

Mechanism of Methyl Transfer Reaction Between CH₃Co(dmgbF₂)py and PPh₃Ni(triphos)

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1. Cartesian coordinates of molecules considered in the calculations

CH₃Ni(Tripfos)Acn-6Acn

Ni	2.198297000	-0.308144000	0.483339000
P	1.494617000	-2.367999000	0.227406000
P	1.297575000	-0.399585000	2.496228000
P	0.854116000	1.382445000	0.115032000
C	-0.647109000	-2.790146000	-1.570583000
H	-1.322796000	-2.523527000	-0.756304000
C	-1.185232000	-3.057903000	-2.832960000
H	-2.265201000	-2.993622000	-2.979467000
C	-0.347041000	-3.391948000	-3.900879000
H	-0.769293000	-3.596342000	-4.886614000
C	1.035685000	-3.467142000	-3.699119000
H	1.698943000	-3.726086000	-4.526947000
C	1.576876000	-3.197684000	-2.440893000
H	2.655908000	-3.258867000	-2.295789000
C	0.740722000	-2.861909000	-1.359738000
C	3.885777000	-3.373141000	1.265259000
H	4.065148000	-2.334744000	1.548430000
C	4.818763000	-4.364736000	1.585050000
H	5.727849000	-4.097998000	2.127561000
C	4.593695000	-5.687712000	1.194601000
H	5.326285000	-6.461104000	1.433323000
C	3.427953000	-6.020051000	0.492464000
H	3.248771000	-7.052889000	0.187016000
C	2.490970000	-5.032933000	0.179755000
H	1.584860000	-5.298989000	-0.367973000
C	2.717121000	-3.698598000	0.560419000
C	0.190631000	-2.698884000	1.508714000
H	-0.736146000	-2.201138000	1.189816000
H	-0.006381000	-3.777591000	1.587350000
C	0.680871000	-2.108081000	2.831194000
H	1.528212000	-2.695406000	3.214288000
H	-0.105173000	-2.092864000	3.600002000
C	2.786321000	1.426341000	3.954425000
H	2.467176000	2.139382000	3.190525000
C	3.657513000	1.844880000	4.960038000
H	3.998244000	2.881855000	4.982162000
C	4.101798000	0.936224000	5.928120000
H	4.787391000	1.262566000	6.712321000
C	3.665526000	-0.390746000	5.885269000
H	4.006852000	-1.105210000	6.636801000
C	2.790162000	-0.814591000	4.879681000
H	2.465160000	-1.855360000	4.865372000
C	2.336152000	0.092844000	3.909488000
C	-0.182060000	0.726834000	2.572033000
H	-0.975268000	0.245106000	3.161820000
H	0.136990000	1.628641000	3.113594000
C	-0.644419000	1.085541000	1.159624000
H	-1.332883000	1.941115000	1.156910000
H	-1.165620000	0.238702000	0.690579000
C	0.633573000	4.042248000	1.120816000
H	-0.439142000	3.871417000	1.224339000
C	1.170656000	5.276012000	1.498400000
H	0.514509000	6.051206000	1.899239000
C	2.542165000	5.519483000	1.361205000
H	2.957253000	6.484921000	1.656904000
C	3.379245000	4.523110000	0.848036000
H	4.450231000	4.704850000	0.738299000
C	2.846681000	3.283288000	0.486672000
H	3.499549000	2.494540000	0.111346000
C	1.470275000	3.033847000	0.614897000
C	0.615926000	2.767004000	-2.342037000
H	1.288189000	3.513018000	-1.914745000
C	0.159676000	2.918452000	-3.655353000

H	0.489817000	3.776387000	-4.244381000
C	-0.719731000	1.982672000	-4.208266000
H	-1.078550000	2.104904000	-5.231815000
C	-1.128346000	0.881916000	-3.445998000
H	-1.805045000	0.138061000	-3.871461000
C	-0.662655000	0.720792000	-2.140097000
H	-0.967605000	-0.158055000	-1.569577000
C	0.200434000	1.671640000	-1.567784000
C	2.822106000	-0.272794000	-1.419516000
H	3.627774000	-1.011929000	-1.515562000
H	3.216260000	0.730399000	-1.624122000
H	2.009260000	-0.505469000	-2.113719000
N	3.991900000	0.109666000	1.101989000
C	5.018545000	0.428638000	1.548465000
C	6.286774000	0.822842000	2.114875000
H	6.438141000	1.903905000	1.982302000
H	6.303187000	0.588163000	3.189229000
H	7.098745000	0.280285000	1.609844000
H	-3.603785000	0.141251000	3.270485000
C	-4.134613000	0.145289000	2.307781000
C	-3.672747000	-0.955131000	1.487664000
H	-5.213443000	0.047540000	2.493514000
N	-3.297601000	-1.833344000	0.820367000
H	-3.942761000	1.102464000	1.799362000
H	-1.674450000	4.697469000	-1.361751000
C	-2.635270000	4.179236000	-1.487333000
C	-3.150114000	3.773901000	-0.196563000
H	-3.347226000	4.853234000	-1.983712000
N	-3.556194000	3.436598000	0.841969000
H	-2.478924000	3.293932000	-2.120008000
H	-4.488705000	1.505153000	-2.326429000
N	-4.559109000	-1.604634000	-2.901142000
C	-4.486515000	-0.591942000	-2.330565000
C	-4.390414000	0.667315000	-1.621955000
H	-5.185064000	0.738360000	-0.866359000
H	-3.414671000	0.737402000	-1.122168000
H	1.296705000	-0.759841000	-4.622584000
C	3.376882000	-0.828771000	-4.842285000
C	2.115143000	-0.139525000	-5.014182000
N	4.392590000	-1.381786000	-4.702778000
H	2.128810000	0.811100000	-4.463661000
H	1.936066000	0.063507000	-6.079194000
H	4.628435000	1.991298000	-3.986761000
C	5.448928000	2.642429000	-2.169724000
C	4.518579000	2.814503000	-3.266782000
N	6.192767000	2.506622000	-1.283760000
H	3.487597000	2.815524000	-2.885062000
H	4.711324000	3.767408000	-3.779219000
H	6.424332000	-3.999579000	-2.347035000
C	6.469840000	-2.306258000	-1.111783000
C	5.741974000	-3.233341000	-1.953108000
N	7.054149000	-1.557479000	-0.437254000
H	4.952329000	-3.723438000	-1.365979000
H	5.283082000	-2.692935000	-2.795327000

PPH3-3Acn

P	3.624020000	1.072450000	-0.447044000
C	6.098667000	2.440657000	-0.831682000
H	6.297516000	2.266619000	0.226783000
C	7.005924000	3.186447000	-1.591935000
H	7.902611000	3.589651000	-1.116928000
C	6.771718000	3.411276000	-2.950922000
H	7.482345000	3.990249000	-3.543323000
C	5.616360000	2.891216000	-3.547069000
H	5.420535000	3.064740000	-4.607072000
C	4.703394000	2.159625000	-2.787057000
H	3.793440000	1.782461000	-3.258273000
C	4.938609000	1.911690000	-1.420372000
C	2.342418000	-1.319667000	-1.010087000
H	1.563284000	-0.894102000	-0.373162000
C	2.167988000	-2.587831000	-1.569285000
H	1.255965000	-3.151042000	-1.363452000
C	3.154797000	-3.128086000	-2.400800000
H	3.016197000	-4.114417000	-2.846715000
C	4.317585000	-2.395853000	-2.664462000

