

SUPPORTING INFORMATION

Computational Details

The computational work was carried out using the Gaussian09 suite of programs.¹ The geometry optimizations were performed without any symmetry constraint using the BP86 functional² in combination with the 6-311G(d,p) basis functions for all the light atoms (O, N, C, H) and the LANL2DZ functions for the metal atoms (Co, Cu), to which were added *f* polarization functions ($\alpha = 2.780$ for Co and 3.325 for Cu).³ The unrestricted formulation was used for all open-shell molecules, yielding negligible spin contamination in all cases. The ZPVE, PV and TS corrections at 298 K were obtained with Gaussian09 from the solution of the nuclear equation using the standard ideal gas and harmonic approximations, which also verified the nature of all optimized geometries as local minima or first order saddle points. A correction of 1.95 kcal/mol was applied to all *G* values to change the standard state from the gas phase (1 atm) to solution (1 M).⁴ Corrections for dispersion were carried out at the fixed BP86 optimized geometries using Grimme's D3 empirical method (BP86-D3), using $S6 = 1$, $SR6 = 1.1390$ and $S8 = 1.6830$.⁵ A solvation correction in methyl acrylate ($\epsilon = 7.03$) or in methyl methacrylate ($\epsilon = 6.32$)⁶ was carried out using the SMD polarizable continuum model.⁷ The energy scans along the hydride quenching pathway were carried out by partial optimizations at fixed C...H distances without any thermal, dispersion or solvent corrections using the BP86 functional, the 6-311+G(d,p) basis set for the light atoms and the LANL2DZ basis set for the metal atoms. The QM/MM calculations of the same hydride quenching pathway for the full (tetramesitylporphyrin)cobalt system were carried out at the same level of QM theory, with the four mesityl groups handled by molecular mechanics at the UFF level. The cutoff between the QM and MM parts was placed at the level of the mesityl-porphyrin rings.

References

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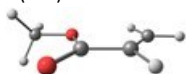
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Cartesian coordinates in Å and energies in hartrees for all optimized (or partially optimized) geometries. E vales are electronic energies in the gas phase. G values are at 298K in solvent (MA for methyl acrylate of MMA for methyl methacrylate) and are corrected for dispersion (see Computational details).

A. Full QM calculations using BP86, LANL2DZ(f) on M and 6-311G(d,p) on O, N, C, H

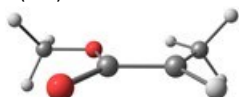
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G(MA) = -306.500713



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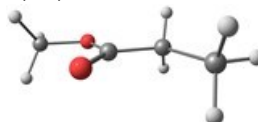
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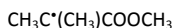
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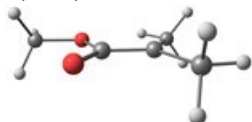
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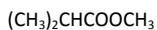


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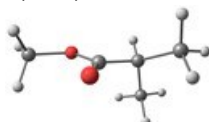


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6	2.576845000	0.232558000	-0.000280000
1	2.789822000	-0.374280000	-0.893849000
1	3.181035000	1.148117000	-0.000657000
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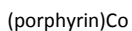
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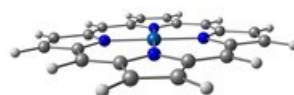
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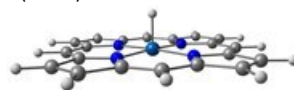
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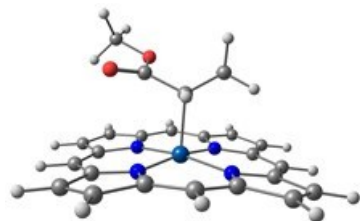
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(porphyrin)Co(CHCH₃COOCH₃)

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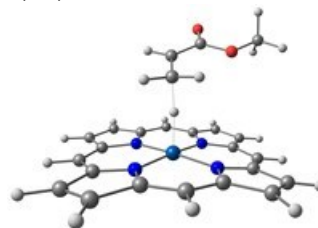
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(porphyrin)Co---H-CH₂CHCOOCH₃ (Broken symmetry)

