

**CHEMISTRY**   
**A EUROPEAN JOURNAL**

Supporting Information

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# Transmetallation Reaction from Fischer Carbene Complexes to Late Transition Metals: a DFT Study<sup>[\*\*]</sup>

Israel Fernández,<sup>\*[a]</sup> María J. Mancheño,<sup>[a]</sup> Rubén Vicente,<sup>[b,c]</sup> Luis A. López,<sup>[b]</sup> and Miguel A.  
Sierra<sup>\*[a]</sup>

*[a] Departamento de Química Orgánica I  
Facultad de Ciencias Químicas  
Universidad Complutense de Madrid, 28040-Madrid (Spain)*

*[b] Instituto Universitario de Química Organometálica “Enrique Moles”  
Unidad Asociada al CSIC, Universidad de Oviedo  
Julián Clavería 8, 33006 Oviedo (Spain)*

*[c] Institut für Organische und Biomolekulare Chemie  
Georg August Universität-Göttingen  
Tammanstr. 2, Göttingen (Germany)*

Cartesian coordinates (in Å) and total energies (in a. u., non corrected zero-point vibrational energies included) of all the stationary points discussed in the text. All calculations have been performed at the BP86/LANL2DZ&6-31G(d) +  $\Delta$ ZPVE level of theory.

### Transmetallation to Palladium

**14:** E= -846.129067

C	-0.164667000	-1.550754000	-1.034732000
Cr	0.371945000	-0.066602000	0.000839000
C	2.091042000	-0.833737000	0.027913000
O	3.158634000	-1.307460000	0.045144000
O	-0.401422000	-2.497062000	-1.680820000
C	0.782793000	0.875771000	-1.583879000
O	1.029090000	1.467356000	-2.559922000
C	1.081574000	1.347921000	1.032947000
O	1.563293000	2.198015000	1.672886000
C	-0.092819000	-0.974080000	1.589872000
O	-0.359266000	-1.533354000	2.581502000
C	-1.426291000	0.892413000	-0.033726000
C	-1.545620000	2.405396000	-0.037782000
O	-2.672154000	0.432821000	-0.033188000
C	-2.984932000	-0.982421000	0.003630000
H	-2.563478000	2.744523000	-0.299041000
H	-0.807605000	2.857281000	-0.720031000
H	-1.303787000	2.777784000	0.976771000
H	-2.406202000	-1.487870000	0.789022000
H	-4.061466000	-1.029209000	0.222132000
H	-2.776031000	-1.429639000	-0.979256000

**Pd(PH<sub>3</sub>)<sub>4</sub>:** E= -1499.423292

Pd	0.001001000	0.001742000	-0.000592000
P	-1.617815000	0.926105000	-1.450950000
H	-1.707550000	0.575137000	-2.840701000
H	-3.028864000	0.777651000	-1.227206000
H	-1.712369000	2.336325000	-1.705501000
P	1.374960000	-1.508594000	-1.192453000
H	1.219446000	-1.757598000	-2.598394000
H	2.799854000	-1.353635000	-1.283649000
H	1.454911000	-2.903812000	-0.860291000
P	1.334189000	1.732373000	0.899563000
H	1.133754000	3.115785000	0.568962000
H	1.429463000	1.987626000	2.309647000
H	2.754937000	1.794432000	0.697548000
P	-1.093125000	-1.153653000	1.745239000
H	-0.888529000	-2.553530000	1.995536000
H	-0.949900000	-0.789360000	3.127452000
H	-2.524332000	-1.252590000	1.822866000

**Pd(PH<sub>3</sub>)<sub>3</sub>:** E= -1156.281290

Pd	-0.005523000	-0.003798000	-0.023833000
P	0.798024000	2.178267000	0.008555000
H	2.025688000	2.604590000	-0.601503000

H	0.066219000	3.326958000	-0.446685000
H	1.110274000	2.753196000	1.284017000
P	1.508408000	-1.767985000	0.009545000
H	2.127294000	-2.092975000	1.260896000
H	1.210792000	-3.134977000	-0.315913000
H	2.741716000	-1.765117000	-0.724190000
P	-2.298107000	-0.402852000	0.009441000
H	-3.299613000	0.515708000	-0.455220000
H	-2.927932000	-1.539426000	-0.600684000
H	-2.925254000	-0.604672000	1.282497000

**Pd(PH<sub>3</sub>)<sub>2</sub>: E= -813.131109**

P	2.276570000	0.004364000	-0.000998000
Pd	0.000064000	-0.003907000	0.000887000
P	-2.276739000	0.004358000	-0.001001000
H	3.023148000	-0.245288000	1.194206000
H	3.023950000	-0.901195000	-0.819302000
H	3.013577000	1.170906000	-0.380342000
H	-3.023985000	-0.887187000	-0.834656000
H	-3.023378000	-0.265516000	1.189770000
H	-3.013710000	1.177181000	-0.360510000

**TS1-Pd: E= -2002.398565**

P	2.596727000	0.307041000	2.133636000
Pd	1.788121000	-0.152673000	-0.008716000
C	-0.931195000	1.478176000	0.475386000
C	-0.684515000	1.959374000	1.888848000
O	-0.750423000	2.397444000	-0.478545000
C	-0.200534000	3.716384000	-0.200036000
P	2.406847000	1.291359000	-1.750235000
P	2.160668000	-2.418356000	-0.588981000
H	1.844193000	0.501744000	3.343188000
H	3.467950000	1.421112000	2.384444000
H	3.485719000	-0.647969000	2.726607000
H	-0.682826000	1.115827000	2.591307000
H	-1.516047000	2.636284000	2.181626000
H	0.255128000	2.528586000	2.006444000
H	0.848817000	3.621856000	0.128932000
H	-0.249656000	4.251919000	-1.158145000
H	-0.796033000	4.247589000	0.560426000
H	3.000610000	0.742608000	-2.933677000
H	3.441486000	2.269403000	-1.566565000
H	1.546308000	2.183653000	-2.475185000
H	2.947991000	-3.267598000	0.255771000
H	2.879091000	-2.755712000	-1.782625000
H	1.132380000	-3.395499000	-0.799454000
C	-0.753590000	-0.513585000	-1.611324000
O	-0.344247000	-0.670551000	-2.696357000
Cr	-1.789740000	-0.285160000	-0.020872000
C	-2.980061000	0.667857000	-1.125064000
O	-3.728848000	1.262353000	-1.795825000
C	-3.020600000	-0.023890000	1.375643000
O	-3.808051000	0.140895000	2.225126000
C	-0.734954000	-1.268492000	1.228016000
O	-0.299823000	-1.942503000	2.081787000
C	-2.633177000	-1.914514000	-0.446241000
O	-3.160707000	-2.924575000	-0.709800000