H	5.090377000	-2.811424000	-3.313971000
C	4.497610000	-1.130520000	-2.095519000
H	5.404752000	-0.563347000	-2.311518000
C	3.512583000	-0.579615000	-1.258446000
C	5.549850000	-0.275284000	1.196246000
H	5.887935000	-0.790322000	0.294918000
C	6.162009000	-0.550762000	2.420231000
H	6.973416000	-1.279810000	2.469889000
C	5.734249000	0.102698000	3.582205000
H	6.210410000	-0.117478000	4.539425000
C	4.696757000	1.036331000	3.513688000
H	4.360347000	1.549267000	4.416705000
C	4.080794000	1.309673000	2.287779000
H	3.270453000	2.040056000	2.232270000
C	4.501256000	0.656217000	1.118599000
N	0.877346000	1.835848000	-3.095298000
H	2.426819000	-0.739457000	-4.072920000
C	1.131212000	0.861730000	-3.681003000
C	1.457680000	-0.346477000	-4.411746000
H	1.512243000	-0.133724000	-5.488054000
H	0.689984000	-1.112120000	-4.236505000
N	2.524932000	-2.405939000	2.697542000
C	3.327414000	-2.922648000	2.030611000
H	4.441592000	-3.025473000	0.258796000
C	4.321585000	-3.575547000	1.201926000
H	5.287544000	-3.604162000	1.723838000
H	4.006467000	-4.602906000	0.973515000
H	3.392306000	4.617738000	-1.971430000
C	2.448874000	4.582146000	-1.408985000
C	2.721811000	4.635409000	0.012978000
N	2.941141000	4.681385000	1.156082000
H	1.821512000	5.434034000	-1.705623000
H	1.930007000	3.645579000	-1.663660000

Ni(Triphos)PPH3-3Acn

Ni	0.373577000	-0.026479000	-1.843902000
P	0.617987000	-1.877225000	-0.743174000
P	2.428441000	0.511362000	-1.391216000
P	-0.299263000	1.690882000	-0.708718000
P	-0.602335000	-0.266131000	-3.768909000
C	-1.595537000	-1.799823000	0.972530000
H	-1.646690000	-0.756234000	0.657291000
C	-2.523237000	-2.303280000	1.889703000
H	-3.291509000	-1.643158000	2.297452000
C	-2.466851000	-3.647159000	2.275295000
H	-3.192481000	-4.045794000	2.986683000
C	-1.474145000	-4.480008000	1.744425000
H	-1.419948000	-5.529761000	2.042361000
C	-0.543254000	-3.972608000	0.833183000
H	0.225015000	-4.629697000	0.420597000
C	-0.593437000	-2.624925000	0.439600000
C	0.179409000	-3.885414000	-2.626071000
H	-0.799820000	-3.411165000	-2.723649000
C	0.494460000	-4.984452000	-3.423479000
H	-0.240872000	-5.364784000	-4.135014000
C	1.758403000	-5.580231000	-3.332586000
H	2.011841000	-6.431516000	-3.967146000
C	2.694004000	-5.074469000	-2.426910000
H	3.682437000	-5.531816000	-2.346721000
C	2.369557000	-3.982367000	-1.613559000
H	3.113194000	-3.617437000	-0.903992000
C	1.108375000	-3.372264000	-1.702236000
C	2.064546000	-1.598885000	0.406974000
H	1.640788000	-1.003843000	1.231642000
H	2.429107000	-2.541859000	0.843116000
C	3.172999000	-0.822995000	-0.307601000
H	3.743939000	-1.495413000	-0.961476000
H	3.886580000	-0.372176000	0.398438000
C	4.466677000	-0.179571000	-3.202317000
H	4.247589000	-1.213382000	-2.926676000
C	5.394437000	0.059515000	-4.216900000
H	5.894011000	-0.783750000	-4.698561000
C	5.677472000	1.369034000	-4.621401000

H	6.399311000	1.556940000	-5.418012000
C	5.024081000	2.433534000	-3.993169000
H	5.234392000	3.461149000	-4.297167000
C	4.099147000	2.195114000	-2.972920000
H	3.602401000	3.048525000	-2.509957000
C	3.805189000	0.883319000	-2.551651000
C	2.409035000	1.984910000	-0.236563000
H	3.266008000	1.935991000	0.453245000
H	2.525960000	2.892950000	-0.844044000
C	1.071368000	2.051236000	0.508809000
H	0.934520000	3.031566000	0.990111000
H	1.013962000	1.281417000	1.292513000
C	0.496509000	3.536823000	-2.651940000
H	1.084640000	2.695746000	-3.026472000
C	0.572614000	4.783709000	-3.274587000
H	1.244763000	4.923959000	-4.123311000
C	-0.233596000	5.837484000	-2.832839000
H	-0.186762000	6.809764000	-3.327378000
C	-1.112581000	5.635655000	-1.762964000
H	-1.750722000	6.452293000	-1.418129000
C	-1.171064000	4.393118000	-1.124116000
H	-1.850120000	4.247836000	-0.281596000
C	-0.364090000	3.330334000	-1.561078000
C	-1.822946000	1.876699000	1.710569000
H	-0.894322000	2.062648000	2.251560000
C	-3.015147000	1.751444000	2.433183000
H	-3.001471000	1.853619000	3.520609000
C	-4.220036000	1.496920000	1.772579000
H	-5.147364000	1.397353000	2.339746000
C	-4.229882000	1.361708000	0.377937000
H	-5.164867000	1.154701000	-0.146812000
C	-3.040359000	1.467238000	-0.341586000
H	-3.044821000	1.313768000	-1.423480000
C	-1.821813000	1.731536000	0.312954000
C	0.100437000	1.576440000	-5.825925000
H	0.919883000	0.895370000	-6.063607000
C	-0.027571000	2.775357000	-6.534362000
H	0.695506000	3.019448000	-7.315739000
C	-1.078058000	3.653539000	-6.252119000
H	-1.178748000	4.587998000	-6.807281000
C	-1.995421000	3.327964000	-5.247560000
H	-2.813249000	4.011279000	-5.009467000
C	-1.860520000	2.137908000	-4.532562000
H	-2.577890000	1.901630000	-3.744355000
C	-0.818596000	1.238171000	-4.820075000
C	-2.802878000	-1.508321000	-2.561405000
H	-2.124803000	-1.576172000	-1.707812000
C	-4.106948000	-2.003317000	-2.470316000
H	-4.443009000	-2.477306000	-1.545534000
C	-4.978873000	-1.876342000	-3.555515000
H	-6.000911000	-2.254070000	-3.486874000
C	-4.539324000	-1.251301000	-4.728614000
H	-5.218032000	-1.141835000	-5.577033000
C	-3.234050000	-0.760854000	-4.817458000
H	-2.908182000	-0.258617000	-5.730123000
C	-2.346183000	-0.890395000	-3.734717000
C	-0.453369000	-2.259688000	-5.860398000
H	-1.543683000	-2.275000000	-5.883679000
C	0.263301000	-3.104316000	-6.713897000
H	-0.275397000	-3.765912000	-7.395780000
C	1.661544000	-3.106975000	-6.695673000
H	2.217663000	-3.767847000	-7.363484000
C	2.342121000	-2.266443000	-5.808380000
H	3.434067000	-2.264400000	-5.778530000
C	1.624531000	-1.440446000	-4.941286000
H	2.148733000	-0.811202000	-4.217974000
C	0.220441000	-1.416970000	-4.964256000
N	3.643137000	-0.077193000	6.110514000
C	3.732086000	0.109802000	4.964553000
C	3.822602000	0.338595000	3.536248000
H	4.595311000	1.086405000	3.315072000
H	4.072354000	-0.598712000	3.019707000
H	2.856473000	0.709439000	3.168025000
N	0.608573000	1.470141000	4.218876000
C	0.535301000	1.462627000	5.381309000
C	0.453629000	1.433781000	6.827279000