E = -1441.01155232

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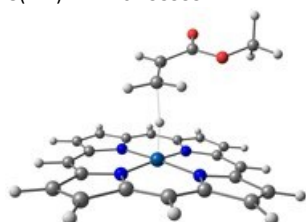
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6	3.147171000	-2.152155000	0.269970000
6	1.959283000	-2.667697000	-0.229036000
6	1.701703000	-4.079405000	-0.394847000
6	0.411713000	-4.195086000	-0.828741000
6	-0.107108000	-2.852460000	-0.950042000
6	-1.378138000	-2.553004000	-1.420510000
6	-1.835075000	-1.263558000	-1.654564000
6	-3.106348000	-0.960120000	-2.269893000
6	-3.167582000	0.398893000	-2.393068000
6	-1.945683000	0.922891000	-1.827843000
6	-1.670668000	2.276934000	-1.702151000
6	-0.548416000	2.784446000	-1.063222000
6	-0.314330000	4.192986000	-0.845659000
6	0.849482000	4.293269000	-0.137536000
6	1.335398000	2.946743000	0.054774000
6	2.538555000	2.640690000	0.675424000
1	5.056676000	1.800916000	1.705143000
1	5.429205000	-0.886561000	1.407734000
1	2.425713000	-4.866665000	-0.191595000
1	-0.150083000	-5.097277000	-1.064469000
1	-3.837553000	-1.706643000	-2.574958000
1	-3.962535000	1.009781000	-2.817517000
1	-0.970968000	4.988479000	-1.194017000
1	1.357778000	5.189002000	0.215454000
1	3.948735000	-2.853760000	0.510241000

1	-2.041621000	-3.383848000	-1.668747000
1	-2.401867000	2.986963000	-2.094051000
1	3.128105000	3.464454000	1.083266000
1	-0.083436000	-0.130753000	0.881492000
6	-0.388553000	-0.098070000	2.191732000
1	-0.632606000	0.967992000	2.233721000
1	0.613258000	-0.364443000	2.543730000
6	-2.848654000	-0.693417000	2.351392000
8	-3.743894000	-1.503250000	2.563977000
8	-3.083867000	0.622888000	2.044199000
6	-4.481764000	0.979375000	1.973744000
1	-4.990136000	0.397844000	1.190150000
1	-4.979437000	0.788631000	2.936706000
1	-4.496871000	2.049054000	1.733223000
6	-1.418703000	-1.006778000	2.423109000
1	-1.206907000	-2.062371000	2.606065000

(porphyrin)Co--H--(CH₂CHCOOCH₃) (TS -Broken symmetry)

E = -1441.0110068

G(MA) = -1440.793953



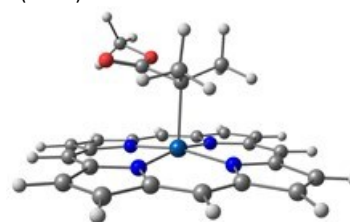
27	0.617628000	0.050104000	-0.564269000
7	2.379945000	0.582120000	0.169066000
7	1.161679000	-1.849980000	-0.489045000
7	-1.087009000	-0.472631000	-1.416687000
7	0.124860000	1.957789000	-0.748415000
6	2.803741000	1.858164000	0.513565000
6	4.140881000	1.830119000	1.057860000
6	4.544978000	0.525344000	1.039567000
6	3.446487000	-0.242057000	0.501182000
6	3.457363000	-1.623922000	0.376711000
6	2.377182000	-2.371639000	-0.069042000
6	2.364175000	-3.815179000	-0.115802000
6	1.121047000	-4.182837000	-0.545592000
6	0.385050000	-2.962362000	-0.779107000
6	-0.910353000	-2.924948000	-1.273950000
6	-1.583701000	-1.755632000	-1.595541000
6	-2.888413000	-1.724385000	-2.214218000
6	-3.190725000	-0.409438000	-2.424941000
6	-2.079769000	0.359235000	-1.913714000
6	-2.045887000	1.745519000	-1.893023000
6	-1.020233000	2.487356000	-1.325972000
6	-1.027625000	3.928454000	-1.233614000
6	0.114172000	4.285786000	-0.574890000
6	0.825706000	3.062837000	-0.285383000
6	2.069216000	3.020723000	0.328334000
1	4.689175000	2.709089000	1.392626000
1	5.494679000	0.101040000	1.361014000
1	3.207139000	-4.448721000	0.154965000
1	0.723817000	-5.183228000	-0.708695000
1	-3.475874000	-2.607522000	-2.459156000
1	-4.082282000	0.021408000	-2.877485000
1	-1.816766000	4.567580000	-1.626131000
1	0.468271000	5.281753000	-0.314252000
1	4.361382000	-2.158213000	0.676271000
1	-1.415430000	-3.874862000	-1.460384000
1	-2.893234000	2.285522000	-2.320516000
1	2.516616000	3.965111000	0.645246000
1	-0.003121000	-0.074199000	0.774382000

