

6	-1.700255000	-2.135887000	-0.000869000
6	-0.949569000	-2.180896000	-2.251365000
6	-2.854190000	-2.879549000	-0.344665000
6	-2.078114000	-2.924535000	-2.656441000
1	-0.133633000	-1.890313000	-2.917604000
6	-3.046873000	-3.272799000	-1.687239000
1	-3.591574000	-3.144408000	0.413022000
1	-2.183041000	-3.217013000	-3.702111000
1	-3.935712000	-3.842856000	-1.967579000
6	-1.374423000	-1.687492000	1.386309000
6	0.115766000	-0.478492000	2.739745000
6	-2.137052000	-2.067263000	2.518838000
6	-0.586612000	-0.817830000	3.915432000
1	1.012039000	0.142431000	2.781543000
6	-1.740612000	-1.627384000	3.799138000
1	-3.013312000	-2.706278000	2.409476000
1	-0.233644000	-0.456668000	4.882663000
1	-2.313526000	-1.916600000	4.683081000
7	-0.265339000	-0.895435000	1.512225000
7	-0.787599000	-1.804691000	-0.962617000
78	0.834799000	-0.680600000	-0.388316000
8	1.793634000	-1.296282000	-1.849459000
7	2.587912000	0.311704000	0.195692000
6	2.558882000	1.467563000	0.913238000
6	3.787305000	-0.219999000	-0.166022000
6	3.735268000	2.126465000	1.324877000
1	1.573243000	1.875716000	1.137187000
6	5.009522000	0.380498000	0.209566000
1	3.730971000	-1.117573000	-0.781683000
6	4.988253000	1.571542000	0.969849000
1	3.658555000	3.054530000	1.894058000
1	5.946838000	-0.085154000	-0.099524000
1	5.919176000	2.058184000	1.272605000
6	-0.150216000	1.127697000	-0.724312000
6	-1.303549000	1.566841000	-0.042901000
6	0.431263000	1.877964000	-1.774136000
6	-1.922596000	2.819789000	-0.391315000
1	-1.737040000	0.971396000	0.755366000
6	-0.185572000	3.107443000	-2.120929000
1	1.306950000	1.524463000	-2.316628000
6	-1.334652000	3.578955000	-1.455328000
1	-1.771499000	4.525958000	-1.769870000
1	0.238679000	3.701273000	-2.935710000
7	-3.044110000	3.284500000	0.299720000
6	-3.771244000	2.367935000	1.181237000
6	-3.758382000	4.461745000	-0.214995000

1	-4.643631000	2.885939000	1.602996000
1	-4.129670000	1.461817000	0.649534000
1	-3.140028000	2.044409000	2.028922000
1	-4.602188000	4.690520000	0.451057000
1	-3.098754000	5.345617000	-0.229044000
1	-4.152702000	4.305248000	-1.238866000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}NO_2\text{-}Py)]^+$

6	3.171551000	0.624871000	-0.428909000
6	2.855315000	-1.329265000	-1.739777000
6	4.572530000	0.550082000	-0.612032000
6	4.243017000	-1.455882000	-1.959914000
1	2.103195000	-1.996223000	-2.167531000
6	5.113430000	-0.504014000	-1.380961000
1	5.232064000	1.291975000	-0.162168000
1	4.617760000	-2.279830000	-2.568685000
1	6.193862000	-0.576515000	-1.525285000
6	2.482740000	1.704509000	0.339665000
6	0.429319000	2.513109000	1.142985000
6	3.163089000	2.828433000	0.870168000
6	1.032409000	3.662943000	1.695042000
1	-0.646996000	2.352679000	1.225183000
6	2.431205000	3.819524000	1.557426000
1	4.239550000	2.938610000	0.739573000
1	0.419716000	4.403161000	2.211892000
1	2.939936000	4.694547000	1.968058000
7	1.129769000	1.560192000	0.489023000
7	2.357050000	-0.318335000	-0.991519000
78	0.342379000	-0.168660000	-0.633282000
8	-0.014111000	-1.156059000	-2.159421000
7	-1.743783000	0.041190000	-0.444115000
6	-2.348175000	0.197926000	0.764994000
6	-2.498170000	0.004862000	-1.576062000
6	-3.741572000	0.355652000	0.899288000
1	-1.701377000	0.175307000	1.641723000
6	-3.902674000	0.155412000	-1.542996000
1	-1.946224000	-0.173732000	-2.498860000
6	-4.506464000	0.335335000	-0.284980000
1	-4.208665000	0.476605000	1.875935000
1	-4.492539000	0.130658000	-2.458686000
6	0.457760000	-1.297618000	1.115375000
6	1.172623000	-0.950213000	2.283755000
6	-0.218881000	-2.542149000	1.028316000
6	1.196514000	-1.849369000	3.383942000
1	1.709605000	-0.005851000	2.373379000
6	-0.186052000	-3.431598000	2.133122000
1	-0.751257000	-2.828673000	0.120834000
6	0.517480000	-3.088092000	3.313038000
1	1.747526000	-1.571612000	4.286930000
1	-0.707072000	-4.390154000	2.059276000
1	0.539768000	-3.777339000	4.161104000
7	-5.990846000	0.507837000	-0.197344000
8	-6.625062000	0.479854000	-1.266779000
8	-6.471042000	0.667318000	0.940215000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}OMe\text{-}Py)]^+$

6	3.019509000	0.628403000	-0.482166000
6	2.632693000	-1.235505000	-1.898227000
6	4.411985000	0.555426000	-0.724810000
6	4.009279000	-1.359193000	-2.181086000
1	1.856091000	-1.867637000	-2.335765000
6	4.911574000	-0.452222000	-1.578815000
1	5.096081000	1.262552000	-0.255904000
1	4.352031000	-2.146278000	-2.854153000
1	5.984789000	-0.523970000	-1.770092000
6	2.372402000	1.661808000	0.381101000
6	0.361561000	2.431979000	1.318032000
6	3.085631000	2.742854000	0.956007000
6	0.999062000	3.537544000	1.919964000
1	-0.712197000	2.274505000	1.430815000
6	2.392836000	3.691946000	1.736561000
1	4.157161000	2.852359000	0.789146000
1	0.415403000	4.246373000	2.509370000
1	2.927175000	4.533366000	2.183403000
7	1.025043000	1.518616000	0.575390000
7	2.173891000	-0.270556000	-1.069318000
78	0.170225000	-0.127247000	-0.620124000
8	-0.256650000	-1.017941000	-2.187690000
7	-1.890428000	0.108784000	-0.326987000
6	-2.450591000	0.219292000	0.914221000
6	-2.708941000	0.149509000	-1.412361000
6	-3.822949000	0.402413000	1.114273000
1	-1.771898000	0.133623000	1.762933000
6	-4.101665000	0.331726000	-1.312991000
1	-2.212681000	0.006667000	-2.372427000
6	-4.686365000	0.465153000	-0.021468000
1	-4.234466000	0.478688000	2.121579000
1	-4.689511000	0.357833000	-2.229399000
6	0.339238000	-1.363467000	1.045301000
6	1.158316000	-1.126027000	2.172203000
6	-0.406692000	-2.566364000	0.942407000
6	1.219337000	-2.090733000	3.213576000
1	1.750214000	-0.215902000	2.272357000
6	-0.336219000	-3.523609000	1.986817000
1	-1.023825000	-2.767441000	0.066174000
6	0.472649000	-3.288745000	3.125257000
1	1.851891000	-1.896341000	4.084488000
1	-0.911510000	-4.449542000	1.899289000
1	0.523534000	-4.029821000	3.927303000
6	-6.919016000	0.693921000	-0.884939000
1	-6.679492000	1.541607000	-1.548810000
1	-7.909975000	0.839041000	-0.438448000
1	-6.896844000	-0.254354000	-1.447652000
8	-5.997208000	0.644866000	0.231279000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}NMe_2\text{-}Py)]^+$

6	3.224138000	0.667027000	-0.420402000
6	2.948333000	-1.279556000	-1.747258000
6	4.627481000	0.621725000	-0.600613000
6	4.338558000	-1.378556000	-1.966008000
1	2.207306000	-1.955607000	-2.181201000
6	5.189805000	-0.415063000	-1.377141000
1	5.271815000	1.372362000	-0.143088000
1	4.730799000	-2.190079000	-2.580525000
1	6.271781000	-0.465883000	-1.519712000
6	2.512685000	1.726184000	0.357165000
6	0.443927000	2.485493000	1.168492000
6	3.171301000	2.858063000	0.898900000
6	1.025172000	3.640763000	1.732771000
1	-0.628818000	2.301764000	1.244731000
6	2.420476000	3.827065000	1.596676000
1	4.245365000	2.990536000	0.768830000
1	0.398402000	4.363197000	2.257927000
1	2.912021000	4.707665000	2.016377000
7	1.162722000	1.553638000	0.504689000
7	2.428889000	-0.285872000	-0.991727000
78	0.401427000	-0.174655000	-0.637707000
8	0.069934000	-1.156992000	-2.172725000
7	-1.667992000	0.029463000	-0.445079000
6	-2.291016000	0.191406000	0.757186000
6	-2.453560000	-0.011943000	-1.562233000
6	-3.673524000	0.346886000	0.898575000
1	-1.652483000	0.172062000	1.641095000
6	-3.844323000	0.136128000	-1.523072000
1	-1.921115000	-0.193045000	-2.495588000
6	-4.521189000	0.327371000	-0.267052000
1	-4.077274000	0.458078000	1.903474000
1	-4.386619000	0.091913000	-2.465937000
6	0.528363000	-1.321752000	1.091811000
6	1.334820000	-1.031412000	2.215705000
6	-0.220200000	-2.526267000	1.041865000
6	1.380018000	-1.941665000	3.305548000
1	1.929660000	-0.119478000	2.276378000
6	-0.166007000	-3.429782000	2.133901000
1	-0.827269000	-2.768952000	0.169170000
6	0.629877000	-3.140299000	3.269026000
1	2.003239000	-1.705570000	4.172956000
1	-0.742726000	-4.357799000	2.085943000
1	0.668939000	-3.840320000	4.107885000
7	-5.877121000	0.476366000	-0.182881000
6	-6.702756000	0.408032000	-1.402429000
6	-6.522007000	0.636926000	1.132030000
1	-6.417482000	1.196223000	-2.120805000
1	-7.756184000	0.556377000	-1.132924000
1	-6.607042000	-0.574408000	-1.898021000
1	-6.353922000	-0.245961000	1.774673000
1	-7.603560000	0.757265000	0.990843000
1	-6.143345000	1.532876000	1.654790000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}NO_2\text{-}Py)]^+$

6	3.091662000	0.571351000	-0.215233000
6	3.088996000	-1.785390000	-0.503956000
6	4.496115000	0.572300000	-0.042886000
6	4.488847000	-1.848208000	-0.342452000
1	2.457388000	-2.650002000	-0.720857000
6	5.200457000	-0.650343000	-0.102293000
1	5.032594000	1.503112000	0.139773000
1	4.994546000	-2.812699000	-0.405111000
1	6.284208000	-0.663826000	0.034605000
6	2.244151000	1.800814000	-0.195663000
6	0.063247000	2.662764000	-0.303424000
6	2.784722000	3.107374000	-0.106720000
6	0.523403000	3.994035000	-0.221263000
1	-1.003488000	2.448655000	-0.382383000
6	1.915582000	4.218575000	-0.118004000
1	3.862051000	3.259411000	-0.042422000
1	-0.192603000	4.817128000	-0.236440000
1	2.316400000	5.232592000	-0.053277000
7	0.893773000	1.596544000	-0.288189000
7	2.430641000	-0.605263000	-0.434355000
78	0.389375000	-0.529344000	-0.618609000
8	0.398523000	-2.138503000	-1.538277000
7	-1.685694000	-0.491356000	-0.982734000
6	-2.535043000	0.186488000	-0.174299000
6	-2.180250000	-1.182144000	-2.048746000
6	-3.917886000	0.211832000	-0.438918000
1	-2.125693000	0.694224000	0.696577000
6	-3.560849000	-1.200454000	-2.353414000
1	-1.434741000	-1.735114000	-2.621876000
6	-4.464627000	-0.488631000	-1.536014000
1	-5.538963000	-0.466272000	-1.726142000
6	0.071685000	-0.718433000	1.432736000
6	0.485448000	0.196857000	2.426372000
6	-0.579562000	-1.926993000	1.791383000
6	0.229440000	-0.092203000	3.793724000
1	0.994367000	1.128316000	2.178822000
6	-0.826949000	-2.204332000	3.160582000
1	-0.877446000	-2.650944000	1.032330000
6	-0.427525000	-1.288663000	4.163821000
1	-0.622407000	-1.506258000	5.217082000
1	-1.326993000	-3.138272000	3.431655000
1	0.545088000	0.624341000	4.557221000
1	-3.908293000	-1.766513000	-3.218672000
7	-4.795717000	0.995873000	0.466841000
8	-4.236856000	1.675241000	1.352260000
8	-6.020998000	0.923364000	0.266977000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}OMe\text{-}Py)]^+$

6	3.000623000	0.591355000	-0.159440000
6	2.943450000	-1.632719000	-0.984700000
6	4.410484000	0.539463000	-0.047397000
6	4.347056000	-1.744969000	-0.898861000

1	2.287184000	-2.416559000	-1.370728000
6	5.089315000	-0.642655000	-0.415986000
1	4.970461000	1.397377000	0.324284000
1	4.832377000	-2.673128000	-1.203765000
1	6.176915000	-0.698135000	-0.328941000
6	2.177696000	1.792388000	0.174810000
6	0.010034000	2.677326000	0.354250000
6	2.745957000	3.040401000	0.531715000
6	0.498707000	3.952086000	0.711186000
1	-1.062020000	2.491958000	0.270851000
6	1.897887000	4.134001000	0.804980000
1	3.827687000	3.163914000	0.582715000
1	-0.200796000	4.766131000	0.907378000
1	2.320068000	5.103986000	1.077147000
7	0.821114000	1.627421000	0.097397000
7	2.309846000	-0.495807000	-0.616712000
78	0.258982000	-0.358658000	-0.690890000
8	0.206335000	-1.709425000	-1.956998000
7	-1.817761000	-0.182597000	-0.950020000
6	-2.614159000	0.282418000	0.040598000
6	-2.359063000	-0.534717000	-2.149341000
6	-4.016935000	0.447660000	-0.122597000
1	-2.155647000	0.507136000	1.003301000
6	-3.742855000	-0.399781000	-2.383322000
1	-1.662408000	-0.944200000	-2.879247000
6	-4.595300000	0.098312000	-1.371978000
1	-5.665351000	0.201094000	-1.557341000
6	0.039006000	-1.026811000	1.267753000
6	0.557667000	-0.398362000	2.422355000
6	-0.647564000	-2.264300000	1.371235000
6	0.374833000	-1.004797000	3.694272000
1	1.095017000	0.548951000	2.371395000
6	-0.822478000	-2.861018000	2.646061000
1	-1.030842000	-2.766005000	0.482243000
6	-0.315432000	-2.233785000	3.810047000
1	-0.452728000	-2.697851000	4.790280000
1	-1.350186000	-3.816158000	2.718304000
1	0.774237000	-0.508996000	4.583694000
1	-4.145263000	-0.687702000	-3.356025000
6	-6.111057000	1.065236000	0.880357000
1	-6.429784000	1.439744000	1.860972000
1	-6.393694000	1.789561000	0.096461000
1	-6.584078000	0.087400000	0.684051000
8	-4.675255000	0.932338000	0.964719000

Oxo - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}NMe_2\text{-}Py)]^+$

6	3.119175000	0.637567000	-0.079566000
6	3.169170000	-1.637647000	-0.750728000
6	4.520324000	0.635231000	0.120622000
6	4.567279000	-1.702816000	-0.572950000
1	2.556386000	-2.463708000	-1.120254000
6	5.250067000	-0.548862000	-0.123791000
1	5.034496000	1.532673000	0.464288000
1	5.094167000	-2.634617000	-0.783068000
1	6.331278000	-0.566371000	0.031914000
6	2.246485000	1.834315000	0.117059000
6	0.049258000	2.664934000	0.089254000
6	2.758451000	3.121984000	0.413407000
6	0.481642000	3.976954000	0.376971000
1	-1.008459000	2.438059000	-0.055249000
6	1.866723000	4.206704000	0.547646000
1	3.831186000	3.282020000	0.521754000
1	-0.248140000	4.783800000	0.460670000
1	2.245588000	5.206731000	0.770417000
7	0.902154000	1.623758000	-0.031009000
7	2.486098000	-0.497818000	-0.501419000
78	0.437443000	-0.423265000	-0.708689000
8	0.497549000	-1.853460000	-1.882652000
7	-1.617350000	-0.302185000	-1.109555000
6	-2.491297000	0.152713000	-0.173201000
6	-2.050416000	-0.667096000	-2.342273000
6	-3.895142000	0.294023000	-0.419773000
1	-2.063360000	0.372720000	0.800889000
6	-3.420334000	-0.558622000	-2.673410000
1	-1.296860000	-1.067451000	-3.017643000
6	-4.345823000	-0.083078000	-1.729091000
1	-5.400057000	-0.017134000	-1.998494000
6	0.123160000	-0.971383000	1.273527000
6	0.563678000	-0.258847000	2.411839000
6	-0.534312000	-2.220620000	1.422668000
6	0.330728000	-0.788936000	3.709656000
1	1.080788000	0.697334000	2.326869000
6	-0.759209000	-2.742410000	2.722274000
1	-0.859332000	-2.786542000	0.549086000
6	-0.331262000	-2.028787000	3.868708000
1	-0.504427000	-2.436465000	4.868240000
1	-1.261457000	-3.708101000	2.828337000
1	0.672124000	-0.228135000	4.584570000
1	-3.749510000	-0.858101000	-3.669936000
7	-4.753701000	0.770626000	0.556217000
6	-4.261759000	0.936690000	1.930785000
6	-6.204417000	0.737973000	0.312051000
1	-3.458050000	1.694022000	1.978167000
1	-5.084135000	1.289054000	2.567350000
1	-3.873737000	-0.009837000	2.354238000
1	-6.722234000	1.166406000	1.180475000
1	-6.470735000	1.347229000	-0.568598000
1	-6.579872000	-0.291781000	0.155166000