H	1.439098000	1.176310000	7.240581000
H	0.141516000	2.414188000	7.211848000
H	-0.272850000	0.670779000	7.139662000
N	-1.030203000	-1.717135000	6.109277000
H	1.514485000	-2.286225000	4.315323000
C	-0.356031000	-1.878130000	5.173236000
H	0.098840000	-2.883092000	3.388115000
C	0.483832000	-2.062404000	4.007441000
H	0.477259000	-1.142494000	3.407985000

CH3NiPPH3Acn-3Acn

Ni	2.256221000	-0.227481000	0.625035000
P	1.262518000	-2.163789000	0.426219000
P	1.270820000	-0.086986000	2.594426000
P	1.234283000	1.668782000	0.155950000
C	-0.894741000	-2.179878000	-1.395871000
H	-1.492314000	-1.696845000	-0.620870000
C	-1.471897000	-2.394989000	-2.651074000
H	-2.502759000	-2.078870000	-2.825680000
C	-0.729009000	-2.992388000	-3.673909000
H	-1.179217000	-3.154894000	-4.654869000
C	0.592387000	-3.384383000	-3.434994000
H	1.177843000	-3.852380000	-4.228569000
C	1.171519000	-3.175798000	-2.181710000
H	2.201454000	-3.489154000	-2.002926000
C	0.431958000	-2.575566000	-1.146536000
C	3.608459000	-3.471472000	1.213269000
H	4.008279000	-2.460118000	1.307316000
C	4.395630000	-4.582699000	1.532959000
H	5.421314000	-4.440243000	1.878211000
C	3.869003000	-5.870791000	1.408601000
H	4.482380000	-6.738913000	1.656659000
C	2.553216000	-6.049362000	0.962700000
H	2.140836000	-7.055194000	0.863727000
C	1.766318000	-4.942451000	0.642253000
H	0.743779000	-5.087890000	0.287237000
C	2.290914000	-3.644200000	0.767695000
C	-0.074726000	-2.290694000	1.708890000
H	-0.945601000	-1.719879000	1.356237000
H	-0.384610000	-3.337739000	1.834287000
C	0.465912000	-1.696536000	3.008514000
H	1.238197000	-2.355801000	3.430434000
H	-0.318048000	-1.556873000	3.766707000
C	2.774845000	1.708602000	4.094650000
H	2.453205000	2.451048000	3.361771000
C	3.668472000	2.087242000	5.096654000
H	4.018093000	3.120098000	5.143816000
C	4.123060000	1.145264000	6.026173000
H	4.825104000	1.440624000	6.807624000
C	3.675373000	-0.176177000	5.947657000
H	4.025769000	-0.917539000	6.667797000
C	2.778772000	-0.559659000	4.945829000
H	2.450394000	-1.598118000	4.901639000
C	2.309646000	0.382320000	4.016396000
C	-0.092285000	1.184102000	2.540419000
H	-0.991502000	0.761838000	3.011437000
H	0.233635000	2.031775000	3.158091000
C	-0.358533000	1.622828000	1.099934000
H	-0.895697000	2.581272000	1.052392000
H	-0.979315000	0.879711000	0.579575000
C	1.461249000	4.192892000	1.476282000
H	0.386572000	4.158314000	1.660606000
C	2.202273000	5.267542000	1.977550000
H	1.699586000	6.049874000	2.548974000
C	3.579361000	5.339884000	1.748806000
H	4.156149000	6.177197000	2.145280000
C	4.216046000	4.335503000	1.011041000
H	5.290811000	4.387070000	0.827560000
C	3.480873000	3.254606000	0.523102000
H	3.983850000	2.457296000	-0.026340000
C	2.095391000	3.171515000	0.750204000
C	0.798032000	3.394807000	-2.063364000
H	1.236084000	4.193776000	-1.463153000
C	0.334799000	3.666772000	-3.354432000
H	0.416437000	4.679097000	-3.754558000

C	-0.232786000	2.650420000	-4.129581000
H	-0.593557000	2.867452000	-5.136499000
C	-0.333408000	1.354603000	-3.611753000
H	-0.774802000	0.553427000	-4.207877000
C	0.135043000	1.078322000	-2.326780000
H	0.056374000	0.065037000	-1.929935000
C	0.694833000	2.097344000	-1.537833000
C	3.012318000	-0.437542000	-1.224114000
H	3.659814000	-1.325415000	-1.215066000
H	3.617420000	0.456933000	-1.423238000
H	2.237455000	-0.543940000	-1.990051000
N	4.045387000	0.029618000	1.346814000
C	5.031629000	0.326618000	1.889277000
C	6.233732000	0.714598000	2.591175000
H	6.509939000	1.744302000	2.321825000
H	6.055515000	0.668838000	3.675493000
H	7.064583000	0.042937000	2.334425000
H	-4.071839000	0.970535000	3.591316000
C	-4.641560000	0.595432000	2.730048000
C	-3.751071000	-0.043513000	1.783772000
H	-5.393853000	-0.122395000	3.084809000
N	-3.038642000	-0.546580000	1.012115000
H	-5.148683000	1.436877000	2.236285000
H	-2.410915000	2.816164000	-1.513682000
C	-3.171032000	2.034307000	-1.647484000
C	-4.322007000	2.296205000	-0.808044000
H	-3.469541000	2.003741000	-2.703575000
N	-5.246532000	2.491649000	-0.126967000
H	-2.737150000	1.061743000	-1.380097000
H	-7.426700000	-1.280823000	-0.920672000
N	-4.766796000	-0.941511000	-2.604020000
C	-5.513906000	-0.930817000	-1.710853000
C	-6.444025000	-0.909533000	-0.599418000
H	-6.071279000	-1.546725000	0.214126000
H	-6.551685000	0.119332000	-0.227921000

Co(dm^gBF₂)₂py-3Acn

Co	2.926131000	-0.628302000	-0.353738000
N	1.661736000	0.544405000	0.348047000
N	1.705428000	-1.980631000	-0.728990000
N	4.070299000	0.472739000	0.623640000
N	4.105351000	-2.061512000	-0.431132000
C	2.195338000	-3.191776000	-1.016209000
C	3.621069000	-3.241957000	-0.833661000
C	2.110444000	1.594623000	1.040158000
C	3.540870000	1.557761000	1.195474000
O	5.427597000	0.306625000	0.783495000
O	5.456220000	-2.029117000	-0.149545000
O	0.294040000	0.429184000	0.242068000
O	0.337822000	-1.854973000	-0.811373000
C	1.314963000	-4.324607000	-1.428700000
C	4.493286000	-4.441468000	-1.004874000
C	1.196474000	2.618869000	1.625306000
C	4.359983000	2.551075000	1.948122000
B	6.073109000	-0.664541000	-0.151742000
B	-0.185129000	-0.454544000	-0.864288000
H	1.743929000	3.527034000	1.902145000
H	0.697445000	2.238682000	2.532162000
H	0.405670000	2.880449000	0.909190000
H	3.841781000	3.514035000	2.027012000
H	4.564131000	2.194293000	2.971314000
H	5.326453000	2.703830000	1.450032000
H	0.709562000	-4.045156000	-2.303905000
H	1.901727000	-5.215461000	-1.676935000
H	0.607084000	-4.588972000	-0.627753000
H	3.951222000	-5.263483000	-1.485020000
H	4.871560000	-4.802000000	-0.034590000
H	5.373245000	-4.193572000	-1.615675000
F	0.091469000	0.131401000	-2.122412000
F	-1.572733000	-0.571789000	-0.670166000
F	6.115501000	-0.141769000	-1.463890000
F	7.373320000	-0.849862000	0.351511000
N	3.159154000	0.148997000	-2.187814000