6	-1.253469000	-0.927684000	2.620220000
6	-0.298369000	0.010032000	2.340578000
1	-0.579554000	1.061606000	2.247066000
1	0.752898000	-0.206740000	2.544192000
1	-0.984890000	-1.962621000	2.843304000
6	-2.708133000	-0.687073000	2.593594000
8	-3.547400000	-1.537799000	2.855429000
8	-3.022759000	0.602898000	2.261586000
6	-4.439776000	0.885215000	2.232476000
1	-4.948155000	0.238559000	1.502003000
1	-4.887591000	0.721061000	3.224362000
1	-4.519354000	1.938921000	1.940104000

(porphyrin)Co(C(CH₃)₂COOCH₃)

E = -1480.36160551

G(MMA) = -1480.128397



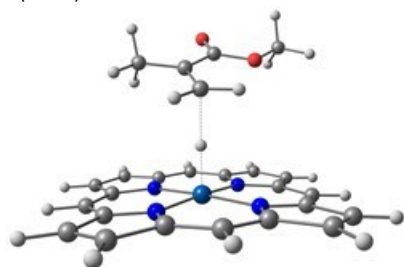
27	0.294603000	0.020737000	-0.392262000
7	2.239820000	0.420059000	-0.270976000
7	0.710025000	-1.917338000	-0.545613000
7	-1.587627000	-0.370953000	-0.930309000
7	-0.069665000	1.966377000	-0.621480000
6	2.848028000	1.664322000	-0.184774000
6	4.280019000	1.533169000	-0.053435000
6	4.554790000	0.195173000	-0.073347000
6	3.289097000	-0.486305000	-0.209200000
6	3.158108000	-1.866365000	-0.272953000
6	1.949222000	-2.528931000	-0.427167000
6	1.824827000	-3.966803000	-0.479419000
6	0.494741000	-4.239568000	-0.625618000
6	-0.186081000	-2.967013000	-0.676782000
6	-1.545954000	-2.832134000	-0.910016000
6	-2.185540000	-1.613995000	-1.075466000
6	-3.573924000	-1.482517000	-1.446322000
6	-3.832498000	-0.143177000	-1.529089000
6	-2.602615000	0.537477000	-1.197843000
6	-2.475852000	1.916530000	-1.145121000
6	-1.288314000	2.578465000	-0.870793000
6	-1.157185000	4.016701000	-0.866841000
6	0.158138000	4.289824000	-0.619985000
6	0.824680000	3.017078000	-0.476549000
6	2.187646000	2.882930000	-0.255503000
1	4.971616000	2.370437000	0.023483000
1	5.520617000	-0.303571000	-0.013199000
1	2.661007000	-4.661231000	-0.417574000
1	0.001602000	-5.206111000	-0.713085000
1	-4.245168000	-2.320024000	-1.628316000
1	-4.761964000	0.357513000	-1.795419000
1	-1.975397000	4.711235000	-1.049813000
1	0.653975000	5.256887000	-0.555052000
1	4.066034000	-2.469175000	-0.203016000
1	-2.141219000	-3.741474000	-1.010933000
1	-3.361497000	2.520273000	-1.353846000
1	2.783886000	3.793699000	-0.168568000
6	0.042028000	-0.015046000	1.713559000
6	0.358804000	1.362501000	2.288083000
1	1.391609000	1.661899000	2.060937000
1	-0.329008000	2.140996000	1.944146000
1	0.272326000	1.305305000	3.391607000

6	-1.404190000	-0.424919000	1.895763000
8	-1.798987000	-1.574114000	2.031214000
8	-2.244796000	0.653091000	1.985189000
6	-3.631416000	0.317033000	2.215775000
1	-3.734633000	-0.302585000	3.119015000
1	-4.145176000	1.278070000	2.342167000
1	-4.042916000	-0.231247000	1.355169000
6	0.951939000	-1.080728000	2.316901000
1	2.005578000	-0.908186000	2.061406000
1	0.867967000	-1.018981000	3.420271000
1	0.657898000	-2.094670000	2.025975000

(porphyrin)Co--H--(CH₂C(CH₃)COOCH₃) (TS Broken symmetry)