Oxo - $[(4,4'\text{-}NO_2\text{-}bpy)Pt^{IV}(Ph)(O)(Py)]^+$

6	1.964537000	-0.303160000	-0.309160000
6	1.257017000	-2.526283000	-0.759984000
6	3.317106000	-0.707622000	-0.248734000
6	2.582554000	-3.009042000	-0.718984000
1	0.389107000	-3.151112000	-0.985585000
6	3.598196000	-2.070865000	-0.451870000

1	4.132407000	-0.014796000	-0.049114000
1	2.809883000	-4.061133000	-0.886351000
6	1.514688000	1.110039000	-0.142489000
6	-0.326820000	2.568180000	-0.023759000
6	2.424067000	2.187707000	-0.023976000
6	0.499353000	3.705637000	0.093536000
1	-1.412455000	2.672029000	-0.032055000
6	1.890073000	3.481721000	0.095720000
1	3.504026000	2.051153000	-0.034481000
1	0.084989000	4.709397000	0.180145000
7	0.159614000	1.311402000	-0.133296000
7	0.978924000	-1.218852000	-0.553905000
78	-0.965670000	-0.539702000	-0.557424000
8	-1.480264000	-2.002480000	-1.566318000
7	-2.933807000	0.147153000	-0.751906000
6	-3.528188000	0.920193000	0.199336000
6	-3.635489000	-0.197232000	-1.867283000
6	-4.844749000	1.403065000	0.059883000
1	-2.942441000	1.129443000	1.094679000
6	-4.958546000	0.249491000	-2.078817000
1	-3.116195000	-0.854260000	-2.564184000
6	-5.576450000	1.065123000	-1.104309000
1	-5.278296000	2.013707000	0.853745000
1	-5.479054000	-0.048579000	-2.990408000
1	-6.599977000	1.423056000	-1.242407000
6	-1.190221000	-0.848066000	1.492242000
6	-0.435408000	-0.215590000	2.504937000
6	-2.156294000	-1.834488000	1.816933000
6	-0.661851000	-0.561915000	3.864497000
1	0.318573000	0.539533000	2.281286000
6	-2.369883000	-2.172394000	3.178308000
1	-2.726429000	-2.341715000	1.038285000
6	-1.628132000	-1.537266000	4.203782000
1	-0.078928000	-0.064894000	4.644940000
1	-3.112897000	-2.935725000	3.424961000
1	-1.797341000	-1.802540000	5.250482000
7	2.824618000	4.642994000	0.219963000
7	5.023352000	-2.526219000	-0.383022000
8	5.232299000	-3.737709000	-0.561928000
8	5.880338000	-1.653093000	-0.152590000
8	4.042379000	4.386684000	0.214610000
8	2.305876000	5.768404000	0.320157000

Oxo - [(4,4'-OMe-bpy)Pt^{IV}(Ph)(O)(Py)]$^{+}$

6	2.202880000	-0.011741000	-0.296227000
6	1.747418000	-2.289159000	-0.736645000
6	3.581520000	-0.269650000	-0.233482000
6	3.110953000	-2.629649000	-0.692247000
1	0.958541000	-3.011172000	-0.961826000
6	4.057436000	-1.598980000	-0.427180000
1	4.306954000	0.518605000	-0.035953000
1	3.401456000	-3.664943000	-0.861490000
6	1.603435000	1.350837000	-0.136571000
6	-0.367238000	2.603942000	-0.029767000
6	2.386283000	2.512471000	-0.018938000
6	0.328470000	3.822741000	0.086744000
1	-1.458860000	2.604051000	-0.041615000
6	1.751511000	3.781068000	0.096281000
1	3.475102000	2.476285000	-0.030589000
1	-0.233988000	4.751756000	0.163505000
7	0.231538000	1.399667000	-0.134971000
7	1.312969000	-1.025121000	-0.537485000
78	-0.689466000	-0.567956000	-0.553934000
8	-1.034416000	-2.074291000	-1.578951000
7	-2.727740000	-0.101561000	-0.759662000
6	-3.399145000	0.630446000	0.170135000
6	-3.390188000	-0.550330000	-1.860381000
6	-4.760532000	0.966599000	0.024687000
1	-2.834233000	0.927508000	1.054001000
6	-4.753733000	-0.252678000	-2.079787000
1	-2.799454000	-1.170663000	-2.534774000
6	-5.453766000	0.520160000	-1.126115000
1	-5.255572000	1.549496000	0.803394000
1	-5.241405000	-0.630086000	-2.980196000
1	-6.509841000	0.763451000	-1.269842000
6	-0.887321000	-0.856775000	1.494416000
6	-0.203368000	-0.143364000	2.505349000
6	-1.753966000	-1.927204000	1.838318000
6	-0.400272000	-0.490267000	3.869058000
1	0.475872000	0.676496000	2.270949000
6	-1.941703000	-2.266786000	3.202649000
1	-2.267642000	-2.498654000	1.064461000
6	-1.269389000	-1.549089000	4.221739000
1	0.129727000	0.071085000	4.644022000
1	-2.608900000	-3.094859000	3.458065000
1	-1.416676000	-1.814535000	5.272001000
6	1.979920000	6.168374000	0.296017000
6	5.942150000	-3.091257000	-0.537275000
1	7.026653000	-2.975704000	-0.424393000
1	5.557454000	-3.785609000	0.228335000
1	5.707879000	-3.462387000	-1.548964000
1	2.827483000	6.861128000	0.358479000
1	1.379415000	6.391763000	-0.601909000
1	1.361551000	6.251273000	1.205738000
8	5.392260000	-1.764452000	-0.342676000
8	2.568569000	4.848385000	0.198577000

Oxo - [(4,4'-NMe$_2$-bpy)Pt^{IV}(Ph)(O)(Py)]$^{+}$

6	1.895942000	-0.341616000	-0.299166000
6	1.199168000	-2.553224000	-0.728656000
6	3.238663000	-0.747374000	-0.223924000
6	2.509191000	-3.034575000	-0.674074000
1	0.339712000	-3.188146000	-0.955905000
6	3.594169000	-2.128967000	-0.403151000
1	4.006850000	-0.006077000	-0.023170000
1	2.674972000	-4.096764000	-0.840707000

6	1.446936000	1.083066000	-0.156215000
6	-0.373596000	2.537067000	-0.065632000
6	2.350694000	2.155951000	-0.055580000
6	0.444355000	3.667566000	0.035510000
1	-1.458752000	2.654854000	-0.080597000
6	1.873394000	3.506447000	0.046723000
1	3.418120000	1.955502000	-0.079430000
1	-0.026079000	4.646746000	0.098257000
7	0.089833000	1.268109000	-0.155023000
7	0.897214000	-1.244278000	-0.537471000
78	-1.040042000	-0.578141000	-0.552337000
8	-1.555022000	-2.043725000	-1.568564000
7	-3.021503000	0.107160000	-0.753974000
6	-3.600246000	0.929185000	0.162080000
6	-3.738923000	-0.289643000	-1.839541000
6	-4.917252000	1.411553000	0.017037000
1	-2.999208000	1.182279000	1.035871000
6	-5.063174000	0.151987000	-2.057965000
1	-3.223754000	-0.987777000	-2.500346000
6	-5.665468000	1.019198000	-1.118754000
1	-5.337738000	2.063333000	0.784947000
1	-5.597357000	-0.189412000	-2.946342000
1	-6.689313000	1.374883000	-1.262015000
6	-1.265570000	-0.812242000	1.499060000
6	-0.516434000	-0.155408000	2.502496000
6	-2.238069000	-1.781895000	1.860975000
6	-0.751538000	-0.454736000	3.871319000
1	0.243344000	0.585902000	2.255302000
6	-2.464333000	-2.075572000	3.230022000
1	-2.805974000	-2.312729000	1.095984000
6	-1.725780000	-1.411776000	4.239807000
1	-0.169437000	0.064133000	4.638723000
1	-3.213931000	-2.826042000	3.496900000
1	-1.903349000	-1.640767000	5.294091000
7	2.724928000	4.574822000	0.139667000
7	4.891849000	-2.557844000	-0.323738000
6	4.181170000	4.362519000	0.128567000
6	2.182652000	5.943451000	0.208229000
6	5.973998000	-1.599081000	-0.051280000
6	5.208694000	-3.984040000	-0.523193000
1	6.290892000	-4.130269000	-0.415398000
1	4.699705000	-4.614840000	0.226480000
1	4.914079000	-4.323302000	-1.531914000
1	6.931054000	-2.134452000	-0.018308000
1	6.040291000	-0.830102000	-0.842559000
1	5.830739000	-1.097094000	0.922687000
1	4.688078000	5.331143000	0.221320000
1	4.499988000	3.728551000	0.975449000
1	4.513319000	3.891078000	-0.814324000
1	3.013743000	6.657054000	0.272463000
1	1.589439000	6.186142000	-0.691442000
1	1.545959000	6.078141000	1.100420000

Oxo - [(5,5'-NO_2-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

6	1.562778000	1.843041000	-0.207338000
6	2.964159000	-0.047002000	-0.522718000
6	2.683671000	2.703395000	-0.105243000
6	4.102215000	0.776592000	-0.425948000
1	2.997678000	-1.121722000	-0.717267000
6	3.982499000	2.165131000	-0.210863000
1	2.556864000	3.772561000	0.059864000
1	4.874627000	2.787630000	-0.132480000
6	0.145743000	2.308733000	-0.134369000
6	-2.110851000	1.656956000	-0.128630000
6	-0.210020000	3.680103000	-0.066876000
6	-2.518946000	3.003622000	-0.063307000
1	-2.847969000	0.856045000	-0.159129000
6	-1.570269000	4.046072000	-0.028559000
1	0.553848000	4.456756000	-0.056956000
1	-1.891708000	5.087126000	0.019873000
7	-0.806606000	1.321942000	-0.159098000
7	1.736211000	0.500235000	-0.406588000
78	0.053451000	-0.690991000	-0.492534000
8	1.010821000	-1.975861000	-1.416239000
7	-1.638520000	-1.886378000	-0.778346000
6	-2.682275000	-1.878599000	0.096900000
6	-1.695922000	-2.683292000	-1.881419000
6	-3.842559000	-2.650482000	-0.111446000
1	-2.567868000	-1.259275000	0.986573000
6	-2.825175000	-3.484819000	-2.157945000
1	-0.808805000	-2.674092000	-2.513962000
6	-3.919752000	-3.468743000	-1.264245000
1	-4.806340000	-4.078766000	-1.455491000
6	0.036489000	-1.013607000	1.566176000
6	-0.100633000	-0.014052000	2.554844000
6	0.251472000	-2.367617000	1.928372000
6	-0.039896000	-0.376937000	3.927539000
1	-0.257992000	1.034964000	2.301993000
6	0.312749000	-2.715346000	3.302475000
1	0.382105000	-3.137870000	1.168104000
6	0.164443000	-1.724943000	4.303622000
1	0.212589000	-1.999391000	5.360482000
1	0.482598000	-3.759661000	3.578264000
1	-0.153890000	0.399085000	4.689642000
1	-2.828225000	-4.103786000	-3.056648000
1	-4.651259000	-2.609758000	0.620133000
7	-3.973786000	3.310114000	-0.025686000
7	5.451405000	0.159069000	-0.551083000
8	6.425193000	0.930437000	-0.470021000
8	5.494710000	-1.071488000	-0.724436000
8	-4.292369000	4.510636000	0.025089000
8	-4.755340000	2.339192000	-0.046372000

Oxo - [(5,5'-OMe-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

6	1.869499000	1.531363000	-0.226391000
6	2.909414000	-0.570931000	-0.606890000

6	3.134741000	2.152776000	-0.125638000
6	4.211071000	0.000248000	-0.516167000
1	2.745184000	-1.627836000	-0.830400000
6	4.316618000	1.394890000	-0.263138000
1	3.210035000	3.223293000	0.066122000
1	5.284931000	1.887878000	-0.175116000
6	0.566183000	2.238883000	-0.123597000
6	-1.774250000	2.011191000	-0.103421000
6	0.444310000	3.645741000	-0.026471000
6	-1.975751000	3.418092000	-0.015058000
1	-2.642024000	1.351013000	-0.138676000
6	-0.826542000	4.252429000	0.030763000
1	1.333435000	4.276502000	-0.009741000
1	-0.906570000	5.337399000	0.099013000
7	-0.555388000	1.450560000	-0.152494000
7	1.807959000	0.181900000	-0.459053000
78	-0.064637000	-0.669122000	-0.526994000
8	0.602340000	-2.090327000	-1.510204000
7	-1.959336000	-1.539860000	-0.773005000
6	-2.957762000	-1.362734000	0.134428000
6	-2.186357000	-2.307180000	-1.873835000
6	-4.237796000	-1.928510000	-0.034795000
1	-2.712264000	-0.774788000	1.019062000
6	-3.442856000	-2.905823000	-2.115304000
1	-1.326864000	-2.442348000	-2.530405000
6	-4.489369000	-2.713976000	-1.185204000
1	-5.471189000	-3.166668000	-1.347079000
6	-0.100867000	-0.992092000	1.528775000
6	-0.084992000	0.003859000	2.531403000
6	-0.084038000	-2.366256000	1.883150000
6	-0.068517000	-0.376893000	3.900302000
1	-0.088368000	1.066239000	2.287062000
6	-0.065306000	-2.734638000	3.252757000
1	-0.073382000	-3.139041000	1.114108000
6	-0.060721000	-1.743643000	4.264468000
1	-0.046542000	-2.032687000	5.318728000
1	-0.049678000	-3.795457000	3.518221000
1	-0.061480000	0.400332000	4.670010000
1	-3.579363000	-3.509008000	-3.014473000
1	-5.002775000	-1.760690000	0.725297000
6	-3.535247000	5.243285000	0.096502000
6	6.585813000	-0.348902000	-0.603618000
1	-3.125773000	5.764413000	-0.786011000
1	-4.627948000	5.335932000	0.107277000
1	-3.116092000	5.670818000	1.023742000
1	6.782383000	0.078962000	0.394876000
1	7.239673000	-1.213178000	-0.771122000
1	6.760894000	0.408337000	-1.387535000
8	-3.268211000	3.824114000	0.020856000
8	5.238269000	-0.864179000	-0.682364000

Oxo - $[(5,5'\text{-}NMe_2\text{-bpy})Pt^{IV}(Ph)(O)(Py)]^+$

6	1.446151000	1.894321000	-0.195765000
6	2.968015000	0.082113000	-0.479305000
6	2.536986000	2.795056000	-0.095545000
6	4.119867000	0.932163000	-0.391084000
1	3.011387000	-0.989839000	-0.672831000
6	3.857051000	2.329871000	-0.185656000
1	2.357987000	3.859919000	0.056366000
1	4.674859000	3.044978000	-0.100576000
6	0.016802000	2.272804000	-0.140685000
6	-2.213041000	1.499315000	-0.175431000
6	-0.445819000	3.613786000	-0.069244000
6	-2.769726000	2.820322000	-0.116540000
1	-2.857125000	0.623611000	-0.221721000
6	-1.817762000	3.894198000	-0.054074000
1	0.265292000	4.440010000	-0.038728000
1	-2.146523000	4.931791000	-0.005327000
7	-0.889374000	1.250765000	-0.182526000
7	1.718447000	0.567415000	-0.380915000
78	0.102898000	-0.696198000	-0.478925000
8	1.120194000	-1.949446000	-1.395457000
7	-1.527937000	-1.998031000	-0.761913000
6	-2.566834000	-2.063836000	0.113621000
6	-1.527054000	-2.806908000	-1.856009000
6	-3.663400000	-2.928700000	-0.081652000
1	-2.498441000	-1.425446000	0.994628000
6	-2.591439000	-3.696320000	-2.125055000
1	-0.639067000	-2.734663000	-2.484169000
6	-3.680183000	-3.761034000	-1.226647000
1	-4.514960000	-4.443415000	-1.407677000
6	0.057248000	-0.966817000	1.581468000
6	-0.120917000	0.046923000	2.549870000
6	0.301327000	-2.305612000	1.985784000
6	-0.073342000	-0.282644000	3.930974000
1	-0.295203000	1.084672000	2.265899000
6	0.347988000	-2.624055000	3.367244000
1	0.464068000	-3.088824000	1.244459000
6	0.157872000	-1.615963000	4.343692000
1	0.195468000	-1.864865000	5.407663000
1	0.538662000	-3.657679000	3.669809000
1	-0.216044000	0.508231000	4.673173000
1	-2.548719000	-4.321250000	-3.018748000
1	-4.467017000	-2.951826000	0.656627000
7	-4.130545000	3.034943000	-0.116092000
7	5.390005000	0.418904000	-0.500792000
6	-4.652004000	4.408461000	-0.043346000
6	-5.054236000	1.898022000	-0.217898000
6	6.548205000	1.321176000	-0.432964000
6	5.581683000	-1.022832000	-0.731991000
1	-4.334227000	5.010916000	-0.914162000
1	-5.749128000	4.376201000	-0.033777000
1	-4.318026000	4.918190000	0.878515000
1	-6.086424000	2.271336000	-0.232696000
1	-4.886942000	1.321531000	-1.146794000
1	-4.952945000	1.213117000	0.645225000