C	3.228012000	1.484300000	-2.366770000
C	3.375982000	2.059551000	-3.625117000
C	3.458173000	1.230766000	-4.746788000
C	3.389921000	-0.151872000	-4.558402000
C	3.240694000	-0.653493000	-3.268980000
H	3.160966000	2.095376000	-1.463867000
H	3.424956000	3.144966000	-3.716467000
H	3.573439000	1.653171000	-5.745752000
H	3.450139000	-0.842971000	-5.399592000
H	3.182795000	-1.727283000	-3.076616000
H	5.392736000	-0.878890000	3.329310000
H	5.525017000	-2.248122000	2.200742000
C	5.669065000	-1.938953000	3.247112000
C	4.848266000	-2.738552000	4.131432000
N	4.172882000	-3.382211000	4.829333000
H	6.730454000	-2.051283000	3.507228000
H	0.745777000	-0.565018000	3.116193000
H	1.665493000	-1.940888000	3.793037000
C	1.752330000	-0.972900000	3.282470000
C	2.541281000	-0.063736000	4.085976000
N	3.189439000	0.657140000	4.732789000
H	2.227937000	-1.115306000	2.295114000
H	2.757145000	-3.939545000	1.568190000
H	2.353332000	-5.669262000	1.757299000
C	2.239276000	-4.672085000	2.204034000
H	2.704321000	-4.664153000	3.199919000
C	0.835798000	-4.324776000	2.302164000
N	-0.289497000	-4.035020000	2.381575000

CH3Co(DmgBF2)Py-3Aen

Co	3.005556000	-0.705353000	-0.431193000
N	1.758755000	0.576214000	0.156352000
N	1.778240000	-1.931073000	-1.166752000
N	4.203422000	0.419936000	0.483469000
N	4.224160000	-2.083310000	-0.833814000
C	2.268995000	-3.085885000	-1.553666000
C	3.716259000	-3.175223000	-1.358523000
C	2.237514000	1.572291000	0.867800000
C	3.682160000	1.475334000	1.068417000
O	5.511024000	0.143873000	0.697919000
O	5.529587000	-2.085025000	-0.477637000
O	0.416993000	0.467229000	0.013660000
O	0.435349000	-1.764041000	-1.164461000
C	1.458410000	-4.209736000	-2.094270000
C	4.496874000	-4.400752000	-1.675613000
C	1.419978000	2.681662000	1.431039000
C	4.447306000	2.446601000	1.896056000
B	6.180715000	-0.732698000	-0.337800000
B	-0.057303000	-0.338369000	-1.176390000
H	1.759273000	3.646150000	1.023378000
H	1.535439000	2.731199000	2.523620000
H	0.362611000	2.544891000	1.185322000
H	4.165970000	3.477422000	1.640764000
H	4.215693000	2.297343000	2.963058000
H	5.523683000	2.313590000	1.747677000
H	0.417751000	-3.901119000	-2.232365000
H	1.867588000	-4.550502000	-3.056554000
H	1.496025000	-5.062204000	-1.397946000
H	4.258839000	-4.757951000	-2.687402000
H	4.227112000	-5.203214000	-0.970495000
H	5.570544000	-4.202630000	-1.601079000
F	0.312029000	0.298746000	-2.365707000
F	-1.436200000	-0.429716000	-1.020277000
F	6.219376000	-0.075013000	-1.571932000
F	7.447602000	-0.988836000	0.175328000
C	2.653803000	-1.627908000	1.326522000
H	2.860173000	-0.925682000	2.140418000
H	1.599518000	-1.927160000	1.336707000
H	3.308140000	-2.502098000	1.405300000
N	3.311505000	0.237033000	-2.233114000
C	3.401096000	1.578973000	-2.303427000
C	3.594794000	2.255072000	-3.503893000
C	3.701507000	1.521983000	-4.685668000
C	3.610529000	0.131967000	-4.613448000

C	3.416000000	-0.470534000	-3.374566000
H	3.315625000	2.128484000	-1.367901000
H	3.658584000	3.342899000	-3.499317000
H	3.852973000	2.023141000	-5.642382000
H	3.687549000	-0.491605000	-5.503777000
H	3.341565000	-1.553281000	-3.292651000
H	4.544272000	-0.129485000	4.281570000
H	5.684034000	-0.520008000	2.956322000
C	5.408155000	-0.749572000	3.996506000
C	5.059143000	-2.149854000	4.116815000
N	4.768620000	-3.273932000	4.210472000
H	6.255718000	-0.512355000	4.654014000
H	-0.081867000	-0.092944000	2.475455000
H	-0.858628000	0.223764000	4.056004000
C	-0.009965000	-0.266062000	3.559469000
C	1.238528000	0.266116000	4.067758000
N	2.245226000	0.699367000	4.462216000
H	-0.061936000	-1.346948000	3.749051000
N	2.458718000	-5.850875000	0.831659000
C	2.186336000	-5.372340000	1.858076000
C	1.856367000	-4.776149000	3.136406000
H	1.106549000	-3.984881000	2.998675000
H	1.448637000	-5.538843000	3.814057000
H	2.760834000	-4.337661000	3.586110000

CH3Co(DmgBF2)2Py

Co	2.613050000	0.028471000	0.022098000
N	2.673450000	1.031977000	1.613511000
N	2.660940000	1.474039000	-1.181817000
N	2.347359000	-1.386837000	1.229173000
N	2.338829000	-0.944740000	-1.561118000
C	2.460879000	1.184649000	-2.449098000
C	2.265939000	-0.246851000	-2.671841000
C	2.481560000	0.364668000	2.730287000
C	2.285018000	-1.065770000	2.501509000
O	2.057213000	-2.658876000	0.875196000
O	2.055046000	-2.265048000	-1.618522000
O	2.755834000	2.380527000	1.670309000
O	2.739194000	2.774467000	-0.819138000
C	2.400472000	2.196956000	-3.538997000
C	1.967091000	-0.856674000	-3.996194000
C	2.432949000	0.986102000	4.082307000
C	1.995581000	-2.049500000	3.580164000
B	2.578162000	-3.103045000	-0.473043000
B	3.423709000	3.056193000	0.496779000
H	3.164138000	0.510522000	4.752348000
H	1.437845000	0.850097000	4.532901000
H	2.649340000	2.056694000	4.018191000
H	2.394918000	-1.709103000	4.542267000
H	0.907599000	-2.184722000	3.692675000
H	2.425213000	-3.026661000	3.327420000
H	2.682638000	3.183286000	-3.158186000
H	3.074666000	1.920540000	-4.362119000
H	1.382232000	2.256276000	-3.953790000
H	2.278723000	-0.199032000	-4.814880000
H	0.885124000	-1.039760000	-4.096488000
H	2.472815000	-1.826319000	-4.089980000
F	4.775112000	2.697247000	0.430683000
F	3.243067000	4.418435000	0.713827000
F	3.977290000	-3.108468000	-0.475173000
F	2.035627000	-4.367545000	-0.672264000
C	0.599355000	0.209940000	0.057663000
H	0.298959000	0.611796000	1.031731000
H	0.291872000	0.885534000	-0.748304000
H	0.177700000	-0.790376000	-0.094746000
N	4.647917000	-0.231117000	-0.026152000
C	5.335543000	-0.503402000	1.099376000
C	6.713974000	-0.692031000	1.106740000
C	7.418207000	-0.597596000	-0.093590000
C	6.706047000	-0.316311000	-1.259515000
C	5.327893000	-0.140636000	-1.185166000
H	4.762367000	-0.571849000	2.022161000
H	7.217936000	-0.909685000	2.048109000
H	8.499104000	-0.740229000	-0.119871000