18: E= -2002.413522

P	-2.757240000	0.664170000	-1.672152000
Pd	-1.230244000	-0.127188000	-0.034439000
C	0.621365000	-1.466041000	1.133449000
O	0.310543000	-2.237211000	1.971096000
Cr	1.560380000	-0.325103000	-0.063925000
C	2.165186000	0.513868000	1.512927000
O	2.568155000	1.004418000	2.493906000
C	0.280185000	1.396632000	-0.380997000
C	0.190687000	2.055814000	-1.756260000
C	2.753329000	0.750665000	-1.026745000
O	3.520277000	1.423298000	-1.601635000
C	0.888243000	-1.126416000	-1.642475000
O	0.566854000	-1.647141000	-2.643950000
C	2.910468000	-1.596368000	-0.000538000
O	3.765347000	-2.397285000	0.023672000
O	0.293054000	2.308713000	0.660727000
C	-0.020924000	3.702388000	0.457663000
P	-1.941020000	0.726910000	2.213384000
H	-2.464858000	0.719558000	-3.074081000
H	-3.315752000	1.982790000	-1.617212000
H	-4.016143000	0.001239000	-1.831257000
H	0.159698000	1.290094000	-2.544552000
H	1.084877000	2.683829000	-1.944980000
H	-0.690111000	2.718513000	-1.870969000
H	-1.066355000	3.839664000	0.123182000
H	0.110475000	4.172615000	1.443709000
H	0.663232000	4.177706000	-0.266706000
H	-2.963656000	0.165965000	3.050137000
H	-2.403829000	2.073529000	2.365589000
H	-0.968827000	0.817334000	3.256897000
P	-2.251662000	-2.380184000	0.047919000
H	-3.441391000	-2.679012000	-0.691699000
H	-2.698774000	-2.970945000	1.270738000
H	-1.522733000	-3.524789000	-0.400351000

19: E= -1659.283949

C	-0.533591000	-1.467009000	-1.160139000
Cr	-1.413313000	-0.276180000	0.029165000
C	-2.805602000	-1.502457000	0.057193000
O	-3.682698000	-2.277461000	0.092483000
Pd	1.297647000	-0.159765000	-0.030686000
P	2.348345000	-2.366593000	-0.058076000
P	3.266964000	1.100156000	0.019910000
C	-0.065796000	1.432147000	0.236923000
O	-0.110191000	2.298420000	-0.837253000
C	0.192410000	3.701093000	-0.692165000
O	-0.225292000	-2.249107000	-1.987111000
C	-2.055652000	0.529427000	-1.555864000
O	-2.484013000	0.996064000	-2.535677000
C	-2.505315000	0.906254000	0.988690000
O	-3.204824000	1.651126000	1.559944000
C	-0.741494000	-1.066469000	1.610937000
O	-0.408171000	-1.579896000	2.612266000
C	0.151818000	2.110038000	1.588121000
H	3.379260000	2.419209000	0.566277000
H	3.882261000	1.416859000	-1.231554000
H	4.457596000	0.604829000	0.640636000

H	0.248704000	1.353660000	2.380963000
H	-0.708981000	2.757365000	1.851622000
H	1.055254000	2.749601000	1.610556000
H	1.249961000	3.863620000	-0.411498000
H	0.010157000	4.138171000	-1.685095000
H	-0.462987000	4.189688000	0.050058000
H	3.499886000	-2.633511000	0.747419000
H	2.873659000	-2.933797000	-1.259705000
H	1.614195000	-3.522956000	0.345052000

**20:** E= -1006.137673

Pd	0.388689000	-0.000035000	-0.008420000
C	-1.589374000	-0.000044000	0.199479000
C	-2.265697000	-0.000049000	1.557215000
O	-2.426962000	-0.000060000	-0.855822000
C	-3.877007000	-0.000097000	-0.704873000
P	1.813107000	-1.851272000	-0.081666000
P	1.812799000	1.851440000	-0.081682000
H	-2.911983000	-0.892833000	1.694421000
H	-2.912004000	0.892722000	1.694418000
H	-1.505207000	-0.000039000	2.351484000
H	-4.223601000	0.902411000	-0.172436000
H	-4.272111000	-0.000094000	-1.730712000
H	-4.223556000	-0.902637000	-0.172459000
H	3.031148000	-1.961838000	-0.839722000
H	1.354513000	-3.159559000	-0.452546000
H	2.409446000	-2.291642000	1.146344000
H	1.354119000	3.159235000	-0.454191000
H	3.031816000	1.961980000	-0.838200000
H	2.407327000	2.293000000	1.146779000

**TS2-Pd:** E= -1852.253042

C	-4.235510000	0.688667000	0.070746000
C	-2.741849000	0.957955000	0.068587000
Pd	-1.487928000	-0.594115000	-0.004567000
Cr	1.947950000	0.260543000	-0.293178000
C	3.219344000	0.135586000	-1.655963000
O	4.021377000	0.072138000	-2.508330000
O	-2.400748000	2.241776000	-0.122370000
C	-3.380137000	3.300726000	-0.351190000
P	-1.093796000	-2.537517000	1.338225000
P	-1.702527000	-1.535670000	-2.190978000
C	0.648037000	0.621488000	1.300635000
O	0.724547000	-0.202825000	2.369166000
C	0.026796000	0.091078000	3.606703000
C	0.086611000	1.996753000	1.596683000
C	1.446658000	-1.500295000	-0.805623000
O	1.369510000	-2.610427000	-1.177990000
C	3.093314000	-0.575876000	0.945601000
O	3.813579000	-1.093520000	1.706458000
C	2.739015000	1.908116000	0.142560000
O	3.270402000	2.918796000	0.401206000
C	0.767210000	1.134118000	-1.488704000
O	0.131998000	1.722167000	-2.276723000
H	-4.733737000	1.040970000	-0.857215000
H	-4.726398000	1.211618000	0.918299000
H	-4.420975000	-0.388843000	0.183799000
H	-4.096100000	3.368734000	0.485183000

H	-2.790456000	4.225522000	-0.418003000
H	-3.920880000	3.134476000	-1.297823000
H	-2.036864000	-3.600870000	1.161848000
H	-1.187706000	-2.540902000	2.768964000
H	0.057555000	-3.389726000	1.300709000
H	-2.916797000	-1.260764000	-2.898382000
H	-1.693639000	-2.931533000	-2.520986000
H	-0.842611000	-1.145351000	-3.264910000
H	-0.136392000	2.524895000	0.662122000
H	0.865306000	2.574485000	2.141040000
H	-0.825336000	1.994093000	2.216409000
H	-1.063116000	0.099087000	3.421617000
H	0.292467000	-0.729980000	4.288106000
H	0.352156000	1.053410000	4.035330000

**21:** E= -1852.283480

C	2.332413000	-1.497167000	0.259480000
C	3.286204000	-0.975431000	1.302328000
O	2.778407000	-2.657939000	-0.199315000
C	2.032005000	-3.333216000	-1.249612000
H	4.104999000	-1.679268000	1.540587000
H	2.721432000	-0.718228000	2.215892000
H	3.708956000	-0.017042000	0.942401000
H	1.729061000	-4.315847000	-0.855824000
H	1.157484000	-2.721207000	-1.530035000
H	2.720138000	-3.465652000	-2.099001000
Pd	0.773318000	-0.395587000	-0.368580000
C	-0.682923000	-1.106323000	0.953967000
C	-0.978846000	-2.591731000	0.740677000
O	-0.446779000	-0.762806000	2.279952000
C	-0.085775000	-1.770462000	3.239003000
P	3.565628000	3.333010000	1.127635000
P	1.881066000	0.639882000	-2.281675000
H	-1.157001000	-2.792193000	-0.326588000
H	-1.891270000	-2.899477000	1.291200000
H	-0.152838000	-3.245954000	1.079999000
H	0.859606000	-2.277045000	2.958240000
H	0.058777000	-1.231674000	4.188011000
H	-0.877372000	-2.530264000	3.369561000
H	4.481500000	4.235167000	1.767593000
H	2.603903000	3.433328000	2.186110000
H	2.948326000	4.375760000	0.362008000
H	2.668009000	-0.171780000	-3.156747000
H	2.887375000	1.622523000	-2.037724000
H	1.198692000	1.357530000	-3.312328000
C	-0.575723000	1.756824000	-0.572119000
O	0.018538000	2.754171000	-0.793878000
Cr	-1.844072000	0.428593000	-0.119040000
C	-1.948927000	1.361655000	1.521509000
O	-2.037591000	1.969069000	2.514280000
C	-3.234125000	-0.664419000	0.502904000
O	-4.107531000	-1.326528000	0.914298000
C	-1.691704000	-0.540688000	-1.728799000
O	-1.661482000	-1.134010000	-2.742489000
C	-3.103285000	1.523692000	-0.922796000
O	-3.903681000	2.205830000	-1.440398000