1	6.595125000	1.846084000	0.538784000
1	7.468503000	0.733846000	-0.545977000
1	6.521829000	2.076343000	-1.240289000
1	6.656946000	-1.236948000	-0.786082000
1	5.152638000	-1.621427000	0.091353000
1	5.115631000	-1.346381000	-1.680040000

Aryl Migration TS - [(bpy)Pt^{IV}(Ph)(O)(Py)]$^{+}$

8	-0.753842000	1.386039000	-1.644876000
7	1.811281000	0.588267000	-0.767321000
6	2.111150000	1.711795000	-1.461087000
6	2.790663000	-0.181680000	-0.198666000
6	3.447719000	2.129751000	-1.629522000
1	1.236905000	2.231109000	-1.866902000
6	4.150361000	0.188329000	-0.330909000
6	4.481643000	1.356033000	-1.052830000
1	3.659878000	3.036893000	-2.197125000
1	4.937554000	-0.418801000	0.115792000
1	5.527541000	1.652188000	-1.162334000
7	-2.056224000	-0.784459000	-0.493541000
6	-2.684593000	-1.151260000	0.656027000
6	-2.730133000	-0.851349000	-1.674818000
6	-4.005090000	-1.641967000	0.666984000
6	-4.055474000	-1.335275000	-1.747746000
6	-4.705059000	-1.742122000	-0.560632000
1	-2.117883000	-1.018928000	1.578992000
1	-2.191178000	-0.495669000	-2.551443000
1	-4.467673000	-1.920705000	1.615403000
1	-4.554602000	-1.377006000	-2.717286000
1	-5.731267000	-2.117584000	-0.586815000
1	4.271282000	-2.151367000	1.130029000
6	3.194586000	-2.320622000	1.140224000
6	2.315953000	-1.400694000	0.516852000
6	2.667888000	-3.465527000	1.772497000
7	0.956127000	-1.593386000	0.524023000
6	1.267486000	-3.664719000	1.757864000
1	3.332520000	-4.184409000	2.256631000
6	0.457555000	-2.702324000	1.121691000
1	0.807162000	-4.538092000	2.222457000
1	-0.625832000	-2.825033000	1.083418000
78	-0.125833000	-0.042220000	-0.527076000
6	-0.729472000	1.686831000	0.610565000
6	0.256973000	2.171963000	1.496989000
6	-2.063572000	2.143168000	0.656858000
6	-0.129936000	3.104184000	2.498999000
1	1.295050000	1.844040000	1.450774000
6	-2.428168000	3.075981000	1.659801000
1	-2.788863000	1.823050000	-0.088437000
6	-1.466559000	3.556388000	2.584087000
1	0.623869000	3.464293000	3.204982000
1	-3.457522000	3.444041000	1.692135000
1	-1.753062000	4.282569000	3.349182000

Aryl Migration TS - [(bpy)Pt^{IV}(*p*-NO_2-Ph)(O)(Py)]$^{+}$

8	0.351990000	0.308242000	-2.239762000
7	-1.558099000	-1.329056000	-0.946315000
6	-1.273683000	-2.074763000	-2.040432000
6	-2.508766000	-1.722302000	-0.041818000
6	-1.948310000	-3.287796000	-2.291758000
1	-0.501225000	-1.645102000	-2.686019000
6	-3.216117000	-2.931984000	-0.238402000
6	-2.931681000	-3.723008000	-1.373665000
1	-1.700852000	-3.865890000	-3.183173000
1	-3.975236000	-3.253685000	0.474253000
1	-3.471150000	-4.659015000	-1.536067000
7	0.208255000	2.337764000	-0.334024000
6	0.791712000	2.747276000	0.825499000
6	0.188275000	3.177291000	-1.406512000
6	1.347093000	4.033363000	0.973498000
6	0.720004000	4.484097000	-1.335871000
6	1.306025000	4.924000000	-0.127516000
1	0.830499000	2.013988000	1.632573000
1	-0.246190000	2.774890000	-2.320311000
1	1.808059000	4.314340000	1.922007000
1	0.676586000	5.124855000	-2.218110000
1	1.728539000	5.928718000	-0.045973000
1	-4.301546000	-1.939739000	2.098453000
6	-3.698570000	-1.031889000	2.112191000
6	-2.738019000	-0.789878000	1.099864000
6	-3.875946000	-0.084775000	3.142072000
7	-1.964741000	0.344851000	1.105591000
6	-3.089753000	1.090601000	3.126662000
1	-4.612389000	-0.257358000	3.929965000
6	-2.150818000	1.258135000	2.088315000
1	-3.194190000	1.861109000	3.892064000
1	-1.531981000	2.155064000	2.037186000
78	-0.598438000	0.447715000	-0.575233000
6	1.322381000	-0.450370000	-0.328181000
6	1.307974000	-1.700191000	0.335057000
6	2.529491000	0.244621000	-0.572852000
6	2.526836000	-2.244924000	0.810422000
1	0.386723000	-2.254190000	0.509691000
6	3.746685000	-0.297753000	-0.104468000
1	2.532566000	1.163951000	-1.153942000
6	3.723579000	-1.532442000	0.586670000
1	2.547794000	-3.193986000	1.346356000
1	4.695689000	0.205800000	-0.289371000
7	5.000121000	-2.101945000	1.087734000
8	6.042342000	-1.446453000	0.883355000
8	4.947842000	-3.196874000	1.685785000

Aryl Migration TS - [(bpy)Pt^{IV}(*p*-OMe-Ph)(O)(Py)]$^{+}$

8	0.604698000	-0.034562000	-2.154333000
7	-1.667226000	-1.147082000	-0.892351000
6	-1.478068000	-2.023705000	-1.907216000
6	-2.720255000	-1.276098000	-0.026076000

6	-2.364168000	-3.101077000	-2.114950000
1	-0.602012000	-1.804691000	-2.526049000
6	-3.641560000	-2.339262000	-0.181981000
6	-3.461076000	-3.261012000	-1.236298000
1	-2.189123000	-3.788971000	-2.943355000
1	-4.484431000	-2.449483000	0.500352000
1	-4.165270000	-4.085935000	-1.367431000
7	0.770048000	2.131831000	-0.425579000
6	1.377949000	2.506248000	0.732245000
6	0.966779000	2.869397000	-1.552890000
6	2.177293000	3.663100000	0.821604000
6	1.752670000	4.043470000	-1.545261000
6	2.365582000	4.452531000	-0.339539000
1	1.234888000	1.844010000	1.587517000
1	0.494566000	2.490792000	-2.457860000
1	2.645510000	3.921450000	1.773054000
1	1.877828000	4.606880000	-2.471447000
1	2.980747000	5.355398000	-0.304792000
1	-4.624736000	-0.963050000	2.000692000
6	-3.852579000	-0.193906000	1.992950000
6	-2.814010000	-0.228716000	1.029945000
6	-3.885723000	0.848134000	2.942037000
7	-1.827800000	0.726911000	1.006335000
6	-2.876341000	1.838677000	2.896915000
1	-4.680215000	0.889157000	3.690363000
6	-1.873467000	1.733533000	1.912301000
1	-2.859593000	2.673062000	3.599819000
1	-1.083419000	2.482730000	1.841261000
78	-0.390787000	0.425535000	-0.579802000
6	1.312892000	-0.820350000	-0.142356000
6	1.013479000	-2.004014000	0.574081000
6	2.645449000	-0.418256000	-0.353359000
6	2.069547000	-2.745184000	1.151413000
1	-0.008372000	-2.353767000	0.719424000
6	3.705685000	-1.163212000	0.222512000
1	2.873584000	0.438772000	-0.984301000
6	3.420618000	-2.333328000	0.981214000
1	1.859702000	-3.642640000	1.737885000
1	4.730682000	-0.837288000	0.042805000
6	5.745851000	-2.792150000	1.393551000
1	6.314435000	-3.556595000	1.939282000
1	6.023809000	-2.819033000	0.324622000
1	5.972980000	-1.795370000	1.813798000
8	4.360979000	-3.128902000	1.577462000

Aryl Migration TS - $[(bpy)Pt^{IV}(p\text{-}NMe_2\text{-}Ph)(O)(Py)]^+$

8	0.259476000	0.399807000	-2.220434000
7	-1.484021000	-1.431276000	-0.959145000
6	-1.114329000	-2.136113000	-2.055378000
6	-2.388395000	-1.933335000	-0.061096000
6	-1.654467000	-3.411771000	-2.318202000
1	-0.387870000	-1.619034000	-2.690719000
6	-2.963007000	-3.210249000	-0.270121000
6	-2.592263000	-3.956655000	-1.409596000
1	-1.342116000	-3.953853000	-3.211933000
1	-3.685881000	-3.616493000	0.437323000
1	-3.029081000	-4.942945000	-1.582925000
7	-0.089454000	2.380957000	-0.309194000
6	0.469821000	2.829521000	0.846494000
6	-0.200221000	3.226043000	-1.370484000
6	0.903912000	4.160630000	1.004403000
6	0.210263000	4.575743000	-1.292020000
6	0.767059000	5.055551000	-0.085182000
1	0.591089000	2.090673000	1.640199000
1	-0.609243000	2.793649000	-2.282143000
1	1.348474000	4.473047000	1.950970000
1	0.097102000	5.218883000	-2.166375000
1	1.094994000	6.094522000	0.003520000
1	-4.159755000	-2.348727000	2.066143000
6	-3.647934000	-1.386763000	2.094086000
6	-2.712777000	-1.041542000	1.087007000
6	-3.919665000	-0.473770000	3.132994000
7	-2.052744000	0.163271000	1.105672000
6	-3.248329000	0.772176000	3.133260000
1	-4.639113000	-0.724634000	3.915523000
6	-2.327890000	1.041353000	2.100916000
1	-3.427896000	1.520258000	3.907048000
1	-1.795988000	1.993310000	2.064160000
78	-0.707383000	0.420936000	-0.563963000
6	1.309192000	-0.284101000	-0.303248000
6	1.443453000	-1.558552000	0.288632000
6	2.450171000	0.510503000	-0.544631000
6	2.711867000	-1.990342000	0.745726000
1	0.592480000	-2.223785000	0.437417000
6	3.715378000	0.079330000	-0.093457000
1	2.370455000	1.440846000	-1.104074000
6	3.882585000	-1.178332000	0.581801000
1	2.769502000	-2.962497000	1.235347000
1	4.573330000	0.718776000	-0.300597000
7	5.124796000	-1.587481000	1.060550000
6	5.289938000	-2.968271000	1.530916000
6	6.326254000	-0.842231000	0.663410000
1	4.621654000	-3.175887000	2.384509000
1	6.322691000	-3.110190000	1.878486000
1	5.083059000	-3.714242000	0.737432000
1	7.204892000	-1.291633000	1.146873000
1	6.488198000	-0.850833000	-0.432960000
1	6.265309000	0.208072000	0.996757000

Aryl Migration TS - $[(bpy)Pt^{IV}(m\text{-}NO_2\text{-}Ph)(O)(Py)]^+$

8	0.556638000	-0.605297000	-1.970461000
7	-1.968302000	-1.044549000	-0.772982000
6	-1.898439000	-2.094814000	-1.625037000
6	-3.083922000	-0.815557000	-0.012060000
6	-2.975232000	-2.995643000	-1.762437000
1	-0.956332000	-2.158155000	-2.178793000

6	-4.194852000	-1.687364000	-0.103575000
6	-4.139291000	-2.788581000	-0.986448000
1	-2.892219000	-3.830525000	-2.459679000
1	-5.088471000	-1.513818000	0.495682000
1	-4.991206000	-3.467831000	-1.066457000
7	1.047067000	1.751861000	-0.575454000
6	1.626677000	2.207622000	0.569045000
6	1.488634000	2.213227000	-1.778668000
6	2.653589000	3.170851000	0.559172000
6	2.510362000	3.184130000	-1.871194000
6	3.104257000	3.673282000	-0.686332000
1	1.273274000	1.762154000	1.500385000
1	1.021377000	1.775078000	-2.658983000
1	3.095151000	3.496530000	1.502487000
1	2.831357000	3.526340000	-2.856350000
1	3.905002000	4.415826000	-0.729226000
1	-5.018513000	0.190228000	1.743626000
6	-4.107929000	0.787152000	1.694545000
6	-3.034073000	0.394751000	0.858582000
6	-3.995126000	1.963365000	2.464484000
7	-1.876527000	1.130194000	0.789915000
6	-2.807173000	2.724953000	2.370492000
1	-4.814710000	2.279129000	3.113716000
6	-1.780048000	2.266992000	1.520053000
1	-2.671290000	3.648694000	2.935013000
1	-0.852662000	2.831643000	1.414727000
78	-0.420620000	0.292587000	-0.582064000
6	0.949003000	-1.142232000	0.205740000
6	0.395193000	-2.146905000	1.031903000
6	2.342678000	-0.974505000	0.092807000
6	1.261573000	-2.973587000	1.799162000
1	-0.680900000	-2.300201000	1.108033000
6	3.169020000	-1.811000000	0.875411000
1	2.793727000	-0.263431000	-0.591517000
6	2.662033000	-2.817631000	1.730159000
1	3.343355000	-3.444526000	2.304587000
1	0.830031000	-3.735972000	2.452515000
7	4.643459000	-1.623031000	0.777513000
8	5.367181000	-2.420846000	1.404687000
8	5.061167000	-0.669522000	0.086199000

Aryl Migration TS - [(bpy)Pt^{IV}(*m*-OMe-Ph)(O)(Py)]$^{+}$

8	0.652166000	-0.573839000	-1.994219000
7	-1.863411000	-1.026968000	-0.787716000
6	-1.799106000	-2.066429000	-1.652764000
6	-2.968781000	-0.815143000	-0.008093000
6	-2.874217000	-2.969098000	-1.789371000
1	-0.861406000	-2.118960000	-2.215301000
6	-4.078516000	-1.689157000	-0.098023000
6	-4.030258000	-2.776779000	-0.997396000
1	-2.796042000	-3.795312000	-2.497423000
1	-4.963983000	-1.528355000	0.516776000
1	-4.880533000	-3.458242000	-1.076550000
7	1.155354000	1.758214000	-0.567447000
6	1.759640000	2.174931000	0.577837000
6	1.566174000	2.263744000	-1.762816000
6	2.775199000	3.151059000	0.579129000
6	2.576758000	3.247449000	-1.845440000
6	3.190462000	3.703639000	-0.657308000
1	1.433845000	1.688864000	1.498683000
1	1.080720000	1.852328000	-2.646272000
1	3.233162000	3.449804000	1.523635000
1	2.870795000	3.628154000	-2.824944000
1	3.978248000	4.460576000	-0.691673000
1	-4.882920000	0.161284000	1.785238000
6	-3.971046000	0.756600000	1.739515000
6	-2.907394000	0.378034000	0.883834000
6	-3.846219000	1.915412000	2.532805000
7	-1.747887000	1.110964000	0.816742000
6	-2.655500000	2.673927000	2.442592000
1	-4.657723000	2.220463000	3.197141000
6	-1.639713000	2.230785000	1.571587000
1	-2.509509000	3.584399000	3.025913000
1	-0.710616000	2.793316000	1.469262000
78	-0.314295000	0.303121000	-0.588466000
6	1.071480000	-1.169375000	0.165694000
6	0.484329000	-2.151517000	0.997946000
6	2.460493000	-1.017301000	0.043417000
6	1.356837000	-2.968041000	1.761476000
1	-0.592378000	-2.284007000	1.088748000
6	3.316527000	-1.847826000	0.824665000
1	2.907965000	-0.329411000	-0.670158000
6	2.763014000	-2.831611000	1.690658000
1	3.397611000	-3.483924000	2.290439000
1	0.925093000	-3.716524000	2.432091000
6	5.578769000	-2.508045000	1.309524000
1	5.415568000	-3.557372000	1.005694000
1	6.580028000	-2.186052000	0.993781000
1	5.493648000	-2.419372000	2.407762000
8	4.656771000	-1.627679000	0.644176000

Aryl Migration TS - [(bpy)Pt^{IV}(*m*-NMe$_2$-Ph)(O)(Py)]$^{+}$

8	0.564202000	-0.509824000	-1.964319000
7	-1.941701000	-1.112256000	-0.807978000
6	-1.796102000	-2.148491000	-1.666885000
6	-3.070402000	-0.970886000	-0.046214000
6	-2.808769000	-3.118554000	-1.817319000
1	-0.847389000	-2.142336000	-2.213251000
6	-4.120545000	-1.914321000	-0.150781000
6	-3.987959000	-2.998638000	-1.045393000
1	-2.666017000	-3.940606000	-2.520132000
1	-5.023774000	-1.808935000	0.449988000
1	-4.791240000	-3.733624000	-1.135835000
7	0.891866000	1.852919000	-0.528385000
6	1.460428000	2.287345000	0.628151000
6	1.271700000	2.409353000	-1.710839000