H	7.203606000	-0.231203000	-2.225280000
H	4.748637000	0.079897000	-2.079962000

CH3Co(DmgBF2)2Acn

Co	0.465236000	-0.130739000	8.070055000
N	0.205499000	-1.997056000	8.029839000
N	-1.349228000	0.370461000	7.987971000
N	2.279252000	-0.644795000	7.985355000
N	0.715181000	1.737417000	7.946400000
C	-1.593905000	1.655371000	7.897675000
C	-0.373739000	2.463695000	7.866365000
C	1.289088000	-2.733270000	7.976706000
C	2.515310000	-1.933972000	7.944190000
O	3.308144000	0.220130000	7.841153000
O	1.919631000	2.335604000	7.808491000
O	-0.997236000	-2.605753000	7.930726000
O	-2.384802000	-0.492941000	7.893555000
C	-2.963683000	2.225448000	7.777912000
C	-0.385918000	3.945159000	7.719875000
C	1.272822000	-4.219533000	7.895547000
C	3.872443000	-2.537146000	7.841240000
B	3.099360000	1.605500000	8.409614000
B	-2.174452000	-1.856307000	8.511691000
H	2.169142000	-4.647403000	8.360280000
H	1.251218000	-4.546399000	6.843214000
H	0.376871000	-4.616439000	8.387146000
H	4.064777000	-3.198622000	8.699314000
H	3.954630000	-3.149793000	6.930950000
H	4.637223000	-1.755139000	7.815268000
H	-3.687352000	1.586054000	8.297329000
H	-3.003352000	3.239927000	8.191632000
H	-3.265644000	2.281076000	6.719368000
H	-0.863623000	4.234112000	6.771383000
H	0.634777000	4.338851000	7.738347000
H	-0.965201000	4.408206000	8.532313000
F	-2.039241000	-1.742350000	9.900030000
F	-3.291979000	-2.597278000	8.141889000
F	2.973300000	1.543513000	9.802101000
F	4.214608000	2.331686000	8.004660000
C	0.516086000	-0.130404000	6.065867000
H	0.578833000	-1.166423000	5.713725000
H	-0.394798000	0.349319000	5.689827000
H	1.405100000	0.435416000	5.763097000
N	0.472377000	-0.091507000	10.030727000
C	0.487967000	-0.056089000	11.188200000
C	0.509556000	-0.008473000	12.630764000
H	1.110758000	0.847735000	12.966816000
H	0.949426000	-0.933359000	13.028713000
H	-0.513636000	0.096134000	13.017184000

CH3Ni(Triphos)Acn-Co(dmgBF2)2Py

Ni	2.625181000	0.288246000	0.478417000
P	1.745112000	-1.613568000	-0.169721000
P	1.410450000	0.042615000	2.314279000
P	1.637134000	2.224094000	0.278083000
C	0.685404000	-0.948326000	-2.643329000
H	0.494769000	0.020193000	-2.176928000
C	0.281915000	-1.172685000	-3.959703000
H	-0.231894000	-0.381059000	-4.508426000
C	0.538129000	-2.406040000	-4.569206000
H	0.226946000	-2.581923000	-5.600422000
C	1.197472000	-3.411604000	-3.855239000
H	1.401048000	-4.374381000	-4.327780000
C	1.594094000	-3.193337000	-2.532042000
H	2.099717000	-3.984991000	-1.976764000

C	1.334407000	-1.960066000	-1.915840000
C	4.054714000	-3.102125000	0.245802000
H	4.546317000	-2.255829000	-0.236325000
C	4.817007000	-4.171021000	0.718477000
H	5.900903000	-4.162212000	0.589648000
C	4.194792000	-5.241753000	1.370195000
H	4.791634000	-6.070962000	1.753912000
C	2.806239000	-5.245179000	1.529762000
H	2.314262000	-6.078159000	2.035188000
C	2.039154000	-4.182583000	1.042434000
H	0.956142000	-4.210179000	1.170018000
C	2.656556000	-3.097032000	0.399606000
C	0.089612000	-1.729728000	0.641110000
H	-0.548474000	-1.004235000	0.114077000
H	-0.361436000	-2.718989000	0.488091000
C	0.218639000	-1.370839000	2.118532000
H	0.621303000	-2.215509000	2.694359000
H	-0.750260000	-1.099910000	2.561696000
C	2.928748000	-1.570775000	3.983514000
H	2.791084000	-2.332066000	3.212162000
C	3.734250000	-1.856601000	5.085902000
H	4.198896000	-2.840325000	5.173501000
C	3.955375000	-0.882609000	6.066196000
H	4.588386000	-1.105208000	6.926746000
C	3.363424000	0.376572000	5.937217000
H	3.531984000	1.142124000	6.696560000
C	2.553251000	0.666273000	4.835218000
H	2.108342000	1.658134000	4.753219000
C	2.316965000	-0.309259000	3.854221000
C	0.365432000	1.540995000	2.596301000
H	-0.544707000	1.273463000	3.152404000
H	0.945626000	2.254783000	3.198076000
C	0.049880000	2.149450000	1.230416000
H	-0.385881000	3.153408000	1.321178000
H	-0.666263000	1.517270000	0.683219000
C	1.912327000	4.961601000	0.945638000
H	1.026540000	5.129400000	0.328902000
C	2.506173000	6.032209000	1.615220000
H	2.080033000	7.033080000	1.523944000
C	3.645395000	5.823547000	2.403249000
H	4.107469000	6.663176000	2.925686000
C	4.190010000	4.542069000	2.517878000
H	5.078603000	4.376194000	3.129832000
C	3.597503000	3.467631000	1.846000000
H	4.014930000	2.462442000	1.928363000
C	2.456093000	3.670008000	1.058174000
C	2.118061000	3.553655000	-2.134721000
H	3.080968000	3.821874000	-1.696138000
C	1.823959000	3.933167000	-3.445445000
H	2.563020000	4.489544000	-4.025040000
C	0.589224000	3.601001000	-4.014361000
H	0.362081000	3.898540000	-5.039728000
C	-0.353754000	2.892947000	-3.263747000
H	-1.325667000	2.631642000	-3.685817000
C	-0.061210000	2.509651000	-1.951991000
H	-0.816897000	1.961253000	-1.389395000
C	1.175068000	2.839907000	-1.373080000
C	3.536227000	0.558230000	-1.292657000
H	4.173725000	-0.316327000	-1.479409000
H	4.162631000	1.456097000	-1.201573000
H	2.819122000	0.680754000	-2.111232000
H	-3.109721000	4.723176000	2.599307000
H	-1.930988000	3.619170000	3.341325000
H	-3.643587000	3.468259000	3.751639000
H	-3.100379000	5.193423000	0.580437000
C	-2.950589000	3.690070000	2.927982000
C	-3.044687000	4.414353000	-0.187731000
H	-2.075129000	4.508771000	-0.703633000
H	-3.825009000	4.599848000	-0.939719000
C	-3.153023000	2.726861000	1.805811000
C	-3.199615000	3.053894000	0.405618000
O	-3.123012000	0.980516000	3.309528000
N	-3.261364000	1.409562000	2.005107000
H	-5.734714000	2.317337000	1.022498000
H	-8.233065000	2.360194000	1.062395000
F	-3.324907000	-0.665138000	4.912512000