E = -1480.339772

G(MMA) = -1480.104333



27	0.670625000	0.158917000	-0.636981000
7	2.463972000	-0.254875000	0.097140000
7	0.414511000	-1.751357000	-1.083531000
7	-1.063166000	0.588239000	-1.484748000
7	0.980361000	2.084256000	-0.294439000
6	3.348262000	0.617282000	0.717207000
6	4.535481000	-0.075991000	1.159438000
6	4.380923000	-1.385394000	0.802729000
6	3.093587000	-1.490551000	0.156788000
6	2.559730000	-2.683197000	-0.308864000
6	1.298548000	-2.800511000	-0.874203000
6	0.721914000	-4.055938000	-1.295570000
6	-0.535636000	-3.777364000	-1.749690000
6	-0.716756000	-2.350334000	-1.619384000
6	-1.862240000	-1.679110000	-2.020654000
6	-2.008841000	-0.300668000	-1.974961000
6	-3.167215000	0.400024000	-2.478311000
6	-2.927598000	1.732601000	-2.298888000
6	-1.631215000	1.840276000	-1.671080000
6	-1.060607000	3.043751000	-1.284557000
6	0.155088000	3.149609000	-0.625396000
6	0.714978000	4.400197000	-0.168790000
6	1.887013000	4.097850000	0.463733000
6	2.047076000	2.665078000	0.377477000
6	3.148728000	1.981629000	0.870851000
1	5.374593000	0.398602000	1.665415000
1	5.063885000	-2.219297000	0.956041000
1	1.229771000	-5.017350000	-1.240053000
1	-1.283033000	-4.459631000	-2.151072000
1	-4.036004000	-0.083832000	-2.921438000
1	-3.558803000	2.580686000	-2.559168000
1	0.253773000	5.374570000	-0.321091000
1	2.598615000	4.770499000	0.939602000
1	3.159820000	-3.589292000	-0.202038000
1	-2.685922000	-2.268926000	-2.427941000
1	-1.613748000	3.962602000	-1.490116000
1	3.923398000	2.558519000	1.380342000
1	0.018742000	-0.043344000	0.663175000
6	-1.328316000	-1.015368000	2.456301000
6	-0.369131000	-0.052884000	2.313912000
1	-0.645481000	1.001251000	2.268704000

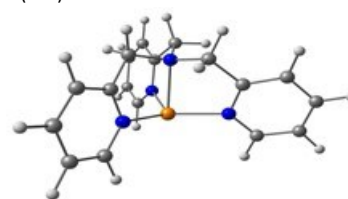
1	0.677955000	-0.289773000	2.518431000
6	-2.780131000	-0.686278000	2.369519000
8	-3.674763000	-1.510407000	2.498991000
8	-3.014717000	0.640481000	2.145899000
6	-4.413163000	0.997510000	2.065118000
1	-4.898702000	0.469949000	1.230910000
1	-4.932506000	0.740302000	3.000604000
1	-4.425802000	2.080851000	1.897455000
6	-1.013845000	-2.471538000	2.640955000
1	-1.556570000	-2.881740000	3.507847000
1	-1.349694000	-3.053938000	1.765836000
1	0.065131000	-2.629983000	2.774880000