6	2.403261000	3.334284000	0.654599000
6	2.209695000	3.464457000	-1.769026000
6	2.782253000	3.941088000	-0.568096000
1	1.163503000	1.762235000	1.537221000
1	0.818531000	1.983732000	-2.604821000
1	2.832019000	3.648081000	1.607955000
1	2.478427000	3.886205000	-2.738993000
1	3.510138000	4.756492000	-0.582390000
1	-5.072190000	-0.111983000	1.712056000
6	-4.197265000	0.537431000	1.681695000
6	-3.098230000	0.224227000	0.844347000
6	-4.156400000	1.701131000	2.476319000
7	-1.984381000	1.026505000	0.795753000
6	-3.012213000	2.530359000	2.405784000
1	-4.995896000	1.956134000	3.126811000
6	-1.957113000	2.150247000	1.552170000
1	-2.931220000	3.447388000	2.991501000
1	-1.061671000	2.767329000	1.465317000
78	-0.483115000	0.309431000	-0.582132000
6	0.983552000	-1.090107000	0.200449000
6	0.419255000	-2.055147000	1.059420000
6	2.366142000	-0.881225000	0.067052000
6	1.331238000	-2.805148000	1.851786000
1	-0.651633000	-2.223767000	1.155732000
6	3.278959000	-1.637304000	0.879642000
1	2.727356000	-0.207700000	-0.702277000
6	2.723439000	-2.611349000	1.776714000
1	3.370317000	-3.225040000	2.402495000
1	0.933063000	-3.548035000	2.549345000
7	4.658466000	-1.436609000	0.786333000
6	5.183272000	-0.625249000	-0.318828000
6	5.556741000	-2.444451000	1.370026000
1	4.780554000	0.401407000	-0.276239000
1	6.276090000	-0.554053000	-0.225453000
1	4.942630000	-1.050931000	-1.314006000
1	5.397054000	-3.454137000	0.941835000
1	6.598323000	-2.147940000	1.182208000
1	5.422949000	-2.505157000	2.463116000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}NO_2\text{-}Py)]^+$

8	0.045822000	1.549761000	-1.622400000
7	2.406121000	0.213642000	-0.837241000
6	2.912212000	1.229992000	-1.575577000
6	3.216953000	-0.749683000	-0.297901000
6	4.297019000	1.331138000	-1.823645000
1	2.156824000	1.927750000	-1.950402000
6	4.615074000	-0.699465000	-0.510314000
6	5.160210000	0.351387000	-1.280700000
1	4.675799000	2.158105000	-2.425894000
1	5.268876000	-1.462773000	-0.088677000
1	6.237933000	0.400283000	-1.452852000
7	-1.652193000	-0.238682000	-0.360799000
6	-2.297332000	-0.419653000	0.823332000
6	-2.368610000	-0.165066000	-1.516323000
6	-3.693039000	-0.583270000	0.906291000
6	-3.773063000	-0.318292000	-1.535601000
6	-4.417357000	-0.534360000	-0.303639000
1	-1.677954000	-0.406010000	1.720670000
1	-1.798046000	0.032392000	-2.422038000
1	-4.194254000	-0.727449000	1.862762000
1	-4.333495000	-0.265162000	-2.468499000
1	4.288315000	-2.977705000	1.015405000
6	3.203360000	-2.899499000	1.083642000
6	2.520909000	-1.817111000	0.476276000
6	2.468567000	-3.883429000	1.776805000
7	1.155237000	-1.697679000	0.556467000
6	1.060755000	-3.760964000	1.838757000
1	2.980467000	-4.724481000	2.249512000
6	0.454263000	-2.652865000	1.213097000
1	0.442439000	-4.498075000	2.353365000
1	-0.629661000	-2.529607000	1.232913000
78	0.395796000	0.038703000	-0.492245000
6	0.254389000	1.885271000	0.621264000
6	1.365811000	2.138229000	1.454497000
6	-0.933564000	2.640777000	0.706581000
6	1.250211000	3.150359000	2.447018000
1	2.295421000	1.575356000	1.376344000
6	-1.026849000	3.647330000	1.700615000
1	-1.742980000	2.492427000	-0.005474000
6	0.060213000	3.902968000	2.573633000
1	2.097412000	3.335223000	3.113509000
1	-1.939028000	4.247224000	1.763417000
1	-0.015101000	4.687504000	3.330869000
7	-5.903133000	-0.709505000	-0.270671000
8	-6.501032000	-0.653628000	-1.359833000
8	-6.420801000	-0.898764000	0.845642000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}OMe\text{-}Py)]^+$

8	-0.179983000	1.503421000	-1.622104000
7	2.239736000	0.237518000	-0.881765000
6	2.702437000	1.251767000	-1.650043000
6	3.086964000	-0.695375000	-0.346233000
6	4.077766000	1.382388000	-1.934344000
1	1.919381000	1.923452000	-2.016765000
6	4.478441000	-0.615516000	-0.593521000
6	4.978239000	0.434024000	-1.395296000
1	4.421787000	2.207248000	-2.559955000
1	5.160982000	-1.354696000	-0.174258000
1	6.050010000	0.506475000	-1.594507000
7	-1.787449000	-0.318644000	-0.265350000
6	-2.393766000	-0.492033000	0.945880000
6	-2.563847000	-0.297895000	-1.381846000
6	-3.770354000	-0.695167000	1.083021000
6	-3.957917000	-0.496227000	-1.347969000
6	-4.588589000	-0.705209000	-0.088361000
1	-1.745911000	-0.437147000	1.821991000

1	-2.043812000	-0.103828000	-2.318788000
1	-4.221145000	-0.825866000	2.067716000
1	-4.511709000	-0.472814000	-2.285439000
1	4.243551000	-2.873573000	0.978159000
6	3.158853000	-2.820727000	1.071273000
6	2.435814000	-1.765437000	0.462915000
6	2.465121000	-3.810143000	1.797915000
7	1.069710000	-1.677361000	0.574433000
6	1.056303000	-3.720762000	1.890822000
1	3.008605000	-4.630189000	2.272346000
6	0.407506000	-2.638590000	1.262242000
1	0.468601000	-4.463870000	2.432070000
1	-0.678140000	-2.539391000	1.304301000
78	0.240148000	0.021197000	-0.476262000
6	0.083724000	1.878935000	0.601336000
6	1.215646000	2.194373000	1.384894000
6	-1.126794000	2.594034000	0.720083000
6	1.104172000	3.227421000	2.356029000
1	2.161417000	1.662881000	1.282848000
6	-1.216930000	3.622765000	1.690719000
1	-1.960460000	2.391120000	0.050978000
6	-0.106035000	3.941022000	2.512086000
1	1.970127000	3.459633000	2.982581000
1	-2.148157000	4.189701000	1.777691000
1	-0.179924000	4.742064000	3.252193000
6	-6.785973000	-0.902978000	-1.046366000
1	-6.753039000	0.074988000	-1.555125000
1	-7.790898000	-1.080662000	-0.645291000
1	-6.513342000	-1.711204000	-1.745680000
8	-5.906037000	-0.907461000	0.104444000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(4\text{-}NMe_2\text{-}Py)]^+$

8	0.147250000	1.571325000	-1.625677000
7	2.484962000	0.190720000	-0.823526000
6	3.018797000	1.201161000	-1.549061000
6	3.271519000	-0.788082000	-0.278085000
6	4.408452000	1.281027000	-1.776800000
1	2.277918000	1.912065000	-1.929606000
6	4.674051000	-0.760861000	-0.469058000
6	5.247545000	0.284353000	-1.225750000
1	4.810435000	2.104331000	-2.369052000
1	5.308777000	-1.536819000	-0.041204000
1	6.328469000	0.316539000	-1.381455000
7	-1.579445000	-0.221881000	-0.366587000
6	-2.241864000	-0.388668000	0.812946000
6	-2.328077000	-0.149215000	-1.507073000
6	-3.628394000	-0.537583000	0.907314000
6	-3.720352000	-0.290557000	-1.517407000
6	-4.437005000	-0.501094000	-0.286471000
1	-1.628814000	-0.374164000	1.715916000
1	-1.774641000	0.041794000	-2.425294000
1	-4.066677000	-0.656872000	1.896693000
1	-4.232643000	-0.222162000	-2.475402000
1	4.283405000	-3.044298000	1.034691000
6	3.198994000	-2.947465000	1.087466000
6	2.545038000	-1.848106000	0.478558000
6	2.436371000	-3.923351000	1.761177000
7	1.180252000	-1.704780000	0.539543000
6	1.029775000	-3.776334000	1.801496000
1	2.925930000	-4.776990000	2.235107000
6	0.451618000	-2.653203000	1.176111000
1	0.391006000	-4.506975000	2.300250000
1	-0.629518000	-2.507695000	1.176775000
78	0.461045000	0.048066000	-0.499474000
6	0.336142000	1.884837000	0.611254000
6	1.450444000	2.148506000	1.438364000
6	-0.852849000	2.639294000	0.704745000
6	1.342507000	3.168663000	2.423458000
1	2.380468000	1.586229000	1.358118000
6	-0.940098000	3.654592000	1.689363000
1	-1.670978000	2.473767000	0.006774000
6	0.153020000	3.921353000	2.552211000
1	2.194671000	3.360562000	3.081850000
1	-1.853779000	4.252229000	1.755597000
1	0.081993000	4.712605000	3.303175000
7	-5.795029000	-0.648423000	-0.248270000
6	-6.581853000	-0.556295000	-1.491823000
6	-6.482995000	-0.821267000	1.043442000
1	-6.476723000	0.437631000	-1.962243000
1	-7.642276000	-0.716656000	-1.259434000
1	-6.269157000	-1.326918000	-2.217686000
1	-6.117480000	-1.719244000	1.571723000
1	-7.558496000	-0.946089000	0.864941000
1	-6.341266000	0.057703000	1.697768000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}NO_2\text{-}Py)]^+$

8	-0.489088000	1.299001000	-1.503819000
7	2.080745000	0.191429000	-1.103424000
6	2.342135000	1.123995000	-2.050253000
6	3.056306000	-0.653875000	-0.644518000
6	3.632661000	1.258016000	-2.603611000
1	1.474886000	1.728382000	-2.334315000
6	4.370800000	-0.564830000	-1.160455000
6	4.661789000	0.401460000	-2.148755000
1	3.813290000	2.015039000	-3.368005000
1	5.153657000	-1.234395000	-0.804632000
1	5.672827000	0.479625000	-2.555227000
7	-1.742031000	-0.373031000	0.301599000
6	-2.119664000	-0.397528000	1.609001000
6	-2.681854000	-0.493653000	-0.671200000
6	-3.458817000	-0.584070000	2.008610000
6	-4.036486000	-0.689403000	-0.328175000
6	-4.454877000	-0.738879000	1.016778000
1	-1.325149000	-0.240136000	2.339847000
1	-2.352837000	-0.424264000	-1.705510000
1	-5.508131000	-0.886224000	1.260718000

1	4.538498000	-2.648390000	0.648300000
6	3.489772000	-2.610099000	0.942798000
6	2.619100000	-1.644770000	0.380235000
6	2.989459000	-3.530902000	1.886350000
7	1.296255000	-1.578470000	0.742507000
6	1.621230000	-3.465559000	2.239717000
1	3.648009000	-4.282013000	2.327967000
6	0.819001000	-2.473727000	1.640069000
1	1.179879000	-4.159566000	2.956669000
1	-0.242578000	-2.396926000	1.881229000
78	0.209045000	-0.029058000	-0.307489000
6	0.167758000	1.940668000	0.579858000
6	1.406057000	2.347252000	1.123246000
6	-1.025862000	2.651811000	0.824376000
6	1.427970000	3.475319000	1.989049000
1	2.336074000	1.818216000	0.917233000
6	-0.981616000	3.776182000	1.686687000
1	-1.951776000	2.378433000	0.322241000
6	0.241133000	4.189117000	2.272890000
1	0.269693000	5.063289000	2.928329000
1	2.379255000	3.781118000	2.433705000
1	-1.899917000	4.341976000	1.867091000
1	-3.710407000	-0.593583000	3.069987000
7	-5.033546000	-0.845995000	-1.422400000
8	-6.223677000	-0.973362000	-1.079997000
8	-4.600577000	-0.841978000	-2.589385000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}OMe\text{-}Py)]^{+}$

8	-0.461750000	1.379580000	-1.558798000
7	2.058402000	0.213739000	-1.041314000
6	2.394654000	1.176907000	-1.931653000
6	2.990279000	-0.662410000	-0.552227000
6	3.720473000	1.311806000	-2.393645000
1	1.554322000	1.804436000	-2.246191000
6	4.337812000	-0.574933000	-0.976403000
6	4.706260000	0.422756000	-1.905353000
1	3.961832000	2.094531000	-3.114182000
1	5.086522000	-1.269152000	-0.595125000
1	5.743067000	0.500600000	-2.240919000
7	-1.846042000	-0.374004000	0.112446000
6	-2.276305000	-0.470045000	1.403208000
6	-2.727482000	-0.479962000	-0.906262000
6	-3.628099000	-0.713627000	1.703005000
6	-4.113665000	-0.732724000	-0.681305000
6	-4.571851000	-0.855062000	0.656055000
1	-1.528117000	-0.312521000	2.179993000
1	-2.345858000	-0.348941000	-1.917501000
1	-5.620629000	-1.044477000	0.887806000
1	4.360153000	-2.721688000	0.759750000
6	3.294765000	-2.680245000	0.986196000
6	2.473849000	-1.683452000	0.403773000
6	2.723412000	-3.627234000	1.860773000
7	1.130784000	-1.611617000	0.680902000
6	1.335683000	-3.555130000	2.125943000
1	3.343081000	-4.402308000	2.317081000
6	0.585185000	-2.531694000	1.512420000
1	0.840201000	-4.267448000	2.787496000
1	-0.488381000	-2.445941000	1.687073000
78	0.130829000	-0.008257000	-0.374182000
6	0.059646000	1.916119000	0.590211000
6	1.267705000	2.302355000	1.211139000
6	-1.145000000	2.619766000	0.800212000
6	1.245796000	3.398200000	2.117370000
1	2.207432000	1.780010000	1.033264000
6	-1.145359000	3.712065000	1.703230000
1	-2.045641000	2.358761000	0.247981000
6	0.045693000	4.102803000	2.365603000
1	0.039963000	4.952456000	3.053317000
1	2.173031000	3.686503000	2.620840000
1	-2.072672000	4.270466000	1.859502000
1	-3.942242000	-0.779116000	2.746247000
6	-6.288703000	-1.048559000	-1.650334000
1	-6.691794000	-1.077195000	-2.669955000
1	-6.483873000	-2.011114000	-1.145900000
1	-6.755349000	-0.220697000	-1.088598000
8	-4.869522000	-0.827852000	-1.802675000

Aryl Migration TS - $[(bpy)Pt^{IV}(Ph)(O)(3\text{-}NMe_2\text{-}Py)]^{+}$

8	0.401147000	1.370527000	1.480249000
7	-2.126305000	0.162848000	1.108706000
6	-2.421409000	1.105167000	2.035033000
6	-3.072789000	-0.721232000	0.664810000
6	-3.716898000	1.209483000	2.582840000
1	-1.573063000	1.743063000	2.304170000
6	-4.392037000	-0.664432000	1.175099000
6	-4.717136000	0.311536000	2.142380000
1	-3.925177000	1.976639000	3.329988000
1	-5.152302000	-1.364657000	0.829374000
1	-5.731993000	0.366457000	2.543294000
7	1.691068000	-0.315600000	-0.352034000
6	1.997935000	-0.414825000	-1.672797000
6	2.656280000	-0.399688000	0.594329000
6	3.328774000	-0.641342000	-2.080224000
6	4.037961000	-0.633220000	0.273674000
6	4.352540000	-0.758642000	-1.120371000
1	1.183219000	-0.267612000	-2.381271000
1	2.316002000	-0.250627000	1.614428000
1	5.377199000	-0.930480000	-1.450056000
1	-4.486050000	-2.791867000	-0.580398000
6	-3.439310000	-2.725550000	-0.877068000
6	-2.601302000	-1.718227000	-0.338753000
6	-2.908686000	-3.651422000	-1.798704000
7	-1.281762000	-1.614398000	-0.705160000
6	-1.543139000	-3.548688000	-2.153163000
1	-3.541920000	-4.434127000	-2.222242000
6	-0.773773000	-2.515808000	-1.579839000

1	-1.078198000	-4.244574000	-2.853269000
1	0.283977000	-2.405473000	-1.822916000
78	-0.243989000	-0.003393000	0.302637000
6	-0.282490000	1.946366000	-0.608768000
6	-1.542813000	2.339984000	-1.109259000
6	0.895069000	2.663205000	-0.908242000
6	-1.607571000	3.460049000	-1.983308000
1	-2.460180000	1.805404000	-0.864341000
6	0.809431000	3.779245000	-1.777005000
1	1.844093000	2.389281000	-0.451882000
6	-0.438210000	4.180040000	-2.318354000
1	-0.497939000	5.047302000	-2.981109000
1	-2.577486000	3.754297000	-2.394550000
1	1.717138000	4.345933000	-2.003180000
1	3.558262000	-0.710787000	-3.145200000
7	4.989145000	-0.724108000	1.264877000
6	6.400440000	-0.913036000	0.899983000
6	4.608503000	-0.519580000	2.671546000
1	7.002802000	-0.975010000	1.815559000
1	6.546870000	-1.850361000	0.333147000
1	6.782977000	-0.071358000	0.292498000
1	3.873521000	-1.275557000	3.003223000
1	5.501464000	-0.617712000	3.302489000
1	4.177483000	0.484744000	2.836853000