**22:** E= -1509.154124

C	2.831767000	0.473769000	-0.351689000
C	3.313067000	0.951835000	-1.698571000
O	3.790286000	0.660253000	0.544615000
C	3.565030000	0.226018000	1.913951000
H	4.205690000	1.602046000	-1.638842000
H	2.488224000	1.461144000	-2.224264000
H	3.563784000	0.061546000	-2.309013000
H	3.661332000	1.113277000	2.558903000
H	2.561699000	-0.225874000	1.994054000
H	4.355800000	-0.501105000	2.155944000
Pd	1.028370000	-0.383528000	-0.164533000
C	-0.062378000	1.367715000	0.215111000
C	0.324901000	1.983912000	1.559302000
O	-0.069752000	2.270561000	-0.841118000
C	0.620600000	3.526928000	-0.732882000
P	1.650499000	-2.743567000	-0.256987000
H	0.308751000	1.213329000	2.344493000
H	-0.392974000	2.774833000	1.858260000
H	1.333311000	2.440163000	1.546006000
H	1.708903000	3.379814000	-0.580934000
H	0.454244000	4.034499000	-1.695347000
H	0.222771000	4.155524000	0.083806000
H	2.667756000	-3.215270000	0.629702000
H	2.232988000	-3.278135000	-1.447195000
H	0.741438000	-3.823917000	-0.033101000
C	-1.088578000	-1.353938000	-1.194529000
O	-0.947432000	-2.126909000	-2.075378000
Cr	-1.699717000	-0.100461000	0.086813000
C	-2.310485000	0.853653000	-1.426726000
O	-2.722718000	1.416340000	-2.362207000
C	-2.520159000	1.213969000	1.141436000
O	-3.047321000	2.046682000	1.773160000
C	-1.054106000	-1.020190000	1.600892000
O	-0.724573000	-1.597484000	2.570046000
C	-3.250165000	-1.110978000	0.177131000
O	-4.228487000	-1.752093000	0.250480000

**23:** E= -855.998743

P	-0.109610000	2.617030000	-0.260100000
Pd	0.010330000	0.298136000	0.070888000
H	-0.934624000	3.470836000	0.546750000
H	0.997899000	3.533720000	-0.274148000
H	-0.645938000	3.071190000	-1.508223000
C	1.831458000	-0.466854000	0.181296000
O	2.524760000	-0.841686000	-0.918353000
C	2.519767000	-0.732510000	1.506738000
C	3.821876000	-1.490067000	-0.831994000
H	1.892725000	-0.355582000	2.328399000
H	2.688661000	-1.817014000	1.674728000
H	3.512200000	-0.236715000	1.566831000
H	4.116332000	-1.688289000	-1.872889000
H	4.571483000	-0.834090000	-0.354861000
H	3.758691000	-2.443237000	-0.277785000
C	-1.794140000	-0.511730000	0.182988000
O	-2.479101000	-0.907477000	-0.913956000
C	-2.468821000	-0.800358000	1.510618000
C	-3.747295000	-1.611420000	-0.822687000
H	-1.849029000	-0.408252000	2.330616000
H	-3.473785000	-0.330726000	1.575154000
H	-2.608696000	-1.889184000	1.676600000



H	-4.043262000	-1.810366000	-1.862961000
H	-3.636663000	-2.567037000	-0.280435000
H	-4.519370000	-0.994001000	-0.330423000

**24:** E= -386.079743

C	0.952338000	0.321811000	-0.062512000
C	-0.382096000	0.587390000	-0.142947000
O	-1.242248000	-0.430397000	-0.567978000
C	-2.389288000	-0.663651000	0.255824000
C	-1.024969000	1.932347000	0.089019000
C	2.041766000	1.347177000	0.130199000
O	1.541352000	-0.920345000	-0.212542000
C	0.840870000	-2.095030000	0.214089000
H	-2.929483000	-1.506653000	-0.204158000
H	-3.066323000	0.212052000	0.293911000
H	-2.099288000	-0.936978000	1.291653000
H	-1.671295000	2.201657000	-0.768767000
H	-0.279936000	2.731248000	0.217680000
H	-1.664034000	1.944637000	0.994276000
H	2.529989000	1.229988000	1.116310000
H	1.684367000	2.383238000	0.038273000
H	2.824581000	1.187077000	-0.634340000
H	1.614686000	-2.874196000	0.318944000
H	0.080379000	-2.414997000	-0.516403000
H	0.351802000	-1.931409000	1.194748000

**25:** E= -1199.126022

C	-2.125187000	-1.832690000	-1.116948000
C	-1.744619000	-0.449408000	-0.628681000
Pd	0.000014000	-0.000020000	0.239538000
P	-0.609163000	1.900446000	1.604356000
O	-2.667177000	0.515148000	-0.870399000
C	-3.928644000	0.233965000	-1.532807000
P	0.608986000	-1.900454000	1.604357000
C	1.744712000	0.449409000	-0.628575000
C	2.125223000	1.832713000	-1.116837000
O	2.667308000	-0.515109000	-0.870263000
C	3.928722000	-0.233906000	-1.532754000
H	0.524362000	-2.075944000	3.032567000
H	0.077663000	-3.212091000	1.339759000
H	1.972391000	-2.339507000	1.536701000
H	-1.336654000	-2.550704000	-0.851022000
H	-3.086091000	-2.186668000	-0.685624000
H	-2.242763000	-1.851180000	-2.221132000
H	-4.437251000	1.205905000	-1.613752000
H	-3.769583000	-0.185656000	-2.541681000
H	-4.550202000	-0.459206000	-0.938402000
H	1.336611000	2.550664000	-0.850976000
H	3.086053000	2.186753000	-0.685396000
H	2.242918000	1.851230000	-2.221009000
H	4.437423000	-1.205810000	-1.613569000
H	3.769582000	0.185535000	-2.541688000
H	4.550239000	0.459419000	-0.938488000
H	-1.973150000	2.338042000	1.538940000
H	-0.522080000	2.076942000	3.032294000
H	-0.079760000	3.212491000	1.337940000

**TS3-Pd:** E= -1199.098522

C	-0.934427000	-1.876273000	1.751579000
C	-1.068843000	-0.812949000	0.676689000
Pd	0.711888000	-0.065445000	-0.049909000
P	2.617415000	1.445073000	0.320212000
O	-2.180849000	-0.916591000	-0.101049000
C	-3.051508000	-2.070161000	-0.043440000
P	1.737833000	-1.978609000	-0.798479000
C	-0.653604000	1.564839000	-0.180137000
C	-0.975397000	2.412800000	1.040206000
O	-1.594754000	1.527809000	-1.141804000
C	-2.958570000	1.984768000	-0.897902000
H	3.080946000	-2.358639000	-0.462229000
H	1.182695000	-3.273372000	-0.517926000
H	1.896376000	-2.239525000	-2.203496000
H	0.031914000	-1.762046000	2.264389000
H	-1.730504000	-1.746032000	2.515686000
H	-1.015930000	-2.922431000	1.380052000
H	-3.885667000	-1.842999000	-0.724101000
H	-2.530810000	-2.978775000	-0.396649000
H	-3.442455000	-2.244222000	0.975718000
H	-0.199785000	2.262139000	1.807159000
H	-0.960449000	3.484239000	0.742356000
H	-1.960423000	2.231240000	1.514727000
H	-3.498866000	1.801166000	-1.838415000
H	-3.423042000	1.409465000	-0.080806000
H	-2.978360000	3.063561000	-0.662849000
H	3.917668000	1.278962000	0.930043000
H	3.149704000	2.039851000	-0.868588000
H	2.350350000	2.703054000	0.955593000