A3. [Cu(TPMA)]⁺ systems

[Cu(TPMA)]⁺

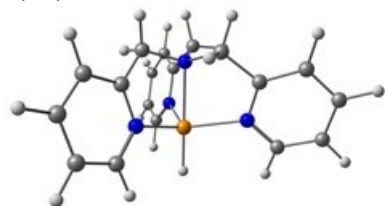
E = -1112.1044056

G(MA) = -1111.947897



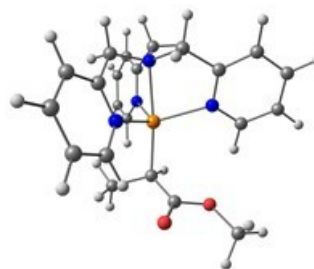
29	-0.001324000	-0.001958000	-0.838316000
7	-1.943548000	-0.575041000	-0.578493000
6	-2.786412000	-1.106818000	-1.495181000
1	-2.420560000	-1.133996000	-2.524162000
6	-4.464662000	-1.555312000	0.166056000
1	-5.442345000	-1.941748000	0.461923000
6	-3.598048000	-1.010042000	1.120065000
1	-3.886087000	-0.960626000	2.173030000
6	-2.351104000	-0.517760000	0.719293000
6	-1.423227000	0.172317000	1.718530000
1	-1.637745000	1.255127000	1.677858000
1	-1.671217000	-0.159942000	2.746545000
7	-0.000273000	-0.000896000	1.391004000
6	0.561234000	-1.320407000	1.716427000
1	-0.268664000	-2.048076000	1.671114000
1	0.970199000	-1.371753000	2.745418000
6	1.625216000	-1.775174000	0.718226000
6	2.678122000	-2.604790000	1.119278000
1	2.780603000	-2.877776000	2.172407000
6	2.352162000	-1.856984000	-1.496573000
1	2.191146000	-1.527528000	-2.525601000
7	1.469426000	-1.394832000	-0.579761000
6	0.862052000	1.144403000	1.717710000
1	1.906959000	0.788499000	1.675597000
1	0.699723000	1.525058000	2.746016000
6	0.727466000	2.292940000	0.718561000
7	0.472507000	1.968261000	-0.578693000
6	0.431227000	2.963918000	-1.495457000
1	0.222537000	2.660499000	-2.523936000
6	0.636241000	4.305744000	-1.170063000
1	0.593244000	5.067191000	-1.950704000
6	0.925108000	3.619053000	1.118907000
1	1.113860000	3.843904000	2.171489000
6	0.884085000	4.642016000	0.164776000
1	1.038454000	5.682070000	0.460091000
6	3.584843000	-3.080339000	0.165169000
1	4.410797000	-3.730665000	0.461184000
6	3.414342000	-2.701933000	-1.170484000
1	4.094827000	-3.046065000	-1.951220000
6	-4.050992000	-1.599810000	-1.169294000
1	-4.690049000	-2.015975000	-1.949961000

[(TPMA)Cu-H]⁺
 E = -1112.6554201
 G(MA) = -1112.498571



29	-0.001446000	-0.001494000	-0.949575000
7	-2.026672000	-0.491956000	-0.545346000
6	-2.907363000	-0.998656000	-1.432973000
1	-2.540263000	-1.102917000	-2.456776000
6	-4.600077000	-1.210692000	0.262785000
1	-5.604861000	-1.495634000	0.582670000
6	-3.686191000	-0.688395000	1.185890000
1	-3.961967000	-0.556496000	2.234887000
6	-2.407653000	-0.329399000	0.744447000
6	-1.387343000	0.330413000	1.657460000
1	-1.501601000	1.424739000	1.563674000
1	-1.582134000	0.073609000	2.716575000
7	-0.000297000	-0.000297000	1.252818000
6	0.408037000	-1.365835000	1.659378000
1	-0.481881000	-2.013225000	1.570388000
1	0.731096000	-1.403233000	2.717632000
6	1.488923000	-1.919363000	0.744730000
6	2.443242000	-2.842393000	1.186862000
1	2.469258000	-3.145384000	2.236333000
6	2.316496000	-2.018124000	-1.433439000
1	2.220265000	-1.650041000	-2.457693000
7	1.436013000	-1.510936000	-0.545959000
6	0.977939000	1.036336000	1.659938000
1	1.983253000	0.588191000	1.573205000
1	0.847488000	1.335338000	2.717962000
6	0.919051000	2.248164000	0.744719000
7	0.592700000	1.997106000	-0.545927000
6	0.593660000	3.012349000	-1.434504000
1	0.322274000	2.744879000	-2.458533000
6	0.920423000	4.321688000	-1.072830000
1	0.911854000	5.113267000	-1.824027000
6	1.242336000	3.536287000	1.185768000
1	1.490180000	3.711129000	2.235469000
6	1.246749000	4.587942000	0.261548000
1	1.498504000	5.601594000	0.581302000
1	-0.001701000	-0.001861000	-2.501045000
6	3.354335000	-3.370033000	0.263896000
1	4.107184000	-4.093606000	0.584491000
6	3.288430000	-2.953881000	-1.070438000
1	3.980247000	-3.340589000	-1.820676000
6	-4.205919000	-1.365562000	-1.070887000
1	-4.887896000	-1.768940000	-1.821364000

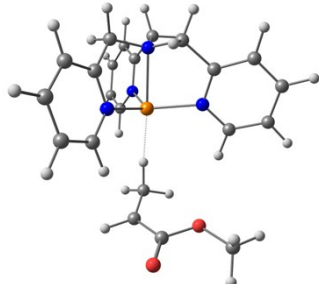
[(TPMA)Cu-CHCH₃COOCH₃]⁺
 E = -1419.2618864
 G(MA) = -1419.044935