Aryl Migration TS - [(4,4'-NO_2-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

8	1.693055000	-1.930784000	-1.119605000
7	-0.955974000	-1.144106000	-0.562656000
6	-1.132052000	-2.457448000	-0.842652000
6	-2.014544000	-0.323803000	-0.272298000
6	-2.416714000	-3.039478000	-0.855213000
1	-0.205467000	-2.998700000	-1.059489000
6	-3.332898000	-0.833502000	-0.261086000
6	-3.506406000	-2.197579000	-0.555791000
1	-2.560129000	-4.094482000	-1.085340000
1	-4.201364000	-0.216763000	-0.037368000
7	2.758207000	0.610874000	-0.757254000
6	3.318979000	1.374613000	0.220277000
6	3.450188000	0.380134000	-1.907575000
6	4.583822000	1.975957000	0.069177000
6	4.722557000	0.949680000	-2.134854000
6	5.299695000	1.764623000	-1.134969000
1	2.745913000	1.475381000	1.143407000
1	2.971761000	-0.277202000	-2.631790000
1	4.993391000	2.578372000	0.881850000
1	5.238160000	0.743018000	-3.074122000
1	6.283914000	2.216160000	-1.283313000
1	-3.710192000	1.846520000	0.345785000
6	-2.648509000	2.078762000	0.282608000
6	-1.669869000	1.099516000	-0.005750000
6	-2.215570000	3.398891000	0.488533000
7	-0.331299000	1.410969000	-0.072739000
6	-0.850547000	3.741175000	0.401048000
6	0.052161000	2.698804000	0.115301000
1	-0.511985000	4.765925000	0.549042000
1	1.119482000	2.903871000	0.029433000
78	0.907905000	-0.285680000	-0.545002000
6	1.627262000	-1.472634000	1.118615000
6	0.658645000	-1.718793000	2.115148000
6	2.992561000	-1.772667000	1.300165000
6	1.098201000	-2.228891000	3.367740000
1	-0.401320000	-1.512414000	1.968652000
6	3.407379000	-2.285972000	2.555133000
1	3.704853000	-1.657159000	0.485867000
6	2.465718000	-2.512057000	3.589948000
1	0.360750000	-2.396950000	4.157551000
1	4.461790000	-2.535141000	2.702675000
1	2.791927000	-2.917353000	4.551055000
7	-3.224109000	4.454440000	0.798075000
7	-4.893646000	-2.760622000	-0.549121000
8	-4.414156000	4.094079000	0.863875000
8	-2.791552000	5.608629000	0.966447000
8	-5.817838000	-1.973493000	-0.272376000
8	-5.008338000	-3.968051000	-0.819453000

Aryl Migration TS - [(4,4'-OMe-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

8	1.299749000	-1.996145000	-1.143643000
7	-1.266058000	-0.977830000	-0.543393000
6	-1.562592000	-2.265043000	-0.834940000
6	-2.262546000	-0.085835000	-0.236938000
6	-2.883348000	-2.747405000	-0.844148000
1	-0.685854000	-2.879757000	-1.065074000
6	-3.606817000	-0.490953000	-0.221014000
6	-3.937221000	-1.843246000	-0.527569000
1	-3.060780000	-3.792871000	-1.090265000
1	-4.414922000	0.199969000	0.016416000
7	2.581694000	0.450565000	-0.762401000
6	3.206659000	1.182247000	0.198695000
6	3.253446000	0.132143000	-1.902941000
6	4.521513000	1.663621000	0.041601000
6	4.572761000	0.580004000	-2.137917000
6	5.218876000	1.361730000	-1.153981000
1	2.641522000	1.353935000	1.116212000
1	2.716826000	-0.499206000	-2.609435000
1	4.982114000	2.243310000	0.843489000
1	5.070461000	0.306019000	-3.069675000
1	6.240619000	1.718618000	-1.307458000
1	-3.773737000	2.183555000	0.422084000
6	-2.699123000	2.349943000	0.355458000
6	-1.806529000	1.310025000	0.044499000
6	-2.201459000	3.662285000	0.587131000
7	-0.447598000	1.515492000	-0.035977000
6	-0.797513000	3.873638000	0.480890000
6	0.016138000	2.768515000	0.168871000
1	-0.335967000	4.848419000	0.629782000
1	1.095014000	2.904325000	0.074206000

78	0.660828000	-0.282946000	-0.540206000
6	1.292138000	-1.553323000	1.075184000
6	0.317792000	-1.734573000	2.081758000
6	2.633127000	-1.952595000	1.261118000
6	0.720284000	-2.286701000	3.329294000
1	-0.724014000	-1.449426000	1.938881000
6	3.014500000	-2.504699000	2.509164000
1	3.351770000	-1.882058000	0.446941000
6	2.062897000	-2.670938000	3.547237000
1	-0.026226000	-2.406510000	4.119840000
1	4.049222000	-2.829408000	2.651435000
1	2.362180000	-3.105271000	4.504725000
6	-5.653339000	-3.508741000	-0.797053000
6	-2.669493000	5.959101000	1.129552000
1	-6.745706000	-3.515024000	-0.702379000
1	-5.364871000	-3.774821000	-1.827705000
1	-5.210618000	-4.217040000	-0.076894000
1	-3.577744000	6.532168000	1.350682000
1	-1.987207000	5.990484000	1.995890000
1	-2.175981000	6.371881000	0.233473000
8	-5.249076000	-2.151344000	-0.490023000
8	-3.119156000	4.604446000	0.884863000

Aryl Migration TS - [(4,4'-NMe_2-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

8	1.815741000	-1.948352000	-1.090264000
7	-0.849489000	-1.161315000	-0.540015000
6	-1.022429000	-2.483990000	-0.796034000
6	-1.935738000	-0.371962000	-0.272742000
6	-2.281913000	-3.087538000	-0.799900000
1	-0.090198000	-3.019141000	-1.001877000
6	-3.235093000	-0.906015000	-0.253576000
6	-3.454307000	-2.302302000	-0.518178000
1	-2.341559000	-4.151834000	-1.017728000
1	-4.075990000	-0.251571000	-0.042159000
7	2.844195000	0.622686000	-0.754845000
6	3.370029000	1.453753000	0.183910000
6	3.571159000	0.325620000	-1.866638000
6	4.633460000	2.058911000	0.031103000
6	4.844408000	0.894026000	-2.095876000
6	5.385616000	1.778450000	-1.135978000
1	2.768134000	1.606117000	1.081206000
1	3.116356000	-0.387593000	-2.552487000
1	5.014385000	2.715833000	0.815081000
1	5.389174000	0.632450000	-3.004650000
1	6.369720000	2.230215000	-1.285849000
1	-3.655305000	1.717356000	0.280602000
6	-2.616856000	2.032541000	0.228854000
6	-1.622282000	1.074662000	-0.035933000
6	-2.273009000	3.412822000	0.419853000
7	-0.289806000	1.398930000	-0.113547000
6	-0.874491000	3.727625000	0.306290000
6	0.042259000	2.704379000	0.045740000
1	-0.501173000	4.744052000	0.415186000
1	1.103018000	2.944437000	-0.047231000
78	0.998305000	-0.290001000	-0.536412000
6	1.727490000	-1.446272000	1.114146000
6	0.762437000	-1.715665000	2.110726000
6	3.100245000	-1.694951000	1.333099000
6	1.198980000	-2.199386000	3.374933000
1	-0.301604000	-1.551184000	1.943961000
6	3.517131000	-2.180210000	2.597217000
1	3.822427000	-1.561684000	0.530027000
6	2.570986000	-2.431117000	3.623222000
1	0.455199000	-2.387659000	4.154844000
1	4.578404000	-2.387552000	2.762391000
1	2.898292000	-2.813323000	4.593819000
7	-3.215844000	4.369896000	0.685682000
7	-4.707990000	-2.852649000	-0.503864000
6	-4.883901000	-4.287201000	-0.795781000
6	-5.882086000	-2.015898000	-0.211354000
6	-4.636888000	4.001011000	0.783814000
6	-2.808288000	5.775229000	0.859366000
1	-5.951191000	-4.536738000	-0.742905000
1	-4.521191000	-4.537092000	-1.808239000
1	-4.346776000	-4.913641000	-0.062134000
1	-6.784913000	-2.638900000	-0.235653000
1	-5.809844000	-1.559260000	0.792412000
1	-6.001330000	-1.211933000	-0.960538000
1	-5.010008000	3.576778000	-0.166154000
1	-4.806140000	3.267056000	1.592339000
1	-5.227978000	4.897049000	1.010883000
1	-3.696300000	6.384101000	1.071131000
1	-2.106238000	5.887279000	1.704554000
1	-2.330050000	6.171317000	-0.054187000

Aryl Migration TS - [(5,5'-NO_2-bpy)Pt^{IV}(Ph)(O)(Py)]$^+$

8	-1.104589000	-1.947230000	-1.023118000
7	-1.617607000	0.741250000	-0.356562000
6	-2.867339000	0.271848000	-0.565509000
6	-1.386213000	2.060060000	-0.058889000
6	-3.962180000	1.152081000	-0.483057000
1	-2.937073000	-0.795293000	-0.801426000
6	-2.465235000	2.974572000	0.034180000
6	-3.781197000	2.518871000	-0.180603000
1	-2.291054000	4.024187000	0.267774000
1	-4.641369000	3.186625000	-0.120133000
7	1.664206000	-1.685238000	-0.866033000
6	2.691062000	-1.827834000	0.016674000
6	1.690462000	-2.373744000	-2.041497000
6	3.812353000	-2.633810000	-0.260742000
6	2.779333000	-3.202210000	-2.391261000
6	3.861941000	-3.332149000	-1.492123000
1	2.590518000	-1.303298000	0.968113000
1	0.819321000	-2.257682000	-2.684235000
1	4.717806000	-3.965976000	-1.737625000
1	-0.257835000	4.556231000	0.528694000

6	0.467844000	3.751584000	0.415736000
6	0.043664000	2.429371000	0.126142000
6	1.840255000	4.032973000	0.555495000
7	0.943857000	1.396219000	-0.016924000
6	2.734010000	2.953481000	0.389340000
1	2.211703000	5.033827000	0.777301000
6	2.263516000	1.659153000	0.104204000
1	2.964790000	0.837992000	-0.031057000
78	0.018487000	-0.497386000	-0.484370000
6	-0.563239000	-1.744348000	1.183116000
6	-1.176870000	-1.045664000	2.244893000
6	-0.160838000	-3.090326000	1.297297000
6	-1.331424000	-1.714469000	3.490274000
1	-1.513219000	-0.013125000	2.152276000
6	-0.329046000	-3.739128000	2.546795000
1	0.227964000	-3.634501000	0.439039000
6	-0.910274000	-3.055440000	3.643729000
1	-1.046657000	-3.566469000	4.600101000
1	-1.780791000	-1.174045000	4.328091000
1	-0.031875000	-4.786989000	2.643113000
1	4.612462000	-2.712775000	0.477159000
1	2.760332000	-3.730841000	-3.345705000
7	-5.332727000	0.621552000	-0.719494000
7	4.200048000	3.165917000	0.517540000
8	4.931085000	2.164994000	0.380253000
8	4.579680000	4.325924000	0.753407000
8	-5.432370000	-0.588410000	-0.988012000
8	-6.268177000	1.438614000	-0.626965000

Aryl Migration TS - [(5,5'-OMe-bpy)Pt^{IV}(Ph)(O)(Py)]$^{+}$

8	-0.688909000	-2.103313000	-1.103323000
7	-1.728839000	0.436217000	-0.419911000
6	-2.855368000	-0.252806000	-0.667795000
6	-1.745574000	1.768427000	-0.088551000
6	-4.132824000	0.373203000	-0.605959000
1	-2.713222000	-1.307752000	-0.923974000
6	-2.986206000	2.440244000	-0.007238000
6	-4.190919000	1.751483000	-0.263118000
1	-3.024856000	3.498156000	0.253242000
1	-5.139498000	2.284507000	-0.196122000
7	1.968445000	-1.319374000	-0.836352000
6	2.966456000	-1.272315000	0.086465000
6	2.162179000	-2.002133000	-1.998149000
6	4.221384000	-1.874091000	-0.132742000
6	3.392945000	-2.629305000	-2.294205000
6	4.442789000	-2.562803000	-1.350573000
1	2.733207000	-0.761546000	1.021873000
1	1.308013000	-2.045629000	-2.671984000
1	5.404847000	-3.041005000	-1.552141000
1	-1.111455000	4.415100000	0.579892000
6	-0.245451000	3.763431000	0.461327000
6	-0.419525000	2.397774000	0.135452000
6	1.044860000	4.303131000	0.633551000
7	0.671235000	1.572404000	-0.008170000
6	2.160749000	3.440471000	0.463666000
1	1.164067000	5.357065000	0.884616000
6	1.909243000	2.077896000	0.140493000
1	2.755661000	1.405121000	-0.002585000
78	0.115048000	-0.459604000	-0.519650000
6	-0.276384000	-1.807537000	1.114119000
6	-1.036098000	-1.242492000	2.161939000
6	0.372872000	-3.052576000	1.253805000
6	-1.095892000	-1.929081000	3.405998000
1	-1.561339000	-0.293975000	2.054045000
6	0.297611000	-3.724018000	2.499602000
1	0.882764000	-3.512180000	0.409453000
6	-0.432314000	-3.165135000	3.578952000
1	-0.493611000	-3.692987000	4.534248000
1	-1.662985000	-1.483978000	4.228682000
1	0.786348000	-4.696432000	2.608113000
1	4.990645000	-1.810382000	0.638783000
1	3.506492000	-3.160130000	-3.240900000
6	3.787446000	5.153366000	0.905615000
6	-6.512551000	0.145158000	-0.839420000
1	3.366325000	5.429585000	1.887687000
1	4.882488000	5.198148000	0.946732000
1	3.416034000	5.837106000	0.122875000
1	-6.611437000	0.959174000	-1.578563000
1	-7.194405000	-0.673992000	-1.097562000
1	-6.744078000	0.516941000	0.174046000
8	-5.187466000	-0.427866000	-0.883768000
8	3.468096000	3.781394000	0.580076000

Aryl Migration TS - [(5,5'-NMe$_2$-bpy)Pt^{IV}(Ph)(O)(Py)]$^{+}$

8	-1.229899000	-1.897986000	-1.028427000
7	-1.562692000	0.829863000	-0.336929000
6	-2.834209000	0.440558000	-0.539985000
6	-1.221092000	2.118426000	-0.023874000
6	-3.932611000	1.358180000	-0.449127000
1	-2.925926000	-0.620137000	-0.785561000
6	-2.257213000	3.079518000	0.090353000
6	-3.596337000	2.714454000	-0.114797000
1	-2.021093000	4.114821000	0.338521000
1	-4.370706000	3.475068000	-0.018678000
7	1.545334000	-1.819041000	-0.840815000
6	2.549501000	-2.035556000	0.050334000
6	1.510081000	-2.539420000	-1.995141000
6	3.587556000	-2.956467000	-0.195071000
6	2.516367000	-3.477659000	-2.317890000
6	3.575587000	-3.689652000	-1.407042000
1	2.493136000	-1.474552000	0.984420000
1	0.651674000	-2.358478000	-2.640129000
1	4.364854000	-4.413083000	-1.627738000
1	0.096003000	4.525737000	0.566716000
6	0.759675000	3.671747000	0.427267000
6	0.222876000	2.389833000	0.138526000

6	2.143305000	3.859978000	0.530041000
7	1.065700000	1.322545000	-0.026771000
6	3.031075000	2.748116000	0.335949000
1	2.529524000	4.854816000	0.749149000
6	2.402624000	1.490022000	0.057557000
1	2.999569000	0.596566000	-0.112305000
78	-0.014917000	-0.504183000	-0.480574000
6	-0.694641000	-1.704085000	1.164475000
6	-1.266368000	-0.965623000	2.224789000
6	-0.368897000	-3.070428000	1.307031000
6	-1.465133000	-1.610165000	3.477036000
1	-1.542202000	0.082809000	2.117924000
6	-0.577475000	-3.696872000	2.560820000
1	-0.007147000	-3.646598000	0.457720000
6	-1.122488000	-2.970539000	3.649949000
1	-1.288333000	-3.461817000	4.612401000
1	-1.884748000	-1.034076000	4.306940000
1	-0.338911000	-4.758832000	2.669592000
1	4.367706000	-3.101104000	0.554502000
1	2.450725000	-4.028049000	-3.257961000
7	-5.223080000	0.940290000	-0.669981000
7	4.401859000	2.873958000	0.411255000
6	4.998453000	4.192836000	0.671771000
6	5.262080000	1.709308000	0.170542000
6	-5.490412000	-0.468912000	-1.006260000
6	-6.327508000	1.904529000	-0.571318000
1	4.665130000	4.601210000	1.642927000
1	6.091072000	4.092967000	0.704352000
1	4.743480000	4.918864000	-0.122247000
1	6.313453000	2.011211000	0.263269000
1	5.073827000	0.907501000	0.909299000
1	5.114506000	1.294453000	-0.844544000
1	-6.210659000	2.729408000	-1.298291000
1	-7.273231000	1.391607000	-0.788547000
1	-6.398228000	2.337919000	0.443574000
1	-6.570863000	-0.604739000	-1.145185000
1	-4.981212000	-0.763440000	-1.941150000
1	-5.157306000	-1.146013000	-0.199685000