**26:** E= -1199.215226

C	1.339384000	1.629477000	1.664591000
C	1.285185000	0.794494000	0.395461000
Pd	-0.754146000	-0.104744000	0.056541000
P	-1.731878000	-2.190257000	-0.379163000
O	1.809454000	1.407986000	-0.749150000
C	1.220637000	2.641806000	-1.146232000
P	-2.419676000	1.516575000	-0.009937000
C	1.358175000	-0.632644000	0.389860000
C	1.517697000	-1.467428000	1.651541000
O	1.836505000	-1.281908000	-0.769447000
C	3.261248000	-1.193158000	-0.933345000
H	-3.706914000	1.287855000	0.582423000
H	-2.296613000	2.841725000	0.532641000
H	-2.948781000	1.966240000	-1.265253000
H	0.922004000	1.082681000	2.523724000
H	2.389230000	1.902710000	1.901439000
H	0.764548000	2.566688000	1.570300000
H	1.726653000	2.934550000	-2.080326000
H	0.135110000	2.511020000	-1.337952000
H	1.361476000	3.446838000	-0.397179000
H	0.962591000	-1.050696000	2.507106000
H	1.143167000	-2.489425000	1.470716000
H	2.583928000	-1.551892000	1.950979000
H	3.494744000	-1.735928000	-1.863906000
H	3.589673000	-0.142485000	-1.028692000
H	3.804491000	-1.677138000	-0.095278000

H	-3.084794000	-2.576467000	-0.092634000
H	-1.771803000	-2.625939000	-1.742202000
H	-1.166301000	-3.410775000	0.117241000

**TS4-Pd:** E= -855.970545

P	-2.698824000	-1.057461000	-0.268481000
Pd	-0.466025000	-0.744148000	-0.003951000
H	-3.434527000	-1.882193000	0.644793000
H	-3.709973000	-0.024953000	-0.306644000
H	-3.169536000	-1.704510000	-1.457091000
C	-0.001315000	1.234983000	0.304197000
O	-0.094378000	2.047339000	-0.763041000
C	-0.385233000	1.844419000	1.633731000
C	-0.613557000	3.412244000	-0.668943000
H	-0.228312000	1.112632000	2.440161000
H	0.214009000	2.751186000	1.859182000
H	-1.456280000	2.145343000	1.654795000
H	-0.589555000	3.802145000	-1.696212000
H	-1.648998000	3.414309000	-0.289232000
H	0.026082000	4.031758000	-0.016963000
C	1.575137000	-0.921813000	0.201226000
O	2.312547000	-0.825674000	-0.926856000
C	2.308037000	-0.658124000	1.504958000
C	3.601252000	-0.155990000	-0.939387000
H	1.579665000	-0.589463000	2.327416000
H	2.951891000	-1.538743000	1.717896000
H	2.966665000	0.233800000	1.535158000
H	3.966998000	-0.244809000	-1.973071000
H	3.480497000	0.911485000	-0.677261000
H	4.319578000	-0.632921000	-0.249472000

**27:** E= -856.066338

P	-3.100098000	-0.067472000	-0.327346000
Pd	-0.876006000	-0.312386000	-0.011770000
H	-3.920942000	-1.214749000	-0.581314000
H	-3.952951000	0.481253000	0.683178000
H	-3.639639000	0.717171000	-1.397543000
C	1.106431000	0.645575000	0.536574000
O	1.534927000	1.535763000	-0.439714000
C	0.985083000	1.205789000	1.942055000
C	0.794503000	2.755531000	-0.560555000
H	0.680599000	0.432607000	2.662283000
H	1.962523000	1.622522000	2.263720000
H	0.239156000	2.015750000	1.999160000
H	1.178957000	3.251792000	-1.465329000
H	-0.284518000	2.534354000	-0.681091000
H	0.943130000	3.426203000	0.308259000
C	1.279389000	-0.725355000	0.231874000
O	1.752675000	-1.099849000	-1.035701000
C	1.418454000	-1.838495000	1.255514000
C	3.146366000	-0.820062000	-1.252792000
H	0.932650000	-1.605750000	2.215691000
H	0.969552000	-2.765486000	0.860089000
H	2.490305000	-2.050805000	1.455138000
H	3.390680000	-1.247186000	-2.238690000
H	3.343692000	0.266535000	-1.259316000
H	3.782362000	-1.307576000	-0.485340000

**28:** E= -193.021801

C	1.886604000	-0.070114000	0.041609000
C	0.613997000	0.353749000	-0.037778000
O	-0.448771000	-0.511633000	-0.072272000
C	-1.729601000	0.112110000	0.048351000
H	0.352826000	1.421671000	-0.100416000
H	-2.476986000	-0.684004000	-0.090303000
H	-1.879000000	0.888345000	-0.728943000
H	-1.867766000	0.569924000	1.047871000
H	2.701844000	0.656306000	0.031204000
H	2.133253000	-1.133656000	0.105669000

**TS5-Pd:** E= -1006.086940

Pd	-0.458326000	-0.118276000	0.121242000
C	1.624465000	-0.150528000	0.555556000
C	1.817897000	-1.491406000	0.987557000
O	2.443992000	0.396046000	-0.377404000
C	3.585209000	-0.352293000	-0.872790000
P	-0.646801000	2.328696000	0.068403000
P	-2.421302000	-1.206208000	-0.410039000
H	2.717425000	-2.096364000	0.759948000
H	0.465919000	-1.621937000	0.276818000
H	1.324730000	-1.766109000	1.926873000
H	3.256843000	-1.254101000	-1.420001000
H	4.110947000	0.330215000	-1.556417000
H	4.258292000	-0.646319000	-0.046665000
H	-1.639596000	3.279711000	-0.363615000
H	0.446052000	3.005321000	-0.557221000
H	-0.458152000	2.936254000	1.349482000
H	-2.466421000	-1.951223000	-1.629921000
H	-3.685141000	-0.558000000	-0.603556000
H	-2.943730000	-2.257086000	0.408968000

**29:** E= -1006.125703

Pd	-0.500476000	-0.296311000	-0.007123000
C	1.495731000	-0.685093000	0.156309000
C	2.066056000	-1.633670000	0.936823000
O	2.212157000	0.236755000	-0.592795000
C	3.637902000	0.077515000	-0.633304000
P	-0.067806000	2.032400000	0.351146000
P	-2.838390000	-0.408765000	-0.241310000
H	3.148798000	-1.715925000	1.094174000
H	-0.502413000	-1.866482000	-0.294276000
H	1.432031000	-2.350511000	1.461174000
H	3.910812000	-0.934965000	-0.987103000
H	4.009710000	0.836459000	-1.339181000
H	4.092461000	0.243219000	0.363779000
H	-1.043160000	2.960973000	0.837835000
H	0.364364000	2.827101000	-0.751327000
H	0.970715000	2.402846000	1.252010000
H	-3.349797000	-0.944847000	-1.460343000
H	-3.778693000	0.669251000	-0.142686000
H	-3.535365000	-1.297877000	0.629480000