B	-3.733125000	-0.351732000	3.603811000
N	-3.339814000	1.959839000	-0.350283000
F	-5.143318000	-0.279255000	3.525524000
C	-6.317800000	1.416953000	0.815997000
C	-7.709116000	1.431008000	0.836667000
O	-3.338339000	2.165671000	-1.711107000
Co	-3.603923000	0.338843000	0.525455000
N	-5.611691000	0.300710000	0.542469000
O	-3.220596000	-1.475461000	2.757012000
C	-8.405494000	0.250173000	0.567670000
H	-9.495982000	0.230500000	0.577263000
N	-3.267130000	-1.270202000	1.395036000
B	-3.817395000	1.020338000	-2.546393000
F	-5.222350000	0.889330000	-2.445361000
F	-3.448522000	1.352165000	-3.864776000
C	-6.281775000	-0.840476000	0.281355000
C	-7.671835000	-0.904765000	0.285645000
N	-3.242208000	-0.719195000	-0.961725000
O	-3.145847000	-0.282722000	-2.265528000
C	-3.109771000	-2.359362000	0.637178000
H	-5.670243000	-1.718843000	0.062632000
H	-8.165836000	-1.852228000	0.068561000
C	-3.075462000	-2.030575000	-0.763642000
H	-2.049667000	-3.770612000	1.867835000
H	-3.803104000	-3.966527000	1.874672000
C	-2.946135000	-3.719428000	1.230008000
H	-1.758057000	-2.889488000	-2.230277000
C	-2.800729000	-2.980249000	-1.881872000
H	-2.859286000	-4.485880000	0.452288000
H	-3.446470000	-2.756329000	-2.741872000
H	-2.966654000	-4.018785000	-1.573713000
H	6.813574000	-1.600069000	2.443707000
C	5.299677000	-0.233146000	1.969271000
C	6.463133000	-0.601873000	2.743472000
N	4.346545000	0.051083000	1.364235000
H	6.200258000	-0.625471000	3.811114000
H	7.274578000	0.122749000	2.588716000

CH3Co(DmgBF2)2Acn

Co	0.464277000	-0.129408000	8.071807000
N	0.204977000	-1.995651000	8.032632000
N	-1.350807000	0.372018000	7.990027000
N	2.279013000	-0.643910000	7.988201000
N	0.714065000	1.737280000	7.943244000
C	-1.595220000	1.656870000	7.896219000
C	-0.374476000	2.464267000	7.864010000
C	1.288317000	-2.732106000	7.977506000
C	2.514718000	-1.933206000	7.946314000
O	3.308568000	0.220638000	7.846746000
O	1.918520000	2.334732000	7.802054000
O	-0.997626000	-2.604519000	7.933570000
O	-2.386050000	-0.491982000	7.897880000
C	-2.964788000	2.226429000	7.771667000
C	-0.384555000	3.945675000	7.717519000
C	1.270058000	-4.218155000	7.893613000
C	3.872006000	-2.536312000	7.843349000
B	3.097418000	1.608397000	8.408963000
B	-2.173581000	-1.854858000	8.516996000
H	2.170896000	-4.648116000	8.347316000
H	1.235517000	-4.543081000	6.841008000
H	0.379256000	-4.615373000	8.394430000
H	4.058659000	-3.210267000	8.692794000
H	3.959085000	-3.135808000	6.924668000
H	4.637721000	-1.754816000	7.832888000
H	-3.690739000	1.585297000	8.285643000
H	-3.007923000	3.239994000	8.187333000
H	-3.260925000	2.284527000	6.711616000
H	-0.824594000	4.234593000	6.750702000
H	0.633888000	4.341716000	7.775242000
H	-0.996498000	4.406700000	8.506465000
F	-2.033921000	-1.739677000	9.904902000
F	-3.292042000	-2.596114000	8.150989000
F	2.968080000	1.552878000	9.801574000

F	4.213205000	2.333157000	8.003141000
C	0.514022000	-0.132523000	6.067015000
H	0.577377000	-1.169283000	5.717284000
H	-0.397498000	0.345612000	5.690547000
H	1.402039000	0.433864000	5.762583000
N	0.472572000	-0.089321000	10.032524000
C	0.491054000	-0.057831000	11.190063000
C	0.516445000	-0.015942000	12.632715000
H	1.107558000	0.846486000	12.970723000
H	0.969568000	-0.936764000	13.025238000
H	-0.506804000	0.073521000	13.022779000

CH3Ni(Triphos)Co(dmgbF2)2Py

Ni	2.118638000	0.175579000	0.248839000
P	1.614608000	-1.903642000	-0.068930000
P	1.191944000	-0.040846000	2.229105000
P	1.637407000	2.284129000	0.442610000
C	0.290971000	-1.673767000	-2.492300000
H	-0.146810000	-0.774874000	-2.052992000
C	-0.071141000	-2.052757000	-3.784674000
H	-0.794449000	-1.450627000	-4.336785000
C	0.486790000	-3.199731000	-4.360805000
H	0.207176000	-3.492952000	-5.374238000
C	1.402585000	-3.969565000	-3.637453000
H	1.839633000	-4.864538000	-4.084008000
C	1.761371000	-3.599761000	-2.337392000
H	2.472810000	-4.205774000	-1.774158000
C	1.203017000	-2.451407000	-1.757788000
C	4.175595000	-2.816576000	0.467416000
H	4.483321000	-1.889280000	-0.021457000
C	5.134751000	-3.692533000	0.978174000
H	6.194945000	-3.452945000	0.881077000
C	4.734921000	-4.866470000	1.625445000
H	5.483790000	-5.546302000	2.035296000
C	3.375182000	-5.167579000	1.750541000
H	3.060816000	-6.081825000	2.256811000
C	2.412120000	-4.299144000	1.229940000
H	1.354966000	-4.549867000	1.330275000
C	2.807107000	-3.116655000	0.585498000
C	0.033550000	-2.146155000	0.857844000
H	-0.715275000	-1.574145000	0.290126000
H	-0.281153000	-3.199224000	0.840217000
C	0.162739000	-1.592986000	2.277728000
H	0.695205000	-2.298772000	2.930572000
H	-0.820142000	-1.387184000	2.725421000
C	3.617355000	-0.615725000	3.463225000
H	3.959451000	-0.841538000	2.451010000
C	4.490434000	-0.758091000	4.544023000
H	5.514601000	-1.094098000	4.372462000
C	4.053730000	-0.462712000	5.839044000
H	4.736787000	-0.568639000	6.683612000
C	2.740141000	-0.030729000	6.052722000
H	2.396358000	0.198096000	7.062984000
C	1.862610000	0.109834000	4.975033000
H	0.838789000	0.443532000	5.154940000
C	2.298959000	-0.180847000	3.672137000
C	0.107054000	1.429010000	2.571620000
H	-0.882043000	1.113829000	2.931953000
H	0.594083000	2.008269000	3.368786000
C	-0.004683000	2.265569000	1.293445000
H	-0.347532000	3.289261000	1.497933000
H	-0.719631000	1.802728000	0.596980000
C	2.282165000	4.559505000	1.986682000
H	1.329992000	4.980476000	1.657270000
C	3.090079000	5.282162000	2.865455000
H	2.763383000	6.260603000	3.221830000
C	4.313963000	4.752115000	3.291899000
H	4.940993000	5.318639000	3.982561000
C	4.732352000	3.499500000	2.835065000
H	5.685012000	3.083342000	3.167003000
C	3.925500000	2.773272000	1.954967000
H	4.243636000	1.790636000	1.600901000
C	2.696529000	3.297398000	1.527004000