Alkoxide - $[(bpy)Pt^{II}(OPh)(Py)]^{+}$

78	0.213065000	0.004971000	-0.244337000
6	3.019174000	0.572841000	0.327056000
6	1.759908000	2.555869000	0.501424000
6	4.206808000	1.268013000	0.653862000
6	2.902585000	3.312095000	0.835234000
1	0.776081000	3.021317000	0.427116000
6	4.151633000	2.654357000	0.911846000
1	5.158448000	0.738862000	0.707180000
1	2.804690000	4.381915000	1.025500000
1	5.060319000	3.204678000	1.165588000
6	2.966343000	-0.889632000	0.041509000
6	1.531420000	-2.677803000	-0.546348000
6	4.085315000	-1.752832000	0.061334000
6	2.606641000	-3.593117000	-0.547390000
1	0.501088000	-2.956493000	-0.779963000
6	3.902262000	-3.122428000	-0.234952000
1	5.078319000	-1.371680000	0.300526000
1	2.420438000	-4.640957000	-0.787085000
1	4.755830000	-3.804053000	-0.223165000
7	1.718704000	-1.370113000	-0.256222000
7	1.811688000	1.225152000	0.253153000
8	-1.128105000	-1.384892000	-0.813853000
6	-3.515908000	-1.639563000	-0.772704000
6	-2.252359000	-1.710103000	1.335874000
6	-4.711390000	-1.883317000	-0.054876000
1	-3.521496000	-1.533186000	-1.860785000
6	-3.455814000	-1.941100000	2.045927000
1	-1.294149000	-1.671196000	1.864529000
6	-4.691677000	-2.028285000	1.356895000
1	-5.657746000	-1.958833000	-0.598611000
1	-3.424565000	-2.068396000	3.132175000
1	-5.617950000	-2.216443000	1.905987000
6	-2.033143000	1.707402000	0.814770000
6	-1.638747000	1.986155000	-1.481687000
6	-3.122888000	2.603013000	0.780246000
1	-1.741466000	1.201566000	1.734827000
6	-2.716088000	2.888521000	-1.602176000
1	-1.034908000	1.701466000	-2.344120000
6	-3.473721000	3.205484000	-0.449978000
1	-3.681676000	2.801476000	1.696333000
1	-2.949944000	3.316912000	-2.578331000
1	-4.318352000	3.896545000	-0.511243000
6	-2.273167000	-1.555867000	-0.081174000
7	-1.300433000	1.414919000	-0.293431000

Alkoxide - $[(bpy)Pt^{II}(p\text{-}NO_2\text{-}OPh)(Py)]^{+}$

78	0.793925000	0.144728000	-0.367314000
6	3.473239000	-0.433517000	0.624530000
6	3.049808000	1.878562000	0.786194000
6	4.760488000	-0.262651000	1.184063000
6	4.321247000	2.123435000	1.345660000
1	2.350178000	2.693583000	0.598526000
6	5.191509000	1.029490000	1.553913000
1	5.417896000	-1.120392000	1.326673000
1	4.609203000	3.143541000	1.603768000
1	6.183205000	1.176817000	1.987236000
6	2.931877000	-1.747861000	0.176499000
6	1.076013000	-2.812846000	-0.833180000
6	3.628981000	-2.974127000	0.261101000
6	1.717565000	-4.069554000	-0.782036000
1	0.080024000	-2.669755000	-1.255370000
6	3.012538000	-4.150576000	-0.222056000
1	4.629997000	-3.017110000	0.690701000
1	1.205519000	-4.950500000	-1.171543000
1	3.536268000	-5.107366000	-0.163515000
7	1.672719000	-1.694110000	-0.361100000

7	2.630388000	0.637231000	0.442925000
8	-0.857764000	-0.539607000	-1.303719000
6	-3.222447000	-0.752028000	-1.480645000
6	-2.181293000	-0.695056000	0.756838000
6	-4.490506000	-0.896330000	-0.888341000
1	-3.114232000	-0.721847000	-2.567137000
6	-3.450145000	-0.834408000	1.355388000
1	-1.285360000	-0.640388000	1.381260000
6	-4.593252000	-0.929384000	0.526741000
1	-5.391960000	-0.976987000	-1.496048000
1	-3.565571000	-0.876234000	2.438404000
6	-0.453836000	2.642402000	0.779204000
6	-0.461257000	2.553160000	-1.567095000
6	-1.147716000	3.869754000	0.780234000
1	-0.177130000	2.146493000	1.711160000
6	-1.151613000	3.781185000	-1.652526000
1	-0.190096000	1.985894000	-2.457683000
6	-1.502589000	4.453938000	-0.459257000
1	-1.409291000	4.338015000	1.730666000
1	-1.409263000	4.182918000	-2.633873000
1	-2.045240000	5.402073000	-0.492748000
6	-2.048554000	-0.645881000	-0.666943000
7	-0.109775000	2.002408000	-0.372702000
7	-5.921129000	-1.065575000	1.150165000
8	-5.980010000	-1.081187000	2.400978000
8	-6.914228000	-1.154632000	0.394650000

Alkoxide - $[(bpy)Pt^{II}(p\text{-OMe-OPh})(Py)]^{+}$

78	0.656374000	0.018301000	-0.261910000
6	3.478441000	0.230119000	0.468005000
6	2.459261000	2.345882000	0.643224000
6	4.721193000	0.766499000	0.879059000
6	3.663958000	2.948335000	1.061186000
1	1.543073000	2.928316000	0.536082000
6	4.819026000	2.141617000	1.180152000
1	5.597566000	0.123902000	0.965291000
1	3.684580000	4.016262000	1.283558000
1	5.771643000	2.569885000	1.499625000
6	3.266818000	-1.207902000	0.134851000
6	1.662755000	-2.797633000	-0.572467000
6	4.274341000	-2.198537000	0.179551000
6	2.621881000	-3.833673000	-0.553886000
1	0.618309000	-2.945146000	-0.858588000
6	3.947006000	-3.528356000	-0.168172000
1	5.292310000	-1.944724000	0.475909000
1	2.326227000	-4.845447000	-0.835050000
1	4.713281000	-4.306404000	-0.139323000
7	1.987756000	-1.529094000	-0.234869000
7	2.364253000	1.026204000	0.352665000
8	-0.794984000	-1.222991000	-0.903601000
6	-3.174681000	-0.924487000	-1.163524000
6	-2.251567000	-1.383778000	1.055182000
6	-4.487540000	-0.927826000	-0.625861000
1	-3.022357000	-0.766497000	-2.234710000
6	-3.550279000	-1.374065000	1.602860000
1	-1.389359000	-1.587680000	1.698323000
6	-4.680704000	-1.147284000	0.766188000
1	-5.333486000	-0.764034000	-1.294780000
1	-3.714732000	-1.559459000	2.667048000
6	-1.451491000	1.944638000	0.693522000
6	-0.800787000	2.291907000	-1.533589000
6	-2.406562000	2.980960000	0.621630000
1	-1.319087000	1.356108000	1.600762000
6	-1.736502000	3.335586000	-1.690855000
1	-0.155382000	1.976840000	-2.354506000
6	-2.554724000	3.690413000	-0.592328000
1	-3.020126000	3.204482000	1.495956000
1	-1.816230000	3.844125000	-2.653269000
1	-3.291046000	4.493226000	-0.682519000
6	-2.044282000	-1.157939000	-0.338159000
7	-0.657440000	1.616210000	-0.360809000
6	-7.075284000	-1.021988000	0.587598000
1	-7.098838000	-0.039386000	0.080050000
1	-7.929237000	-1.096108000	1.274695000
1	-7.139438000	-1.827509000	-0.166807000
8	-5.902325000	-1.162812000	1.399516000

Alkoxide - $[(bpy)Pt^{II}(p\text{-NMe}_2\text{-OPh})(Py)]^{+}$

78	0.865033000	0.011148000	-0.253469000
6	3.678360000	0.196210000	0.535752000
6	2.663070000	2.308550000	0.757289000
6	4.917663000	0.717502000	0.976678000
6	3.863510000	2.895860000	1.207574000
1	1.749101000	2.896059000	0.657963000
6	5.015596000	2.083260000	1.316952000
1	5.791297000	0.070248000	1.055795000
1	3.883467000	3.956683000	1.461921000
1	5.965376000	2.499810000	1.659563000
6	3.467657000	-1.232911000	0.164885000
6	1.871475000	-2.802619000	-0.600757000
6	4.472639000	-2.226888000	0.202370000
6	2.827877000	-3.841188000	-0.591126000
1	0.830731000	-2.940187000	-0.905459000
6	4.148040000	-3.547727000	-0.179668000
1	5.486630000	-1.982158000	0.519287000
1	2.534475000	-4.845664000	-0.899594000
1	4.912384000	-4.327920000	-0.157288000
7	2.193811000	-1.542608000	-0.230864000
7	2.568220000	0.998291000	0.426651000
8	-0.565632000	-1.232874000	-0.937523000
6	-2.881939000	-0.692357000	-1.394664000
6	-2.237683000	-1.451179000	0.828515000
6	-4.233003000	-0.637364000	-0.989548000
1	-2.609897000	-0.432157000	-2.421827000
6	-3.584567000	-1.391671000	1.249244000
1	-1.467031000	-1.783784000	1.531919000

6	-4.627367000	-0.999364000	0.343605000
1	-4.979261000	-0.326417000	-1.721202000
1	-3.820101000	-1.677153000	2.274856000
6	-1.330276000	1.875574000	0.625368000
6	-0.438104000	2.404833000	-1.477965000
6	-2.260422000	2.934157000	0.544546000
1	-1.303500000	1.206765000	1.484738000
6	-1.343029000	3.474121000	-1.643385000
1	0.291591000	2.151735000	-2.248446000
6	-2.270442000	3.748830000	-0.610526000
1	-2.959708000	3.095519000	1.366547000
1	-1.314857000	4.064172000	-2.561164000
1	-2.984108000	4.571173000	-0.707144000
6	-1.861091000	-1.110639000	-0.499404000
7	-0.428701000	1.626535000	-0.361411000
7	-5.969236000	-0.990841000	0.734594000
6	-6.305795000	-1.184229000	2.146895000
6	-6.972995000	-0.409530000	-0.160102000
1	-5.969905000	-2.173840000	2.504584000
1	-7.397339000	-1.142425000	2.269531000
1	-5.853653000	-0.411287000	2.802761000
1	-6.777588000	0.660104000	-0.382526000
1	-7.964817000	-0.487572000	0.307315000
1	-7.014533000	-0.955337000	-1.119310000

Alkoxide - $[(bpy)Pt^{II}(m\text{-}NO_2\text{-}OPh)(Py)]^+$

78	0.591039000	0.147947000	-0.497436000
6	3.249055000	0.047470000	0.692208000
6	2.395596000	2.238941000	0.836152000
6	4.435183000	0.438598000	1.354776000
6	3.551679000	2.699338000	1.500132000
1	1.572075000	2.914359000	0.602719000
6	4.590600000	1.779346000	1.767584000
1	5.224755000	-0.288032000	1.546850000
1	5.500648000	2.095748000	2.282004000
6	2.988091000	-1.336696000	0.205085000
6	1.424440000	-2.709411000	-0.921500000
6	3.886824000	-2.418604000	0.341085000
6	2.276372000	-3.830888000	-0.822291000
1	0.447683000	-2.742329000	-1.407645000
6	3.525050000	-3.682531000	-0.177317000
1	4.847745000	-2.284664000	0.838137000
1	4.206789000	-4.530378000	-0.079378000
7	1.779042000	-1.505414000	-0.417104000
7	2.242281000	0.950727000	0.447232000
8	-0.850479000	-0.834797000	-1.517477000
6	-3.144478000	-1.450338000	-1.805911000
6	-2.298292000	-0.972544000	0.447246000
6	-4.422716000	-1.725868000	-1.268729000
1	-2.960540000	-1.527353000	-2.880419000
6	-3.597302000	-1.227540000	0.944187000
1	-1.495924000	-0.718260000	1.137874000
6	-4.677724000	-1.614076000	0.122021000
1	-5.233111000	-2.021300000	-1.940185000
1	-5.659788000	-1.807607000	0.551409000
6	-1.245443000	2.309204000	0.530189000
6	-0.846995000	2.412025000	-1.782350000
6	-2.126941000	3.408600000	0.471308000
1	-1.053493000	1.789184000	1.469742000
6	-1.712536000	3.517244000	-1.925141000
1	-0.336966000	1.971546000	-2.639517000
6	-2.364491000	4.028141000	-0.778492000
1	-3.045468000	4.879419000	-0.857503000
6	-2.062872000	-1.066172000	-0.950694000
7	-0.610170000	1.829104000	-0.575166000
1	3.623542000	3.747817000	1.792800000
1	1.957614000	-4.786807000	-1.240134000
1	-1.868506000	3.950750000	-2.914424000
1	-2.617469000	3.749510000	1.384593000
7	-3.820339000	-1.061711000	2.402079000
8	-2.890245000	-0.561622000	3.080245000
8	-4.919890000	-1.414313000	2.871799000

Alkoxide - $[(bpy)Pt^{II}(m\text{-}OMe\text{-}OPh)(Py)]^+$

78	0.531632000	0.136797000	-0.392111000
6	3.254565000	0.070768000	0.654890000
6	2.327390000	2.208994000	0.996799000
6	4.468288000	0.472239000	1.259894000
6	3.506377000	2.677380000	1.612991000
1	1.460158000	2.857813000	0.868006000
6	4.599256000	1.790556000	1.746143000
1	5.297185000	-0.229874000	1.351943000
1	5.530344000	2.115033000	2.215990000
6	3.009832000	-1.296971000	0.114381000
6	1.414567000	-2.676057000	-0.960900000
6	3.951881000	-2.350235000	0.136575000
6	2.308212000	-3.769299000	-0.971810000
1	0.405458000	-2.717361000	-1.377225000
6	3.595256000	-3.602842000	-0.411992000
1	4.941806000	-2.202825000	0.568829000
1	4.310443000	-4.428523000	-0.402071000
7	1.766610000	-1.483072000	-0.429745000
7	2.200540000	0.944079000	0.529631000
8	-0.903253000	-0.858239000	-1.391391000
6	-3.277051000	-0.936307000	-1.715933000
6	-2.346003000	-1.223549000	0.544652000
6	-4.569577000	-1.130490000	-1.183584000
1	-3.118565000	-0.763671000	-2.782692000
6	-3.657782000	-1.397044000	1.065882000
1	-1.493634000	-1.302792000	1.224803000
6	-4.785821000	-1.354280000	0.202827000
1	-5.433503000	-1.102411000	-1.854081000
1	-5.799634000	-1.493954000	0.577469000
6	-1.515829000	2.089226000	0.643407000
6	-0.779888000	2.551924000	-1.536973000
6	-2.424535000	3.168266000	0.611075000

1	-1.441305000	1.434281000	1.511173000
6	-1.664282000	3.644714000	-1.651173000
1	-0.126241000	2.259310000	-2.359311000
6	-2.502141000	3.962276000	-0.556329000
1	-3.201667000	4.800137000	-0.614934000
6	-2.149549000	-0.988282000	-0.841634000
7	-0.701707000	1.797186000	-0.406841000
1	3.555371000	3.706605000	1.971548000
1	1.992207000	-4.717600000	-1.408754000
1	-1.692069000	4.217186000	-2.579888000
1	-3.058467000	3.359738000	1.478442000
6	-5.008507000	-1.871015000	3.000584000
1	-4.833518000	-2.032617000	4.073294000
1	-5.695529000	-1.015428000	2.866253000
1	-5.460553000	-2.778349000	2.561077000
8	-3.720702000	-1.602013000	2.426996000

Alkoxide - $[(bpy)Pt^{II}(m\text{-}NMe_2\text{-}OPh)(Py)]^+$

78	0.674757000	0.164344000	-0.387803000
6	3.374132000	-0.027564000	0.710827000
6	2.453054000	2.072662000	1.246159000
6	4.575755000	0.299867000	1.381589000
6	3.619538000	2.465460000	1.934560000
1	1.592252000	2.737955000	1.167427000
6	4.704004000	1.560822000	2.001871000
1	5.397153000	-0.415826000	1.421878000
1	5.625554000	1.827839000	2.523778000
6	3.133793000	-1.333594000	0.032873000
6	1.554134000	-2.591196000	-1.202150000
6	4.072201000	-2.388766000	-0.033406000
6	2.445118000	-3.681498000	-1.308111000
1	0.550890000	-2.584094000	-1.635726000
6	3.722438000	-3.578050000	-0.711452000
1	5.054895000	-2.289705000	0.428141000
1	4.435595000	-4.403306000	-0.772817000
7	1.899691000	-1.459406000	-0.547429000
7	2.329372000	0.863406000	0.647785000
8	-0.736602000	-0.768515000	-1.476503000
6	-3.008765000	-0.162139000	-1.982046000
6	-2.450487000	-1.205224000	0.184353000
6	-4.367950000	-0.157903000	-1.589084000
1	-2.688789000	0.204799000	-2.959908000
6	-3.822615000	-1.182623000	0.593137000
1	-1.676986000	-1.636684000	0.821104000
6	-4.782886000	-0.648213000	-0.329582000
1	-5.125165000	0.231380000	-2.276312000
1	-5.843897000	-0.627671000	-0.083611000
6	-1.466068000	2.004959000	0.667691000
6	-0.421771000	2.787548000	-1.282202000
6	-2.343117000	3.110372000	0.691852000
1	-1.524689000	1.216473000	1.416789000
6	-1.263159000	3.917731000	-1.333516000
1	0.339669000	2.610243000	-2.042782000
6	-2.243590000	4.084943000	-0.327015000
1	-2.915138000	4.947263000	-0.341294000
6	-2.050620000	-0.699769000	-1.082821000
7	-0.517902000	1.854361000	-0.295538000
1	3.665601000	3.451980000	2.398260000
1	2.135487000	-4.578894000	-1.845674000
1	-1.149777000	4.634282000	-2.148917000
1	-3.089307000	3.182692000	1.484731000
7	-4.209928000	-1.645372000	1.864148000
6	-3.274658000	-2.503549000	2.601281000
6	-5.639882000	-1.886491000	2.106304000
1	-2.344590000	-1.959543000	2.841422000
1	-3.733264000	-2.801095000	3.555471000
1	-3.001345000	-3.422335000	2.041643000
1	-5.774115000	-2.243981000	3.137788000
1	-6.216077000	-0.952286000	2.005319000
1	-6.072390000	-2.637845000	1.414518000