**Transmetallation to copper:**

**Cu (MeCN)<sub>4</sub><sup>+</sup>: E= -726.978791**

Cu	-0.005005000	0.009164000	-0.003490000
C	-0.311089000	-1.883111000	2.559143000
C	1.380588000	2.760630000	0.851540000
C	1.829551000	-1.470723000	-2.171250000
C	-2.894918000	0.588301000	-1.238295000
N	0.874910000	1.751933000	0.536878000
N	1.158275000	-0.930361000	-1.377859000
N	-1.836828000	0.374482000	-0.783656000
N	-0.195320000	-1.186813000	1.624470000
C	2.666018000	-2.146628000	-3.157186000
H	3.622339000	-1.608707000	-3.276094000
H	2.876743000	-3.179914000	-2.831917000
H	2.152560000	-2.179991000	-4.133605000
C	2.011098000	4.015243000	1.246840000
H	3.108632000	3.932122000	1.165409000
H	1.666068000	4.837575000	0.596657000
H	1.752927000	4.254952000	2.292798000
C	-0.451499000	-2.752785000	3.721816000
H	0.385540000	-3.470973000	3.761027000
H	-0.448349000	-2.154614000	4.649309000
H	-1.400094000	-3.314041000	3.664533000
C	-4.214021000	0.853202000	-1.802334000
H	-4.960970000	0.172084000	-1.359125000
H	-4.514037000	1.894319000	-1.592841000
H	-4.197835000	0.701974000	-2.895413000

**Cu (MeCN)<sub>3</sub><sup>+</sup>: E= -594.251521**

Cu	0.000159000	-0.000170000	-0.004223000
C	-2.248137000	-2.165082000	0.001000000
C	2.999815000	-0.864637000	0.000713000
C	-0.753249000	3.028974000	0.001636000
N	-0.472676000	1.891594000	-0.002555000
N	1.874249000	-0.539737000	-0.001743000
N	-1.404764000	-1.352026000	-0.003101000
C	-3.297731000	-3.175271000	0.005283000
H	-3.647958000	-3.349350000	1.037669000
H	-4.151040000	-2.837069000	-0.607908000
H	-2.914003000	-4.124290000	-0.407735000
C	-1.098946000	4.444183000	0.004833000
H	-2.011039000	4.613768000	-0.593333000
H	-1.281606000	4.784258000	1.039124000
H	-0.272930000	5.036678000	-0.425472000
C	4.399494000	-1.268060000	0.004825000
H	4.766762000	-1.339595000	1.043481000
H	4.512237000	-2.252392000	-0.481900000
H	5.009827000	-0.526539000	-0.539412000

**Cu (MeCN)<sub>2</sub><sup>+</sup>: E= -461.516109**

C	-4.467718000	0.000975000	0.000098000
C	-3.014701000	0.000139000	0.000004000
N	-1.844007000	-0.000435000	-0.000035000
Cu	-0.000012000	-0.000535000	-0.000061000
N	1.843979000	-0.000299000	-0.000070000
C	3.014684000	0.000188000	0.000038000

C	4.467802000	0.000923000	0.000126000
H	-4.843756000	-0.927815000	-0.463750000
H	-4.842910000	0.064015000	1.036670000
H	-4.842561000	0.867590000	-0.572351000
H	4.842515000	1.036595000	0.078886000
H	4.843443000	-0.584799000	0.857470000
H	4.843407000	-0.448291000	-0.936004000

**TS1-Cu:** E= -1440.373907

N	-2.315507000	-0.223838000	1.820316000
Cu	-1.731597000	0.053628000	-0.062994000
N	-2.083011000	-1.460253000	-1.301818000
N	-2.014780000	1.875298000	-0.790514000
C	-2.369929000	-2.189086000	-2.172771000
C	-2.7821429000	-3.082428000	-3.269311000
C	-2.783105000	-0.216885000	2.894611000
C	-3.360591000	-0.195229000	4.232656000
C	-2.137540000	2.961094000	-1.211375000
C	-2.279840000	4.313803000	-1.733973000
H	-1.927473000	-3.064223000	-4.035938000
H	-3.668867000	-2.755408000	-3.731716000
H	-2.843924000	-4.115869000	-2.902379000
H	-3.301514000	-1.196096000	4.693797000
H	-4.420100000	0.109930000	4.180816000
H	-2.813954000	0.524584000	4.866280000
H	-2.057658000	4.327727000	-2.814938000
H	-1.579293000	4.992057000	-1.216682000
H	-3.310191000	4.675914000	-1.575234000
C	1.150200000	-1.463101000	0.692656000
C	0.884486000	-1.810046000	2.139069000
O	1.099397000	-2.489902000	-0.156341000
C	0.836780000	-3.864273000	0.268525000
C	0.712356000	0.227387000	-1.591389000
O	0.234334000	0.171187000	-2.657890000
Cr	1.729206000	0.340119000	0.003130000
C	3.079125000	-0.545431000	-0.995040000
O	3.911448000	-1.090792000	-1.597235000
C	2.981768000	0.411952000	1.423755000
O	3.767531000	0.456220000	2.282567000
C	0.557623000	1.291994000	1.140968000
O	-0.025837000	1.958571000	1.908706000
C	2.333899000	2.025848000	-0.608063000
O	2.688737000	3.069389000	-0.988998000
H	0.807881000	-0.904087000	2.754316000
H	1.721146000	-2.419996000	2.539231000
H	-0.037319000	-2.410086000	2.265613000
H	-0.196840000	-3.964066000	0.638936000
H	0.975434000	-4.468378000	-0.638012000
H	1.553456000	-4.179496000	1.043385000

**31:** E= -1440.382619

N	-2.160339000	-0.303039000	1.723872000
C	-2.921845000	-0.220199000	2.609191000
C	-3.866715000	-0.110720000	3.714885000
H	-3.771269000	0.878840000	4.194243000
H	-3.664662000	-0.891262000	4.468357000
H	-4.899648000	-0.231164000	3.345772000
Cu	-0.917732000	-0.097037000	0.042117000

C	0.638060000	0.599353000	-1.646808000
O	0.220323000	0.737434000	-2.732231000
Cr	1.623379000	0.414849000	-0.032439000
C	2.713332000	-0.731111000	-1.080392000
O	3.390270000	-1.421293000	-1.725855000
C	0.813179000	-1.306877000	0.796340000
C	2.904452000	0.246655000	1.352211000
O	3.710929000	0.142161000	2.184526000
C	0.638017000	1.587076000	1.084835000
O	0.146456000	2.365727000	1.807757000
C	2.600817000	1.919466000	-0.612168000
O	3.190140000	2.858626000	-0.966730000
O	0.826419000	-2.417445000	0.038431000
C	0.627777000	-3.752101000	0.591411000
H	-0.395786000	-3.857790000	0.988014000
H	0.775348000	-4.431253000	-0.258838000
H	1.368539000	-3.967462000	1.378153000
N	-1.847012000	-1.491959000	-1.288513000
C	-2.273401000	-2.079402000	-2.206899000
C	-2.798799000	-2.805968000	-3.357620000
H	-2.064645000	-2.786148000	-4.181432000
H	-3.736387000	-2.339272000	-3.705050000
H	-3.003445000	-3.855954000	-3.087192000
N	-2.032496000	1.605249000	-0.650536000
C	-2.487702000	2.614344000	-1.030007000
C	-3.043125000	3.876069000	-1.506415000
H	-2.692596000	4.077389000	-2.533294000
H	-2.718056000	4.702422000	-0.851144000
H	-4.145653000	3.833254000	-1.507536000
C	0.645354000	-1.542480000	2.282791000
H	-0.207329000	-2.204503000	2.521060000
H	1.557585000	-2.035269000	2.678508000
H	0.517353000	-0.592195000	2.818437000