C	2.252431000	4.288681000	-1.446406000
H	3.084558000	4.561286000	-0.795434000
C	2.060387000	4.968447000	-2.652764000
H	2.748302000	5.766563000	-2.937605000
C	0.993292000	4.629158000	-3.489679000
H	0.843812000	5.163482000	-4.429496000
C	0.117589000	3.602391000	-3.119812000
H	-0.719698000	3.330192000	-3.764776000
C	0.309209000	2.914464000	-1.921158000
H	-0.383045000	2.112558000	-1.657630000
C	1.370513000	3.264936000	-1.067513000
C	2.919326000	0.397931000	-1.561354000
H	3.412015000	-0.520460000	-1.911314000
H	3.647103000	1.223498000	-1.523506000
H	2.119448000	0.662434000	-2.267918000
H	-3.185710000	4.890802000	2.083890000
H	-2.205661000	3.825916000	3.117050000
H	-3.965324000	3.807125000	3.271086000
H	-3.232260000	5.136809000	0.002978000
C	-3.145010000	3.897611000	2.544658000
C	-2.893159000	4.293156000	-0.609430000
H	-1.827386000	4.448622000	-0.844010000
H	-3.435901000	4.303245000	-1.564113000
C	-3.234442000	2.819828000	1.516531000
C	-3.113028000	2.994917000	0.092973000
O	-3.400736000	1.250822000	3.192561000
N	-3.379710000	1.532377000	1.842884000
H	-5.669309000	2.404321000	0.521016000
H	-8.156044000	2.532489000	0.315932000
F	-3.731212000	-0.225878000	4.931387000
B	-4.017334000	-0.060544000	3.564784000
N	-3.164341000	1.823151000	-0.550040000
F	-5.414121000	-0.027792000	3.345576000
C	-6.268667000	1.505573000	0.358309000
C	-7.654110000	1.567339000	0.242716000
O	-2.958908000	1.865177000	-1.912096000
Co	-3.586134000	0.313922000	0.454996000
N	-5.589664000	0.343593000	0.276807000
O	-3.411944000	-1.250920000	2.891220000
C	-8.372554000	0.387530000	0.034658000
H	-9.459036000	0.404685000	-0.059763000
N	-3.390343000	-1.201443000	1.513021000
B	-3.484714000	0.694245000	-2.679043000
F	-4.899667000	0.716852000	-2.701104000
F	-2.966011000	0.844759000	-3.978839000
C	-6.280494000	-0.796787000	0.075795000
C	-7.666325000	-0.814756000	-0.049712000
N	-3.183363000	-0.916590000	-0.881744000
O	-2.990692000	-0.638249000	-2.215886000
C	-3.265804000	-2.376220000	0.888646000
H	-5.690471000	-1.714254000	0.015645000
H	-8.178071000	-1.763825000	-0.211582000
C	-3.145009000	-2.208410000	-0.536101000
H	-2.311057000	-3.727670000	2.265209000
H	-4.075889000	-3.766077000	2.303599000
C	-3.210355000	-3.669302000	1.631663000
H	-1.892638000	-3.358649000	-1.856325000
C	-2.944241000	-3.301361000	-1.532316000
H	-3.198938000	-4.522549000	0.944863000
H	-3.544388000	-3.109019000	-2.432353000
H	-3.228167000	-4.274788000	-1.116468000

Ni(Triphos)

Ni	2.269717000	0.150444000	0.918907000
P	1.713240000	-1.765682000	0.174859000
P	1.385923000	-0.135705000	2.841488000
P	1.218404000	1.963855000	0.546165000
C	0.691509000	-1.003496000	-2.310615000
H	0.887708000	0.003257000	-1.933362000
C	0.119894000	-1.190271000	-3.572728000
H	-0.139004000	-0.322552000	-4.183673000
C	-0.106577000	-2.484730000	-4.052324000
H	-0.542612000	-2.634873000	-5.041939000

C	0.233714000	-3.589172000	-3.261682000
H	0.061195000	-4.601211000	-3.634318000
C	0.793252000	-3.401083000	-1.994583000
H	1.056960000	-4.266881000	-1.382898000
C	1.026278000	-2.104233000	-1.507455000
C	3.984118000	-3.297516000	-0.321143000
H	4.200628000	-2.512897000	-1.051493000
C	4.888326000	-4.344056000	-0.140235000
H	5.804236000	-4.378722000	-0.733810000
C	4.627048000	-5.343084000	0.806776000
H	5.338059000	-6.157597000	0.956334000
C	3.450901000	-5.288531000	1.559108000
H	3.237408000	-6.063637000	2.298169000
C	2.537048000	-4.245949000	1.366952000
H	1.619930000	-4.231847000	1.957682000
C	2.790353000	-3.236895000	0.423719000
C	0.190565000	-2.114595000	1.206105000
H	-0.597266000	-1.508217000	0.734135000
H	-0.117604000	-3.167871000	1.107260000
C	0.379687000	-1.711590000	2.673377000
H	0.951369000	-2.480348000	3.213481000
H	-0.587525000	-1.603282000	3.189657000
C	2.974661000	-1.352579000	4.766159000
H	3.273364000	-1.990077000	3.928093000
C	3.552626000	-1.546922000	6.020232000
H	4.286349000	-2.343314000	6.161596000
C	3.204573000	-0.713425000	7.091647000
H	3.664114000	-0.856180000	8.071307000
C	2.267912000	0.304791000	6.894171000
H	1.988394000	0.958535000	7.723242000
C	1.674655000	0.489404000	5.640037000
H	0.934873000	1.281485000	5.517771000
C	2.016577000	-0.339272000	4.556968000
C	0.117391000	1.221347000	2.999743000
H	-0.753015000	0.902812000	3.594755000
H	0.608932000	2.046711000	3.538616000
C	-0.303534000	1.710485000	1.608839000
H	-0.890352000	2.640000000	1.675270000
H	-0.923100000	0.952328000	1.105965000
C	1.259906000	4.810437000	0.891983000
H	0.429567000	4.853359000	0.183642000
C	1.743845000	5.987700000	1.468797000
H	1.287716000	6.945978000	1.211250000
C	2.809764000	5.940813000	2.375179000
H	3.186658000	6.861781000	2.824143000
C	3.392681000	4.711591000	2.700211000
H	4.227087000	4.669493000	3.403298000
C	2.912495000	3.535175000	2.117169000
H	3.361861000	2.567512000	2.360370000
C	1.839594000	3.571598000	1.211786000
C	1.424613000	2.827565000	-2.088256000
H	2.495153000	2.842564000	-1.864801000
C	0.982551000	3.125848000	-3.376302000
H	1.705177000	3.391872000	-4.150455000
C	-0.384368000	3.066691000	-3.681228000
H	-0.731103000	3.283426000	-4.693217000
C	-1.298386000	2.725616000	-2.681959000
H	-2.365443000	2.678673000	-2.909437000
C	-0.855797000	2.445007000	-1.383530000
H	-1.589725000	2.187712000	-0.619235000
C	0.512712000	2.487143000	-1.070285000

CH3Ni(triphos)Acn

Ni	2.205153000	-0.072968000	0.528223000
P	1.126348000	-1.949148000	0.220619000
P	1.219267000	-0.012551000	2.505226000
P	1.284314000	1.896378000	0.194506000
C	-0.942535000	-1.897648000	-1.702182000
H	-1.572818000	-1.444781000	-0.935509000
C	-1.462018000	-2.076387000	-2.987367000
H	-2.487887000	-1.769721000	-3.201001000
C	-0.673190000	-2.643650000	-3.992472000