Alkoxide - $[(bpy)Pt^{II}(OPh)(4\text{-}NO_2\text{-}Py)]^+$

78	-0.701266000	0.078715000	-0.221495000
6	-3.126362000	-1.454151000	0.324273000
6	-1.239456000	-2.832233000	0.621186000
6	-3.990533000	-2.521534000	0.662328000
6	-2.039416000	-3.940208000	0.969461000
1	-0.151606000	-2.909086000	0.590677000
6	-3.444053000	-3.781057000	0.989027000
1	-5.070679000	-2.374620000	0.671628000
1	-1.565977000	-4.892178000	1.214145000
1	-4.098791000	-4.614856000	1.251723000
6	-3.598548000	-0.085845000	-0.032787000
6	-2.891844000	2.078265000	-0.683549000
6	-4.954424000	0.309684000	-0.078109000
6	-4.225704000	2.536776000	-0.751177000
1	-2.026684000	2.705171000	-0.912030000
6	-5.271532000	1.638642000	-0.439570000
1	-5.748923000	-0.397659000	0.160572000
1	-4.424855000	3.569660000	-1.040220000
1	-6.314399000	1.961452000	-0.478324000
7	-2.601258000	0.805260000	-0.330166000
7	-1.762756000	-1.623312000	0.305762000
8	0.060101000	1.843886000	-0.821662000
6	2.238701000	2.858052000	-0.730332000
6	0.908327000	2.645865000	1.327441000
6	3.257579000	3.510371000	0.005576000
1	2.333064000	2.700093000	-1.808137000
6	1.938183000	3.288478000	2.056800000
1	-0.015883000	2.335382000	1.825898000
6	3.118783000	3.722106000	1.402126000
1	4.158542000	3.852676000	-0.511789000
1	1.811278000	3.463714000	3.129168000
1	3.908544000	4.226033000	1.965110000
6	1.998684000	-0.573331000	0.938584000
6	1.790598000	-1.113848000	-1.339381000

6	3.356229000	-0.956813000	0.959671000
1	1.512789000	-0.176920000	1.828916000
6	3.139733000	-1.514363000	-1.423072000
1	1.139604000	-1.144054000	-2.213231000
6	3.909527000	-1.427938000	-0.246151000
1	3.953224000	-0.878325000	1.867498000
1	3.569638000	-1.869720000	-2.358962000
6	1.052417000	2.423682000	-0.073057000
7	1.233999000	-0.661922000	-0.182551000
7	5.346625000	-1.844347000	-0.280002000
8	5.791733000	-2.238527000	-1.373227000
8	5.979696000	-1.766594000	0.788252000

Alkoxide - $[(bpy)Pt^{II}(OPh)(4\text{-}OMe\text{-}Py)]^{+}$

78	-0.547356000	0.065081000	-0.215164000
6	-3.040508000	-1.360600000	0.300570000
6	-1.212709000	-2.802206000	0.662367000
6	-3.951497000	-2.389428000	0.635395000
6	-2.061826000	-3.873351000	1.010053000
1	-0.127936000	-2.916945000	0.655828000
6	-3.459706000	-3.662508000	0.994825000
1	-5.025389000	-2.202568000	0.617225000
1	-1.630050000	-4.837938000	1.281098000
1	-4.150814000	-4.467034000	1.255773000
6	-3.452757000	0.018709000	-0.088274000
6	-2.650392000	2.143244000	-0.754825000
6	-4.791679000	0.464606000	-0.168015000
6	-3.963709000	2.651704000	-0.857166000
1	-1.756556000	2.732295000	-0.973884000
6	-5.049758000	1.798822000	-0.555399000
1	-5.617514000	-0.208088000	0.064544000
1	-4.117225000	3.687123000	-1.164510000
1	-6.078378000	2.160762000	-0.621003000
7	-2.415874000	0.865556000	-0.378152000
7	-1.683915000	-1.580410000	0.316338000
8	0.306166000	1.775897000	-0.841904000
6	2.448364000	2.851575000	-0.701174000
6	1.104337000	2.558273000	1.336835000
6	3.436788000	3.523185000	0.057578000
1	2.561881000	2.710672000	-1.779399000
6	2.105122000	3.220646000	2.088645000
1	0.187198000	2.207263000	1.821296000
6	3.277018000	3.706057000	1.455938000
1	4.332460000	3.902047000	-0.443796000
1	1.961635000	3.369269000	3.163135000
1	4.044194000	4.224434000	2.037016000
6	2.064411000	-0.779859000	1.051015000
6	1.939011000	-1.224502000	-1.240896000
6	3.379219000	-1.254927000	1.121218000
1	1.567910000	-0.377521000	1.933813000
6	3.257147000	-1.715364000	-1.277009000
1	1.341126000	-1.182318000	-2.152292000
6	4.008156000	-1.735234000	-0.065676000
1	3.926885000	-1.239656000	2.064339000
1	3.665487000	-2.054385000	-2.228030000
6	1.268963000	2.365450000	-0.066297000
7	1.340035000	-0.773989000	-0.107574000
6	5.974465000	-2.630490000	-1.122967000
1	5.465821000	-3.507114000	-1.559006000
1	6.975796000	-2.915432000	-0.778632000
1	6.050956000	-1.819728000	-1.866862000
8	5.276806000	-2.171192000	0.059577000

Alkoxide - $[(bpy)Pt^{II}(OPh)(4\text{-}NMe_2\text{-}Py)]^{+}$

78	-0.736178000	0.060429000	-0.228214000
6	-3.089770000	-1.568878000	0.330053000
6	-1.139062000	-2.855798000	0.631890000
6	-3.903176000	-2.672663000	0.677016000
6	-1.887477000	-3.996699000	0.989315000
1	-0.049030000	-2.877169000	0.596203000
6	-3.298009000	-3.903009000	1.011259000
1	-4.989022000	-2.575799000	0.687278000
1	-1.370431000	-4.924417000	1.239024000
1	-3.912912000	-4.764468000	1.281095000
6	-3.624791000	-0.225700000	-0.035964000
6	-3.019246000	1.962811000	-0.700620000
6	-4.998028000	0.106060000	-0.082601000
6	-4.372608000	2.359902000	-0.769662000
1	-2.183530000	2.626290000	-0.935424000
6	-5.376246000	1.416510000	-0.451992000
1	-5.758782000	-0.636040000	0.160823000
1	-4.619371000	3.380810000	-1.064632000
1	-6.432896000	1.690843000	-0.492126000
7	-2.669154000	0.707228000	-0.340201000
7	-1.719718000	-1.675069000	0.310508000
8	-0.034922000	1.837429000	-0.860937000
6	1.939392000	3.192690000	-0.743391000
6	0.719105000	2.655699000	1.322207000
6	2.848469000	3.975540000	0.007150000
1	2.037052000	3.096235000	-1.827953000
6	1.642216000	3.431400000	2.065154000
1	-0.121867000	2.164347000	1.822653000
6	2.711848000	4.096288000	1.415011000
1	3.664598000	4.490681000	-0.508601000
1	1.514959000	3.527867000	3.147753000
1	3.416469000	4.703268000	1.989663000
6	1.979396000	-0.562910000	0.950857000
6	1.811179000	-1.052283000	-1.321212000
6	3.332051000	-0.917540000	0.981515000
1	1.487411000	-0.193406000	1.850751000
6	3.157065000	-1.424437000	-1.396664000
1	1.183539000	-1.075750000	-2.213273000
6	3.986967000	-1.365236000	-0.220472000
1	3.865924000	-0.819694000	1.925041000
1	3.548677000	-1.737841000	-2.362811000
6	0.860128000	2.527464000	-0.091236000

7	1.207077000	-0.633585000	-0.171359000
7	5.310149000	-1.707597000	-0.244986000
6	6.129088000	-1.570702000	0.972896000
6	5.943513000	-2.114175000	-1.512050000
1	5.448249000	-3.004623000	-1.937064000
1	6.994460000	-2.368023000	-1.323957000
1	5.912048000	-1.300488000	-2.258913000
1	6.153605000	-0.524339000	1.325976000
1	7.157533000	-1.883342000	0.751992000
1	5.744088000	-2.210661000	1.786198000

Alkoxide - $[(bpy)Pt^{II}(OPh)(3\text{-}NO_2\text{-}Py)]^+$

78	-0.666257000	-0.153688000	0.313620000
6	-3.179649000	1.190105000	-0.316035000
6	-1.469095000	2.791135000	-0.073851000
6	-4.125325000	2.205072000	-0.591507000
6	-2.355509000	3.854093000	-0.344053000
1	-0.414664000	2.976050000	0.136045000
6	-3.711989000	3.554311000	-0.606469000
1	-5.165475000	1.949171000	-0.793973000
1	-4.430468000	4.348981000	-0.819014000
6	-3.508082000	-0.263522000	-0.286775000
6	-2.605508000	-2.427265000	0.046061000
6	-4.794068000	-0.802068000	-0.517705000
6	-3.863892000	-3.029153000	-0.172512000
1	-1.698417000	-2.991208000	0.275963000
6	-4.973621000	-2.202647000	-0.460582000
1	-5.639741000	-0.149628000	-0.735926000
1	-5.960922000	-2.635635000	-0.636772000
7	-2.446664000	-1.085351000	-0.012749000
7	-1.864724000	1.495538000	-0.057816000
8	0.229842000	-1.922097000	0.679963000
6	2.529484000	-2.556201000	0.995103000
6	1.688892000	-2.104368000	-1.271589000
6	3.800809000	-2.865472000	0.453192000
1	2.340573000	-2.626479000	2.069870000
6	2.967438000	-2.400410000	-1.802699000
1	0.859479000	-1.838170000	-1.934772000
6	4.030571000	-2.779800000	-0.944848000
1	4.610262000	-3.172642000	1.121891000
1	3.129017000	-2.345786000	-2.882944000
1	5.014410000	-3.016164000	-1.358118000
6	2.034616000	1.015059000	-0.282467000
6	1.513455000	1.007066000	2.003923000
6	3.326136000	1.498254000	0.006520000
1	1.728160000	0.816466000	-1.306555000
6	2.795555000	1.481880000	2.354626000
1	0.762048000	0.790211000	2.763826000
6	3.738546000	1.734734000	1.333815000
1	4.746748000	2.096542000	1.541785000
6	1.461887000	-2.174929000	0.133463000
7	1.143082000	0.782109000	0.712632000
1	-1.983433000	4.879663000	-0.346115000
1	-3.957480000	-4.114562000	-0.116194000
1	3.043101000	1.639858000	3.405138000
7	4.255842000	1.757035000	-1.123546000
8	5.411741000	2.112466000	-0.830485000
8	3.804437000	1.607190000	-2.275706000

Alkoxide - $[(bpy)Pt^{II}(OPh)(3\text{-}OMe\text{-}Py)]^+$

78	-0.546245000	-0.124332000	0.295989000
6	-3.075065000	1.185375000	-0.340650000
6	-1.362902000	2.796935000	-0.196855000
6	-4.028838000	2.187273000	-0.635591000
6	-2.258036000	3.846956000	-0.488813000
1	-0.304882000	2.989226000	-0.013940000
6	-3.618984000	3.535448000	-0.711522000
1	-5.072744000	1.922178000	-0.804330000
1	-4.343824000	4.320303000	-0.938602000
6	-3.400780000	-0.266218000	-0.242740000
6	-2.491768000	-2.411410000	0.174028000
6	-4.690511000	-0.814365000	-0.426953000
6	-3.753119000	-3.022998000	0.004691000
1	-1.580555000	-2.963366000	0.416704000
6	-4.868223000	-2.210723000	-0.302990000
1	-5.540104000	-0.172268000	-0.660225000
1	-5.858028000	-2.651300000	-0.442709000
7	-2.333987000	-1.073937000	0.050132000
7	-1.755382000	1.502444000	-0.123896000
8	0.359483000	-1.862885000	0.750944000
6	2.609446000	-2.685641000	0.917785000
6	1.666989000	-2.169731000	-1.294319000
6	3.806489000	-3.118129000	0.297719000
1	2.488604000	-2.724765000	2.003669000
6	2.873758000	-2.590319000	-1.903473000
1	0.825486000	-1.826954000	-1.905324000
6	3.950031000	-3.067020000	-1.113196000
1	4.626187000	-3.494105000	0.917297000
1	2.966701000	-2.559040000	-2.993148000
1	4.876347000	-3.402452000	-1.587059000
6	2.078553000	1.133115000	-0.424198000
6	1.630341000	1.149239000	1.881618000
6	3.355350000	1.734986000	-0.234022000
1	1.755218000	0.859112000	-1.427951000
6	2.878849000	1.741281000	2.151068000
1	0.930302000	0.886817000	2.674061000
6	3.763282000	2.045669000	1.089832000
1	4.733166000	2.498543000	1.299028000
6	1.526115000	-2.211646000	0.123479000
7	1.247593000	0.859512000	0.605682000
1	-1.889063000	4.872590000	-0.535964000
1	-3.845190000	-4.104605000	0.113161000
1	3.157105000	1.954956000	3.184520000
6	5.401613000	2.491263000	-1.238732000
1	6.036720000	1.817840000	-0.637686000
1	5.793028000	2.554506000	-2.261460000

1	5.377686000	3.498767000	-0.787431000
8	4.066995000	1.954099000	-1.368464000

Alkoxide - $[(bpy)Pt^{II}(OPh)(3\text{-}NMe_2\text{-}Py)]^+$

78	-0.664751000	0.068885000	-0.365742000
6	-3.152557000	-1.185495000	0.497647000
6	-1.434443000	-2.796233000	0.422316000
6	-4.082700000	-2.159815000	0.928484000
6	-2.306306000	-3.818529000	0.851992000
1	-0.383772000	-2.997971000	0.210359000
6	-3.657959000	-3.493625000	1.108369000
1	-5.119555000	-1.884843000	1.123003000
1	-4.364712000	-4.257147000	1.440860000
6	-3.494544000	0.250526000	0.284638000
6	-2.623727000	2.354585000	-0.358028000
6	-4.781378000	0.804819000	0.470757000
6	-3.883102000	2.971643000	-0.192904000
1	-1.730088000	2.888124000	-0.690214000
6	-4.977307000	2.183550000	0.230737000
1	-5.615330000	0.180513000	0.792155000
1	-5.965199000	2.628670000	0.369654000
7	-2.447073000	1.035052000	-0.119591000
7	-1.842657000	-1.516733000	0.246349000
8	0.229665000	1.760671000	-0.999842000
6	2.456388000	2.655431000	-1.045083000
6	1.284775000	2.431850000	1.104442000
6	3.557260000	3.240672000	-0.375118000
1	2.461573000	2.520265000	-2.129845000
6	2.395807000	3.009593000	1.766675000
1	0.396137000	2.136227000	1.671407000
6	3.538599000	3.417443000	1.033619000
1	4.429078000	3.560051000	-0.953923000
1	2.358780000	3.156534000	2.850474000
1	4.387747000	3.879377000	1.544436000
6	2.106460000	-0.911648000	0.205640000
6	1.254419000	-1.616956000	-1.876897000
6	3.374410000	-1.553194000	-0.005832000
1	1.905020000	-0.336174000	1.104944000
6	2.464480000	-2.281435000	-2.170143000
1	0.418859000	-1.587107000	-2.575702000
6	3.525096000	-2.258970000	-1.246025000
1	4.458450000	-2.765534000	-1.491645000
6	1.303026000	2.252374000	-0.311358000
7	1.099741000	-0.955484000	-0.698834000
1	-1.926503000	-4.833644000	0.976855000
1	-3.990135000	4.038366000	-0.394909000
1	2.572250000	-2.800146000	-3.124525000
7	4.374312000	-1.484945000	0.940628000
6	5.692810000	-2.060627000	0.636820000
6	4.225811000	-0.577307000	2.091017000
1	6.173251000	-1.566301000	-0.229420000
1	6.346382000	-1.937806000	1.510420000
1	5.614526000	-3.141554000	0.426231000
1	3.383940000	-0.887237000	2.736444000
1	5.140482000	-0.616317000	2.697221000
1	4.059914000	0.468100000	1.771837000