**32:** E= -1307.662552

N	2.586612000	-1.327447000	-0.343346000
Cu	1.097234000	0.015700000	0.015882000
C	-0.302571000	0.877948000	-1.632337000
O	0.257250000	1.376371000	-2.531854000
Cr	-1.444753000	0.098134000	-0.319493000
C	-1.237131000	1.592207000	0.838150000
O	-1.138861000	2.533548000	1.515500000
C	-0.373245000	-1.116199000	0.999308000
C	-2.831283000	-0.597953000	0.768844000
O	-3.680180000	-1.033753000	1.432839000
C	-1.623575000	-1.352869000	-1.520526000
O	-1.749065000	-2.215788000	-2.293023000
C	-2.837424000	1.005354000	-1.215777000
O	-3.697268000	1.569554000	-1.756042000
O	-0.121657000	-0.590422000	2.225331000
C	0.162527000	-1.413074000	3.401245000
N	2.114674000	1.765318000	0.207419000
C	3.439855000	-2.013736000	-0.759126000
C	4.500661000	-2.866958000	-1.278075000
C	2.605562000	2.819055000	0.342618000
C	3.210531000	4.133848000	0.506152000
H	1.120345000	-1.945269000	3.282282000
H	0.228138000	-0.696287000	4.230200000
H	-0.657304000	-2.127099000	3.577889000
H	4.081841000	-3.830770000	-1.615435000

H	5.252891000	-3.057143000	-0.493131000
H	4.994143000	-2.373484000	-2.133308000
H	4.125805000	4.057834000	1.117939000
H	2.499818000	4.814799000	1.005586000
H	3.472740000	4.551720000	-0.481233000
C	-0.272997000	-2.621783000	0.917166000
H	-0.302887000	-2.969076000	-0.123423000
H	0.649382000	-3.005648000	1.391817000
H	-1.126839000	-3.086311000	1.451679000

**30:** E= -654.545210

Cu	0.125213000	-0.001849000	-0.122495000
C	2.011518000	-0.012351000	-0.446195000
C	2.583057000	-0.018669000	-1.831812000
O	2.976771000	-0.015211000	0.438442000
C	2.663549000	-0.010136000	1.860593000
N	-1.132751000	1.558876000	0.012463000
C	-1.800457000	2.520551000	0.049087000
C	-2.631357000	3.716665000	0.093643000
N	-1.151627000	-1.546819000	0.013222000
C	-1.832279000	-2.499295000	0.051892000
C	-2.678589000	-3.684493000	0.097626000
H	2.199585000	0.863860000	-2.379974000
H	3.686319000	-0.024777000	-1.854143000
H	2.189813000	-0.899375000	-2.375933000
H	1.570011000	0.004915000	2.007280000
H	3.112149000	-0.918162000	2.290073000
H	3.136649000	0.886158000	2.288322000
H	-3.171044000	3.766003000	1.055149000
H	-3.368355000	3.694669000	-0.727701000
H	-2.004802000	4.619133000	-0.011803000
H	-2.063302000	-4.584947000	0.267188000
H	-3.220037000	-3.796619000	-0.857698000
H	-3.414332000	-3.593604000	0.915264000

**TS2-Cu:** E= -1500.658383

Cu	1.413229000	0.094516000	-0.282440000
C	-0.956183000	0.533670000	1.608660000
O	-0.548746000	0.759891000	2.680657000
Cr	-1.826008000	0.218043000	-0.042437000
C	-3.120247000	-0.762228000	0.941209000
O	-3.917426000	-1.361001000	1.539673000
C	-0.946953000	-1.590447000	-0.359619000
C	-2.861090000	-0.078216000	-1.601813000
O	-3.518010000	-0.236054000	-2.551003000
C	-0.773019000	1.357401000	-1.130522000
O	-0.331657000	2.175796000	-1.846307000
C	-2.848056000	1.771314000	0.303401000
O	-3.474025000	2.726916000	0.531554000
O	-0.714287000	-2.366805000	0.700470000
C	-0.315829000	-3.768728000	0.590618000
C	-0.776689000	-2.268282000	-1.699888000
C	2.202651000	-0.315002000	-2.029614000
C	1.670659000	0.155211000	-3.349437000
O	3.355244000	-0.911665000	-2.234802000
C	4.145947000	-1.406928000	-1.116630000
H	0.706803000	-3.846364000	0.185996000
H	-0.344876000	-4.149303000	1.620329000
H	-1.022269000	-4.332866000	-0.038427000



H	0.158053000	-2.854479000	-1.778490000
H	-1.615615000	-2.978443000	-1.859115000
H	-0.811811000	-1.536825000	-2.517070000
H	1.739733000	1.261921000	-3.357717000
H	2.223355000	-0.250016000	-4.214526000
H	0.592729000	-0.060938000	-3.436558000
H	3.556005000	-1.368331000	-0.187780000
H	4.437860000	-2.435726000	-1.374441000
H	5.041155000	-0.770002000	-1.048313000
N	1.822976000	-0.904564000	1.542734000
C	2.010804000	-1.164289000	2.669530000
C	2.216872000	-1.466649000	4.080592000
H	1.366603000	-1.075814000	4.666241000
H	3.145995000	-0.992345000	4.440602000
H	2.290212000	-2.556343000	4.237454000
N	1.782942000	1.980302000	0.506638000
C	1.960382000	3.099867000	0.800208000
C	2.168141000	4.497151000	1.160757000
H	1.705315000	5.152269000	0.402530000
H	3.247363000	4.721181000	1.214328000
H	1.709411000	4.708573000	2.141969000

**33:** E= -1500.664969

Cu	0.971292000	-0.092665000	-0.214247000
C	-0.696036000	1.700000000	0.787994000
O	-0.283639000	2.606144000	1.402522000
Cr	-1.668240000	0.341306000	-0.103544000
C	-2.002646000	-0.319617000	1.643774000
O	-2.204479000	-0.680623000	2.731761000
C	-0.607689000	-1.466338000	-0.493929000
C	-3.029911000	-0.777692000	-0.782285000
O	-3.898084000	-1.446861000	-1.176395000
C	-1.186869000	0.987536000	-1.809124000
O	-0.899102000	1.389315000	-2.868253000
C	-3.064643000	1.591282000	-0.009451000
O	-3.934796000	2.363600000	0.031794000
O	-0.556922000	-2.342993000	0.545356000
C	-0.543138000	-3.784622000	0.349160000
H	0.364311000	-4.110649000	-0.187315000
H	-0.551614000	-4.206931000	1.363337000
H	-1.440807000	-4.114036000	-0.199176000
N	1.539212000	0.034668000	1.974154000
C	1.600424000	0.260232000	3.122191000
C	1.660598000	0.552597000	4.550272000
H	1.259308000	1.562859000	4.741340000
H	2.703188000	0.509219000	4.908788000
H	1.057169000	-0.180188000	5.112918000
N	1.869233000	1.834964000	-0.596900000
C	2.285244000	2.901782000	-0.840738000
C	2.789235000	4.237481000	-1.138329000
H	2.340107000	4.969309000	-0.444918000
H	2.525722000	4.519684000	-2.172238000
H	3.886746000	4.266774000	-1.027700000
C	-0.585076000	-2.113332000	-1.871288000
H	0.261176000	-2.812465000	-2.006445000
H	-1.509727000	-2.701800000	-2.035431000
H	-0.541011000	-1.352195000	-2.662527000
C	2.384204000	-1.100617000	-1.217588000
C	2.726214000	-0.712591000	-2.623496000
H	3.046820000	0.346983000	-2.608484000