H	-1.079489000	-2.782202000	-4.996221000
C	0.638513000	-3.036282000	-3.704658000
H	1.261016000	-3.480809000	-4.483817000
C	1.159334000	-2.861429000	-2.421212000
H	2.182180000	-3.176067000	-2.206266000
C	0.371751000	-2.293904000	-1.403570000
C	3.301885000	-3.416873000	1.190057000
H	3.741486000	-2.434706000	1.372278000
C	3.990972000	-4.581688000	1.544281000
H	4.977721000	-4.509809000	2.006284000
C	3.417281000	-5.832891000	1.303530000
H	3.954798000	-6.743228000	1.576686000
C	2.151544000	-5.919900000	0.709354000
H	1.701445000	-6.896794000	0.520909000
C	1.462078000	-4.758801000	0.356943000
H	0.476708000	-4.832187000	-0.108488000
C	2.036107000	-3.498101000	0.594917000
C	-0.279582000	-2.026029000	1.431396000
H	-1.069549000	-1.346229000	1.080130000
H	-0.694335000	-3.043307000	1.474660000
C	0.263896000	-1.568994000	2.784808000
H	0.953834000	-2.324842000	3.186706000
H	-0.533073000	-1.401572000	3.523770000
C	2.838475000	1.521074000	4.168401000
H	2.549332000	2.360347000	3.532812000
C	3.768313000	1.731704000	5.187095000
H	4.178741000	2.731236000	5.343694000
C	4.180208000	0.665796000	5.994639000
H	4.909684000	0.830286000	6.789904000
C	3.656322000	-0.611229000	5.775420000
H	3.974702000	-1.449269000	6.398529000
C	2.724483000	-0.826417000	4.755670000
H	2.338408000	-1.833898000	4.597811000
C	2.295076000	0.241365000	3.951560000
C	-0.032968000	1.365429000	2.559178000
H	-0.947174000	0.996994000	3.046797000
H	0.382094000	2.159573000	3.194732000
C	-0.304396000	1.886814000	1.147019000
H	-0.785468000	2.875511000	1.155184000
H	-0.964903000	1.202347000	0.594108000
C	1.651119000	4.343097000	1.615355000
H	0.574375000	4.363052000	1.790411000
C	2.447925000	5.355963000	2.157502000
H	1.985669000	6.146828000	2.751705000
C	3.829063000	5.357720000	1.939486000
H	4.449037000	6.148493000	2.366439000
C	4.413967000	4.343235000	1.173391000
H	5.491550000	4.340182000	0.997117000
C	3.622194000	3.322263000	0.645364000
H	4.083766000	2.518048000	0.070305000
C	2.232903000	3.312696000	0.859750000
C	1.163503000	3.662321000	-2.031741000
H	1.782823000	4.353073000	-1.457325000
C	0.753191000	4.007377000	-3.323831000
H	1.059161000	4.965475000	-3.749143000
C	-0.047072000	3.134292000	-4.066865000
H	-0.366119000	3.407360000	-5.074643000
C	-0.433548000	1.906325000	-3.516362000
H	-1.052597000	1.214539000	-4.091719000
C	-0.016829000	1.555309000	-2.232130000
H	-0.300357000	0.586002000	-1.816860000
C	0.775584000	2.435021000	-1.474581000
C	2.908085000	-0.160790000	-1.350905000
H	3.496318000	-1.084670000	-1.443648000
H	3.560686000	0.711065000	-1.495742000
H	2.099456000	-0.153291000	-2.089965000
N	4.013319000	0.027548000	1.243605000
C	5.031739000	0.217183000	1.775465000
C	6.280261000	0.471578000	2.456688000
H	6.633429000	1.487314000	2.225009000
H	6.131043000	0.386290000	3.543199000
H	7.044226000	-0.253494000	2.141393000

Table S1.. Total energies of molecules considered in the calculations

	BP86	BP86-D3Bj	PBE	PBE-D3BJ	PBE-D3BJ	PBE-D3BJ	PBE-D4	PBE-SCNL
	ENERGY	ENERGY	ENERGY	ENERGY	GIBBS ENERGY	GIBBS ENER- SCAL	ENERGY	ENERGY
acn	-132,8078107	-132,8119348	-132,6387351	-132,641543	-132,621598	-132,6078715	-132,6443	-132,5597166
codmg-acn	-2797,866398	-2797,952152	-2795,850641	-2795,903416	-2795,689638	-2795,670827	-2795,91959	-2795,114146
codmg-acn-r	-2797,701109	-2797,79698	-2795,700279	-2795,753434	-2795,689638		-2795,76747	-2794,963897
codmg	-2665,043769	-2665,115229	-2663,194231	-2663,238207	-2663,063689	-2663,045075	-2663,2508	-2662,527696
codmg-met-acn	-2837,626714	-2837,726506	-2835,556509	-2835,618231	-2835,367075	-2835,348234	-2835,63477	-2834,799153
codmg-met-acn-m	-2837,84854	-2837,846858	-2835,742719	-2835,745868			-2835,75188	-2834,914384
codmg-met	-2704,797632	-2704,882271	-2702,893056	-2702,945279	-2702,73138	-2702,712706	-2951,07211	-2950,16329
codmg-met-m	-2704,95122	-2705,035207	-2703,042443	-2703,094088			-2951,18947	-2950,277862
codmgpy-	-2913,433665	-2913,541151	-2911,273759	-2911,339836	-2911,082064	-2911,063105	-2911,35722	-2910,478473
codmgpy-met	-2953,192993	-2953,315397	-2950,978602	-2951,054263	-2950,760066	-2950,741064	-2951,0721	-2950,163274
codmgpy-met-m	-2953,315865	-2953,43605	-2951,096881	-2951,171167	-2950,881761	-2950,862759	-2951,18947	-2950,277861
codmgpy-r	-2913,279364	-2913,38739	-2911,124029	-2911,190431	-2910,933619	-2910,914661	-2911,20585	-2910,328975
codmg-r	-2664,88662	-2664,958314		-2663,086146			-2663,09638	-2662,375795
codmg-t								
nip3-0	-3848,76939	-3848,984919	-3846,018213	-3846,14546	-3845,664212	-3845,644514	-3846,15891	-3844,98609
nip3+	-3848,632893	-3848,848085	-3845,885591	-3846,013054	-3845,528584	-3845,508903	-3846,02592	-3844,854511
nip3-met-acn	-4021,373482	-4021,629429	-4018,402225	-4018,554394	-4017,993995	-4017,97421	-4018,57272	-4017,286332
nip3-met	-3888,560248	-3888,795397	-3885,75407	-3885,892082	-3885,373481	-3885,353797	-3885,90945	-3884,704301
nip4	-4885,355445	-4885,719689	-4881,529208	-4881,746253	-4881,015856	-4880,995586	-4881,76891	-4880,074307
nip4-p	-4885,206526	-4885,57741	-4881,38456	-4881,603381	-4880,871139	-4880,850869	-4881,62655	-4879,93363
PPh3	-1036,555136	-1036,636485	-1035,469844	-1035,519604	-1035,301409	-1035,283275	-1035,52726	-1035,00602
Met	-39,8509738	-39,85210465	-39,78801963	-39,78886796	-39,779709	-39,76828475	-39,7893726	-39,75440168
Py	-248,3666269	-248,3819298	-248,0521125	-248,0620265	-248,003394	-247,9880532	-248,064567	-247,9068591

Table S2.Reaction energies in kcal/mol. Entries *b* and *d* are redox potentials in Volts..

Reaction	BP86 ΔE	BP86-D3BJ ΔE	PBE ΔE	PBE-D3BJ ΔE	ΔG	PBE-D4 ΔE	PBE-SCNL ΔE
Total reaction energy							
4	0.4	-38.9	-6.4	-30.7	-22.88	-29.5	-30.6
5	–	-15.2	–	-12.2	-7.08	-13.0	-12.3
6	3.8	-25.1	-0.4	-17.7	-15.01	-17.6	-16.6
7	–	-1.1	–	1.1	1.85	-0.3	2.9
18	-1.5	-37.0	-6.6	-27.7	-22.94	-28.5	-27.3
19	–	-13.1	–	-8.9	-6.08	-11.1	-7.8
Elementary reactions energy							
8	19.4	61.6	25.8	50.9	42.54	51.9	51.6
9	11.6	58.2	18.3	44.4	36.82	46.0	45.7
10	19.6	26.8	22.0	26.6	19.68	26.9	28.2
11	39.3	47.6	41.8	47.0	36.46	48.2	50.1
12	47.9	59.7	50.5	56.6	48.07	59.0	59.8
13	3.4	13.8	5.9	13.0	7.86	11.9	14.0
14	5.3	11.9	6.1	10.0	7.93	10.8	10.7
15 ^{a)}	-0.3	-0.48	-0.4	-0.5	-0.42	-0.4	-0.5
16 ^{b)}	-1.0	-1.07	-1.1	-1.2	-1.04	-1.1	-1.2

a) Expt -0.1 V (Ref.[31]). b) Expt -1.1 V (Ref.[31]).