Alkoxide - $[(4,4'\text{-}NO_2\text{-}bpy)Pt^{II}(OPh)(Py)]^+$

78	-0.622099000	-0.024056000	-0.260876000
6	2.182755000	0.709720000	0.070229000
6	0.842130000	2.650169000	0.136884000
6	3.358825000	1.471643000	0.245358000
6	1.961804000	3.487260000	0.317403000
1	-0.164085000	3.066624000	0.087176000
6	3.224616000	2.865704000	0.366849000
1	4.348119000	1.018974000	0.290439000
1	1.856465000	4.567264000	0.413269000
6	2.181164000	-0.774366000	-0.059127000
6	0.794685000	-2.674493000	-0.352228000
6	3.342811000	-1.575006000	-0.022633000
6	1.904982000	-3.547172000	-0.331251000
1	-0.234455000	-3.018601000	-0.481509000
6	3.175574000	-2.965781000	-0.160060000
1	4.341712000	-1.161244000	0.104950000
1	1.783542000	-4.624040000	-0.442248000
7	0.941631000	-1.336711000	-0.218822000
7	0.942766000	1.303703000	0.014473000
8	-1.905782000	-1.528943000	-0.586273000
6	-4.304157000	-1.719490000	-0.567943000
6	-3.069888000	-1.618482000	1.559336000
6	-5.514504000	-1.867052000	0.151427000
1	-4.291926000	-1.719057000	-1.661082000
6	-4.287092000	-1.754638000	2.269534000
1	-2.116475000	-1.554582000	2.094137000
6	-5.514647000	-1.878523000	1.570668000
1	-6.455342000	-1.974802000	-0.395889000
1	-4.274391000	-1.782113000	3.362953000
1	-6.451909000	-1.995705000	2.120689000
6	-2.898396000	1.700938000	0.700700000
6	-2.564622000	1.776444000	-1.622991000
6	-4.012883000	2.561276000	0.610872000
1	-2.572645000	1.290768000	1.656113000
6	-3.670283000	2.633933000	-1.798128000
1	-1.972563000	1.430794000	-2.471236000
6	-4.409487000	3.036518000	-0.660568000
1	-4.554721000	2.831151000	1.518809000
1	-3.938757000	2.963779000	-2.803188000
1	-5.274314000	3.696863000	-0.763466000
6	-3.072647000	-1.599180000	0.135012000
7	-2.183321000	1.326905000	-0.395080000
7	4.450591000	3.699457000	0.554197000
7	4.389143000	-3.841814000	-0.123588000
8	4.280474000	4.926789000	0.658939000
8	5.539021000	3.096935000	0.590022000
8	5.486435000	-3.273026000	0.025368000
8	4.200523000	-5.063886000	-0.245047000

Alkoxide - [(4,4'-OMe-bpy)Pt^{II}(OPh)(Py)]$^{+}$

78	0.396967000	-0.043720000	-0.315552000
6	-2.435723000	-0.630153000	0.129651000
6	-1.209146000	-2.629551000	0.166068000
6	-3.632131000	-1.323707000	0.367112000
6	-2.357548000	-3.406715000	0.406790000
1	-0.232438000	-3.108462000	0.078308000
6	-3.611064000	-2.740206000	0.511036000
1	-4.587452000	-0.805467000	0.446280000
1	-2.254857000	-4.486140000	0.504067000
6	-2.362244000	0.853378000	-0.033517000
6	-0.906835000	2.665231000	-0.429338000
6	-3.471170000	1.710155000	0.024449000
6	-1.963076000	3.594825000	-0.388265000
1	0.128616000	2.962891000	-0.610898000
6	-3.281627000	3.112194000	-0.153159000
1	-4.480070000	1.337604000	0.199816000
1	-1.741954000	4.650344000	-0.536412000
7	-1.097335000	1.338842000	-0.254928000
7	-1.226956000	-1.284692000	0.028648000
8	1.777996000	1.368468000	-0.727697000
6	4.119500000	1.797997000	-0.445691000
6	2.697793000	1.514899000	1.539974000
6	5.231331000	2.041254000	0.395308000
1	4.218145000	1.820388000	-1.534242000
6	3.820284000	1.747779000	2.372273000
1	1.709723000	1.335644000	1.976667000
6	5.093189000	2.011824000	1.807838000
1	6.206942000	2.250432000	-0.053807000
1	3.695402000	1.736219000	3.459359000
1	5.956014000	2.198991000	2.452388000
6	2.602878000	-1.847030000	0.663702000
6	2.294697000	-1.903812000	-1.660678000
6	3.699498000	-2.731582000	0.583403000
1	2.276444000	-1.431834000	1.616887000
6	3.381612000	-2.787266000	-1.828245000
1	1.721474000	-1.537530000	-2.513038000
6	4.099266000	-3.211497000	-0.685099000
1	4.226705000	-3.014511000	1.496060000
1	3.653775000	-3.118298000	-2.831984000
1	4.950706000	-3.890163000	-0.781462000
6	2.837028000	1.537063000	0.120533000
7	1.908519000	-1.450865000	-0.436749000
6	-4.841243000	-4.772998000	0.890562000
6	-4.268283000	5.304221000	-0.258282000
1	-5.286605000	5.698959000	-0.161336000
1	-3.622900000	5.735243000	0.525354000
1	-3.869407000	5.537749000	-1.259635000
1	-5.896384000	-5.017315000	1.061111000
1	-4.485409000	-5.270766000	-0.027210000
1	-4.239179000	-5.086812000	1.759941000
8	-4.799959000	-3.333117000	0.736545000
8	-4.393312000	3.871174000	-0.082664000

Alkoxide - [(4,4'-NMe$_2$-bpy)Pt^{II}(OPh)(Py)]$^{+}$

78	0.735166000	-0.075471000	-0.342603000
6	-2.102215000	-0.677740000	0.057293000
6	-0.871606000	-2.667239000	0.094904000
6	-3.299816000	-1.377680000	0.272120000
6	-2.013574000	-3.444730000	0.311152000
1	0.107392000	-3.143340000	0.016997000
6	-3.299130000	-2.807815000	0.408645000
1	-4.231510000	-0.821909000	0.335400000
1	-1.896033000	-4.522969000	0.398238000
6	-2.032100000	0.810860000	-0.094312000
6	-0.584126000	2.627299000	-0.457828000
6	-3.146810000	1.662078000	-0.045242000
6	-1.638937000	3.544437000	-0.423457000
1	0.450232000	2.934538000	-0.625782000
6	-2.983821000	3.081853000	-0.208067000
1	-4.134311000	1.237499000	0.114669000
1	-1.409069000	4.598574000	-0.563318000
7	-0.765719000	1.292844000	-0.294265000
7	-0.887782000	-1.316628000	-0.032446000
8	2.131042000	1.333534000	-0.736133000
6	4.411842000	1.942440000	-0.341720000
6	2.940664000	1.493684000	1.575327000
6	5.466815000	2.247513000	0.549874000
1	4.552125000	2.000645000	-1.424395000
6	4.008400000	1.790815000	2.458312000
1	1.954122000	1.226452000	1.967756000
6	5.277771000	2.168610000	1.954993000
1	6.439881000	2.543360000	0.145762000
1	3.841501000	1.738660000	3.538741000
1	6.097756000	2.403268000	2.638825000
6	2.925972000	-1.883670000	0.668640000
6	2.680063000	-1.906325000	-1.662262000
6	4.028771000	-2.762151000	0.604663000
1	2.572807000	-1.483903000	1.618996000
6	3.774702000	-2.783233000	-1.814566000
1	2.128462000	-1.528368000	-2.523689000
6	4.463607000	-3.222308000	-0.659548000
1	4.533369000	-3.055878000	1.526683000
1	4.074680000	-3.097889000	-2.815675000
1	5.320022000	-3.896441000	-0.743411000
6	3.130717000	1.564328000	0.162391000
7	2.258674000	-1.473724000	-0.443047000
7	-4.449793000	-3.519107000	0.617694000
7	-4.047884000	3.942360000	-0.162920000
6	-4.393413000	-4.985431000	0.754430000
6	-5.744125000	-2.823501000	0.703842000
6	-5.409136000	3.426729000	0.050818000
6	-3.830404000	5.389800000	-0.339621000
1	-4.793833000	5.909857000	-0.265314000
1	-3.161316000	5.792041000	0.441169000

1	-3.394507000	5.612079000	-1.329624000
1	-6.116735000	4.265164000	0.054066000
1	-5.707630000	2.731464000	-0.754825000
1	-5.494024000	2.905113000	1.021425000
1	-5.407236000	-5.370602000	0.921292000
1	-3.992137000	-5.458834000	-0.159242000
1	-3.767254000	-5.283935000	1.613788000
1	-6.540043000	-3.560619000	0.867727000
1	-5.761104000	-2.108951000	1.546570000
1	-5.970060000	-2.278566000	-0.230531000

Alkoxide - $[(5,5'\text{-}NO_2\text{-bpy})Pt^{II}(OPh)(Py)]^+$

78	-0.057216000	0.161614000	-0.211237000
6	0.873541000	-2.588573000	0.172431000
6	2.711607000	-1.115296000	0.133845000
6	1.725085000	-3.704996000	0.353217000
6	3.596539000	-2.194814000	0.317669000
1	3.084815000	-0.096646000	0.044547000
6	3.120122000	-3.516672000	0.429233000
1	1.312945000	-4.710197000	0.435803000
1	3.813616000	-4.346597000	0.568846000
6	-0.611164000	-2.688688000	0.091472000
6	-2.600619000	-1.434483000	-0.185827000
6	-1.336741000	-3.899842000	0.184606000
6	-3.360692000	-2.618489000	-0.103393000
1	-3.038972000	-0.444831000	-0.335056000
6	-2.743966000	-3.871470000	0.087421000
1	-0.825500000	-4.851136000	0.329074000
1	-3.347621000	-4.777351000	0.153711000
7	-1.256461000	-1.491051000	-0.085716000
7	1.377399000	-1.310865000	0.061398000
8	-1.665467000	1.317368000	-0.510481000
6	-1.974412000	3.700633000	-0.648188000
6	-1.755643000	2.619230000	1.552346000
6	-2.162518000	4.948653000	-0.006717000
1	-2.004275000	3.614031000	-1.737558000
6	-1.932717000	3.873558000	2.184005000
1	-1.631505000	1.707540000	2.145948000
6	-2.135696000	5.043749000	1.408979000
1	-2.332039000	5.844123000	-0.611438000
1	-1.931413000	3.933791000	3.276191000
1	-2.284706000	6.009350000	1.899111000
6	1.555888000	2.556042000	0.641929000
6	1.588184000	2.168039000	-1.674429000
6	2.358189000	3.707796000	0.502621000
1	1.186999000	2.234343000	1.615340000
6	2.386631000	3.308257000	-1.898318000
1	1.250063000	1.539054000	-2.498799000
6	2.782454000	4.093533000	-0.789804000
1	2.626246000	4.283349000	1.390075000
1	2.679102000	3.565941000	-2.917640000
1	3.400175000	4.984109000	-0.930465000
6	-1.774777000	2.527345000	0.131375000
7	1.189417000	1.796399000	-0.426062000
7	5.055728000	-1.914483000	0.390826000
7	-4.842599000	-2.531763000	-0.223325000
8	5.806351000	-2.892461000	0.550117000
8	5.407417000	-0.723238000	0.286622000
8	-5.470517000	-3.603712000	-0.145551000
8	-5.329692000	-1.399647000	-0.390444000

Alkoxide - $[(5,5'\text{-OMe-bpy})Pt^{II}(OPh)(Py)]^+$

78	0.139710000	-0.033931000	-0.275073000
6	-2.731819000	0.100837000	0.203251000
6	-2.027878000	-2.150249000	0.170552000
6	-4.063723000	-0.306000000	0.441905000
6	-3.346671000	-2.628098000	0.411781000
1	-1.209858000	-2.862621000	0.058777000
6	-4.389660000	-1.673559000	0.548923000
1	-4.853087000	0.438971000	0.546410000
1	-5.421558000	-1.972368000	0.733030000
6	-2.292838000	1.512973000	0.080752000
6	-0.413514000	2.908536000	-0.290071000
6	-3.134810000	2.641442000	0.181476000
6	-1.210523000	4.087257000	-0.200123000
1	0.661122000	2.951370000	-0.482130000
6	-2.602707000	3.941614000	0.044517000
1	-4.202746000	2.519377000	0.365569000
1	-3.262417000	4.805469000	0.126309000
7	-0.950102000	1.685546000	-0.150313000
7	-1.736086000	-0.840268000	0.070055000
8	1.825816000	0.992513000	-0.679652000
6	4.197535000	0.660295000	-0.526666000
6	2.859788000	0.799119000	1.531512000
6	5.370315000	0.526884000	0.254419000
1	4.243843000	0.674314000	-1.618852000
6	4.038128000	0.652735000	2.303567000
1	1.888580000	0.932769000	2.019217000
6	5.299732000	0.515059000	1.672028000
1	6.338962000	0.429823000	-0.245059000
1	3.970816000	0.661479000	3.395694000
1	6.208826000	0.411189000	2.270157000
6	1.817162000	-2.373271000	0.611279000
6	1.451450000	-2.294590000	-1.704798000
6	2.634067000	-3.516956000	0.486779000
1	1.634307000	-1.907659000	1.579324000
6	2.257025000	-3.433003000	-1.915731000
1	0.977483000	-1.769982000	-2.535145000
6	2.859870000	-4.059006000	-0.799344000
1	3.085744000	-3.951713000	1.379991000
1	2.406354000	-3.803469000	-2.931378000
1	3.493861000	-4.939866000	-0.929459000
6	2.929138000	0.803300000	0.107299000
7	1.229765000	-1.782294000	-0.463582000
6	-4.788447000	-4.525025000	0.725943000
6	-1.289206000	6.487120000	-0.275640000

1	-5.480041000	-4.251249000	-0.089423000
1	-4.652414000	-5.613038000	0.746406000
1	-5.184067000	-4.180800000	1.697086000
1	-1.751633000	6.595816000	0.720794000
1	-0.553464000	7.285117000	-0.431697000
1	-2.060473000	6.531554000	-1.064113000
8	-3.472594000	-3.975520000	0.486005000
8	-0.542603000	5.252606000	-0.360180000

Alkoxide - $[(5,5'\text{-}NMe_2\text{-bpy})Pt^{II}(OPh)(Py)]^+$

78	-0.010675000	0.191328000	-0.291179000
6	1.072925000	-2.453448000	0.211208000
6	2.830602000	-0.869351000	0.121069000
6	2.013491000	-3.486569000	0.452898000
6	3.844909000	-1.852218000	0.366304000
1	3.082485000	0.178578000	-0.025167000
6	3.382769000	-3.202036000	0.530834000
1	1.673700000	-4.515206000	0.579279000
1	4.083885000	-4.015101000	0.715720000
6	-0.387687000	-2.648530000	0.111849000
6	-2.451688000	-1.530259000	-0.261000000
6	-1.071228000	-3.882284000	0.242877000
6	-3.216927000	-2.739463000	-0.142214000
1	-2.897748000	-0.558277000	-0.468092000
6	-2.467918000	-3.936799000	0.121686000
1	-0.516554000	-4.800679000	0.439654000
1	-2.970396000	-4.897512000	0.229542000
7	-1.112649000	-1.513148000	-0.133311000
7	1.514559000	-1.165201000	0.050352000
8	-1.648700000	1.305445000	-0.700426000
6	-2.546485000	3.508308000	-0.413246000
6	-1.896639000	2.205221000	1.567422000
6	-2.979618000	4.558643000	0.430107000
1	-2.630549000	3.585765000	-1.500578000
6	-2.322637000	3.268600000	2.401339000
1	-1.499147000	1.282681000	2.002885000
6	-2.865738000	4.451541000	1.841322000
1	-3.402070000	5.464001000	-0.016397000
1	-2.240985000	3.164936000	3.487735000
1	-3.199567000	5.267562000	2.487575000
6	1.402476000	2.707415000	0.576959000
6	1.420113000	2.367696000	-1.742989000
6	2.060287000	3.949144000	0.444284000
1	1.096143000	2.326987000	1.551205000
6	2.076193000	3.597114000	-1.963309000
1	1.131870000	1.718776000	-2.570655000
6	2.404684000	4.404991000	-0.849182000
1	2.274421000	4.539722000	1.336667000
1	2.307806000	3.906279000	-2.984094000
1	2.905972000	5.366652000	-0.986479000
6	-2.002178000	2.314556000	0.148297000
7	1.099298000	1.928859000	-0.495847000
7	5.178412000	-1.511970000	0.437821000
7	-4.584716000	-2.729076000	-0.275568000
6	5.594689000	-0.118806000	0.233667000
6	6.186233000	-2.560731000	0.657620000
6	-5.289159000	-1.462880000	-0.539277000
6	-5.338293000	-3.984508000	-0.145149000
1	6.685196000	-0.048991000	0.337912000
1	5.324078000	0.244977000	-0.775777000
1	5.139153000	0.553152000	0.984641000
1	6.177732000	-3.309905000	-0.155426000
1	7.182501000	-2.100931000	0.687018000
1	6.023152000	-3.081413000	1.618527000
1	-6.367104000	-1.659483000	-0.604449000
1	-5.121064000	-0.730851000	0.270986000
1	-4.963125000	-1.011066000	-1.493336000
1	-5.207644000	-4.433329000	0.856864000
1	-6.406722000	-3.778965000	-0.289184000
1	-5.026524000	-4.723844000	-0.905592000

Full reference for # 22:

Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.