H	3.514798000	-1.336107000	-3.079367000
H	1.812620000	-0.727757000	-3.245672000
O	3.179330000	-2.056677000	-0.818177000
C	3.076749000	-2.581208000	0.542535000
H	2.144685000	-2.236426000	1.012011000
H	3.121746000	-3.675927000	0.449367000
H	3.957540000	-2.216429000	1.091928000

**34:** E= -714.829738

Cu	-0.085994000	-0.099650000	0.211949000
C	1.794164000	0.327715000	0.306540000
O	2.480366000	0.343870000	-0.815094000
C	3.935933000	0.577431000	-0.863535000
H	4.461002000	-0.176209000	-0.256505000
H	4.199694000	0.473785000	-1.923311000
H	4.164019000	1.594031000	-0.506820000
N	-1.277323000	1.549154000	-0.029184000
C	-1.955625000	2.493202000	-0.175063000
C	-2.799111000	3.668016000	-0.356841000
H	-2.415613000	4.283838000	-1.188635000
H	-2.801033000	4.276335000	0.564155000
H	-3.834870000	3.362803000	-0.585017000
C	2.549156000	0.560891000	1.582918000
H	3.266217000	-0.267143000	1.765298000
H	3.146475000	1.494090000	1.547210000
H	1.862608000	0.611638000	2.441028000
C	-1.118137000	-1.734135000	0.384305000
C	-1.661825000	-2.222065000	1.693592000
H	-2.302370000	-1.433551000	2.133451000
H	-2.226358000	-3.166949000	1.612576000
H	-0.820248000	-2.351317000	2.401887000
O	-1.394921000	-2.593767000	-0.564954000
C	-0.965898000	-2.315341000	-1.930097000
H	-0.199524000	-1.521685000	-1.929826000
H	-0.564286000	-3.258511000	-2.327283000
H	-1.856125000	-2.010502000	-2.500978000

**35:** E= -847.548582

Cu	-0.082923000	0.012410000	0.207695000
C	-1.175189000	-1.485424000	-0.369615000
O	-2.385445000	-1.249314000	-0.839628000
C	-3.322900000	-2.320402000	-1.217179000
H	-3.512521000	-2.984149000	-0.359111000
H	-4.242561000	-1.798611000	-1.510791000
H	-2.918939000	-2.892449000	-2.067331000
N	0.150019000	1.425551000	-1.340653000
C	0.278681000	2.203218000	-2.206977000
C	0.438905000	3.173230000	-3.285504000
H	0.997847000	2.721424000	-4.123118000
H	0.991781000	4.057755000	-2.924733000
H	-0.549366000	3.497969000	-3.654333000
N	2.042103000	-0.745499000	-0.068298000
C	3.140830000	-1.131865000	-0.198203000
C	4.510287000	-1.612301000	-0.360279000
H	4.627295000	-2.106947000	-1.339749000
H	4.757001000	-2.336664000	0.434836000
H	5.218960000	-0.768399000	-0.302792000
C	-0.772580000	-2.925743000	-0.219850000
H	-1.414261000	-3.436522000	0.528609000

H	-0.884590000	-3.488582000	-1.168828000
H	0.272312000	-2.995738000	0.114327000
C	-0.004182000	0.844676000	1.970408000
C	1.085774000	0.581444000	2.968285000
H	2.037724000	0.959268000	2.547246000
H	0.904419000	1.042532000	3.954866000
H	1.222680000	-0.510601000	3.075391000
O	-0.899513000	1.645237000	2.504225000
C	-2.048027000	2.052823000	1.705982000
H	-2.174125000	1.364654000	0.853793000
H	-2.916489000	2.026590000	2.380031000
H	-1.867196000	3.082875000	1.362008000

**TS3-Cu:** E=-847.514527

N	1.511127000	-0.320198000	0.978190000
C	2.206061000	-0.364482000	1.921313000
C	3.070537000	-0.434761000	3.092867000
H	3.456079000	0.567482000	3.348021000
H	3.925224000	-1.103360000	2.890401000
H	2.507654000	-0.831823000	3.955345000
Cu	0.296865000	-0.533695000	-0.557532000
C	-1.394975000	0.878869000	-0.485548000
O	-2.108591000	0.843668000	0.612174000
C	-1.111675000	2.219037000	-1.099634000
C	-2.626800000	2.056428000	1.284414000
C	-1.294490000	-1.410825000	-1.172075000
O	-2.070546000	-1.998292000	-0.262324000
C	-1.844302000	-1.240869000	-2.573745000
C	-3.503534000	-2.197129000	-0.482400000
H	-0.584645000	2.098654000	-2.057268000
H	-2.042072000	2.798927000	-1.267478000
H	-0.468737000	2.830928000	-0.429925000
H	-3.131563000	1.685639000	2.185071000
H	-1.791482000	2.722787000	1.548911000
H	-3.340410000	2.571235000	0.622076000
H	-1.205402000	-0.553152000	-3.148843000
H	-1.779701000	-2.233658000	-3.066428000
H	-2.895952000	-0.909220000	-2.655236000
H	-3.863040000	-2.700564000	0.425099000
H	-4.011824000	-1.225646000	-0.603115000
H	-3.680040000	-2.835830000	-1.362778000
N	1.641535000	0.174262000	-2.101027000
C	2.418758000	0.220406000	-2.977785000
C	3.386625000	0.265587000	-4.068741000
H	4.057890000	1.133365000	-3.950010000
H	2.865252000	0.348350000	-5.037841000
H	3.994154000	-0.655964000	-4.071399000

**36:** E= -847.613412

C	-0.144222000	-2.438592000	1.482409000
C	-0.706371000	-1.630513000	0.333039000
Cu	0.339707000	0.324938000	0.168932000
N	-0.000664000	2.291991000	-0.022218000
O	-0.646744000	-2.160377000	-0.935907000
C	0.430985000	-3.059049000	-1.256678000
N	2.294132000	0.063481000	0.005609000
C	-1.566431000	-0.521903000	0.483313000
C	-2.121807000	-0.024901000	1.805365000
O	-2.248646000	-0.028326000	-0.629886000

C	-3.312491000	-0.880832000	-1.122984000
C	3.462695000	-0.005113000	-0.045086000
C	4.915786000	-0.088888000	-0.109741000
C	-0.323977000	3.402857000	-0.200599000
C	-0.728400000	4.784625000	-0.424223000
H	-0.223428000	-1.895668000	2.434908000
H	-0.714233000	-3.382696000	1.583164000
H	0.915633000	-2.702114000	1.333217000
H	0.290175000	-3.308402000	-2.318009000
H	1.411254000	-2.564846000	-1.121581000
H	0.388854000	-3.984295000	-0.655901000
H	-1.471592000	-0.237262000	2.668721000
H	-2.284118000	1.064183000	1.752451000
H	-3.105581000	-0.495371000	2.001416000
H	-3.814047000	-0.299593000	-1.910657000
H	-2.912183000	-1.817166000	-1.545264000
H	-4.037590000	-1.106571000	-0.318716000
H	5.248800000	-0.045734000	-1.161259000
H	5.264566000	-1.035704000	0.337639000
H	5.366966000	0.754371000	0.441355000
H	-0.129080000	5.227778000	-1.238084000
H	-0.576160000	5.376914000	0.494528000
H	-1.795494000	4.824158000	-0.703221000

**TS4-Cu:** E= -714.793877

N	-2.414285000	-0.342987000	-0.085057000
Cu	-0.567283000	-0.671130000	0.058722000
C	0.759835000	1.096892000	0.430860000
O	1.134739000	1.687418000	-0.671598000
C	0.456820000	1.944864000	1.629788000
C	1.266207000	3.159928000	-0.809368000
C	1.223117000	-1.256927000	0.171908000
O	1.898593000	-1.314552000	-0.970007000
C	1.968950000	-1.460563000	1.470982000
C	3.361938000	-1.263904000	-1.006222000
C	-3.575893000	-0.257624000	-0.217010000
C	-5.018894000	-0.171207000	-0.384099000
H	0.195287000	1.318327000	2.496051000
H	1.325575000	2.579233000	1.901435000
H	-0.390187000	2.635975000	1.431256000
H	1.560579000	3.317587000	-1.853997000
H	0.299294000	3.640172000	-0.595572000
H	2.045756000	3.524001000	-0.122591000
H	1.342508000	-1.163471000	2.326563000
H	2.146600000	-2.551608000	1.569665000
H	2.952302000	-0.962629000	1.550433000
H	3.619648000	-1.336725000	-2.070923000
H	3.721589000	-0.306821000	-0.592575000
H	3.794446000	-2.112469000	-0.452940000
H	-5.489608000	0.163040000	0.556812000
H	-5.425808000	-1.161203000	-0.655545000
H	-5.265904000	0.548581000	-1.183798000

**37:** E= -714.878879

N	-2.520992000	0.008775000	-0.031840000
Cu	-0.666648000	-0.167809000	0.193548000
C	1.446877000	0.560296000	0.421840000
O	1.676841000	1.218400000	-0.751995000
C	1.642432000	1.295098000	1.728472000

C	1.627761000	2.664249000	-0.775445000
C	1.262998000	-0.840184000	0.315844000
O	1.304066000	-1.459395000	-0.932176000
C	1.377040000	-1.824022000	1.469141000
C	2.571413000	-1.418946000	-1.645307000
C	-3.681778000	0.046278000	-0.182385000
C	-5.123011000	0.094086000	-0.367633000
H	1.369884000	0.671105000	2.590715000
H	2.710155000	1.568941000	1.834738000
H	1.054046000	2.225833000	1.781915000
H	1.834829000	2.936281000	-1.819391000
H	0.624734000	3.030321000	-0.490280000
H	2.395889000	3.105995000	-0.119247000
H	1.100666000	-1.401181000	2.447229000
H	0.737996000	-2.700657000	1.273129000
H	2.420152000	-2.190170000	1.537619000
H	2.448024000	-2.112836000	-2.488748000
H	2.793362000	-0.405592000	-2.014527000
H	3.387311000	-1.774783000	-0.990574000
H	-5.498771000	1.106336000	-0.137247000
H	-5.612270000	-0.632939000	0.303990000
H	-5.375918000	-0.154792000	-1.413129000

**Transmetallation to Rhodium:**

**40:** E= -874.537400

N	1.347580	1.203119	-0.142227
C	2.686600	1.046413	0.200149
C	2.896108	-0.289424	0.416459
N	1.679455	-0.930312	0.206615
C	0.698194	-0.019900	-0.157650
Rh	-1.102862	-0.389735	-0.563227
Cl	-2.048755	0.539560	1.281101
C	1.426923	-2.357522	0.388821
C	0.702301	2.479447	-0.445914
H	3.370993	1.890179	0.255305
H	3.796416	-0.832201	0.696067
H	0.329206	-2.486835	0.379423
H	1.881882	-2.948624	-0.425446
H	1.834443	-2.690017	1.358369
H	-0.370127	2.273337	-0.590940
H	0.834910	3.178603	0.396563
H	1.129915	2.917394	-1.364723

**41:** E= -1720.752811

N	2.947584000	-1.119167000	-0.741521000
C	3.870429000	-1.908245000	-0.060161000
C	3.587489000	-1.795159000	1.270703000
N	2.496256000	-0.936523000	1.379357000
C	2.075185000	-0.527151000	0.139588000
Rh	0.634050000	0.747529000	-0.322468000
C	-0.343587000	-0.706754000	-1.464506000
O	0.044085000	-1.100585000	-2.519163000
Cr	-1.721679000	-0.596712000	-0.039705000
C	-2.694982000	0.398149000	-1.334669000
O	-3.347305000	0.945323000	-2.131617000
C	-1.061685000	1.153515000	0.815729000

C	-3.202162000	-0.443288000	1.087993000
O	-4.116506000	-0.310711000	1.806246000
C	-0.918615000	-1.711407000	1.234291000
O	-0.498198000	-2.468960000	2.027255000
C	-2.398812000	-2.166759000	-0.805155000
O	-2.813364000	-3.152921000	-1.277690000
O	-1.150343000	2.239937000	-0.083620000
C	-0.853560000	3.608627000	0.333118000
Cl	2.332477000	2.390778000	-0.436315000
C	1.972509000	-0.466168000	2.660743000
C	3.015763000	-0.872635000	-2.187577000
C	-1.017982000	1.537557000	2.275656000
H	4.643200000	-2.466527000	-0.583077000
H	4.060980000	-2.235079000	2.144992000
H	0.203904000	3.702727000	0.633600000
H	-1.038040000	4.216767000	-0.563266000
H	-1.538967000	3.907760000	1.142646000
H	1.393023000	0.446882000	2.474618000
H	1.329926000	-1.231774000	3.122960000
H	2.817884000	-0.227738000	3.326050000
H	2.664883000	0.150052000	-2.387094000
H	4.068529000	-0.957755000	-2.498795000
H	2.393387000	-1.590924000	-2.740393000
H	-1.988083000	1.991511000	2.564714000
H	-0.886120000	0.637493000	2.893548000
H	-0.222355000	2.267098000	2.520184000

**42:** E= -1180.974601

Rh	-0.416888000	0.024317000	-0.002468000
C	-2.376198000	-0.277083000	-0.063560000
C	-0.634444000	1.788532000	0.450571000
C	1.683331000	0.184410000	0.051692000
Cl	0.094719000	-2.275937000	-0.593656000
O	-0.721207000	2.920804000	0.751889000
C	-3.061506000	-1.598433000	-0.282563000
O	-3.191441000	0.771684000	0.125031000
C	-4.641045000	0.647469000	0.122061000
N	2.518513000	-0.224251000	1.055385000
N	2.527966000	0.609288000	-0.938454000
C	2.049280000	-0.845676000	2.293370000
C	3.855714000	-0.080400000	0.692125000
C	3.862747000	0.448270000	-0.569714000
C	2.075429000	1.101819000	-2.238245000
H	-2.313321000	-2.369775000	-0.516551000
H	-3.608306000	-1.898483000	0.635630000
H	-3.807344000	-1.538970000	-1.100477000
H	-5.007285000	0.351784000	-0.875446000
H	-4.979143000	-0.081315000	0.877106000
H	-5.010865000	1.651183000	0.373908000
H	2.127580000	-1.943251000	2.221804000
H	0.989984000	-0.575863000	2.423364000
H	2.643600000	-0.474631000	3.144949000
H	4.672273000	-0.359690000	1.354310000
H	4.686189000	0.725447000	-1.224158000
H	2.484226000	2.108710000	-2.429811000
H	0.975265000	1.140602000	-2.211136000
H	2.392875000	0.412307000	-3.038614000