29	0.011882000	0.059626000	-0.338197000
7	-0.581364000	-1.597892000	0.969885000
6	-1.193169000	-2.748045000	0.614851000
1	-1.510197000	-2.812432000	-0.428566000
6	-1.023854000	-3.627686000	2.849508000
1	-1.192654000	-4.418257000	3.584215000
6	-0.381512000	-2.440616000	3.220820000
1	-0.037993000	-2.284973000	4.246291000
6	-0.179491000	-1.446863000	2.256550000
6	0.478681000	-0.121508000	2.594127000
1	-0.307433000	0.630555000	2.778994000
1	1.075774000	-0.207146000	3.523056000
7	1.291173000	0.358557000	1.453668000
6	2.528731000	-0.426943000	1.276416000
1	2.305594000	-1.467199000	1.571500000
1	3.341273000	-0.073036000	1.940711000
6	2.991171000	-0.445820000	-0.168465000
6	4.343217000	-0.606481000	-0.496743000
1	5.095594000	-0.639857000	0.294910000
6	2.385084000	-0.504125000	-2.409104000
1	1.576161000	-0.455663000	-3.141188000
7	2.023410000	-0.378545000	-1.114393000
6	1.545368000	1.814563000	1.494242000
1	2.286995000	2.037984000	0.706810000
1	1.986867000	2.132911000	2.459339000
6	0.275137000	2.592162000	1.208492000
7	-0.593513000	2.014429000	0.340946000
6	-1.739965000	2.665043000	0.037479000
1	-2.420854000	2.144308000	-0.645536000
6	-2.048345000	3.920847000	0.570543000
1	-2.985659000	4.406757000	0.294069000
6	0.027736000	3.841055000	1.787263000
1	0.747816000	4.270460000	2.487894000
6	-1.149447000	4.522304000	1.456013000
1	-1.363451000	5.500577000	1.892541000
6	4.709465000	-0.730461000	-1.840712000
1	5.757629000	-0.858300000	-2.120056000
6	3.708397000	-0.687356000	-2.816677000
1	3.942606000	-0.785670000	-3.878013000
6	-1.434162000	-3.784496000	1.522327000
1	-1.931516000	-4.696054000	1.186224000
6	-2.447922000	-0.298396000	-1.896335000
6	-1.011222000	-0.109150000	-2.165922000
8	-3.279634000	0.593024000	-1.731722000
8	-2.800295000	-1.628694000	-1.856225000
6	-4.211922000	-1.876311000	-1.622023000
1	-4.819754000	-1.375876000	-2.388542000
1	-4.513029000	-1.506959000	-0.630394000
1	-4.330094000	-2.964444000	-1.686328000
1	-0.537942000	-1.037350000	-2.520038000
6	-0.678902000	1.138056000	-2.969678000
1	-0.868384000	0.970594000	-4.048220000
1	-1.312204000	1.982197000	-2.665765000
1	0.373294000	1.448613000	-2.871190000

[(TPMA)Cu...H-CH₂CHCOOCH₃]⁺

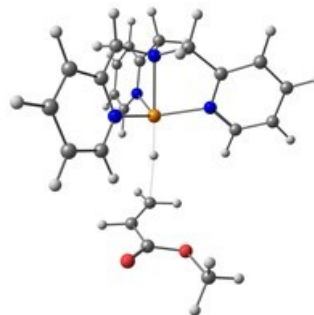
E = -1419.23767411
G(MA) = -1419.022562



29	-0.392090000	0.022255000	0.267941000
7	0.341158000	-1.627514000	-0.733329000
6	1.268540000	-2.511556000	-0.297414000
1	1.801601000	-2.237778000	0.615811000
6	0.861474000	-3.991662000	-2.149289000
1	1.052430000	-4.916622000	-2.697855000
6	-0.088263000	-3.074560000	-2.613161000
1	-0.647379000	-3.264995000	-3.532548000
6	-0.319105000	-1.898160000	-1.891510000
6	-1.269114000	-0.826957000	-2.420692000
1	-0.664907000	-0.098992000	-2.990705000
1	-1.981003000	-1.279043000	-3.139660000
7	-1.942337000	-0.086461000	-1.343105000
6	-3.049458000	-0.807638000	-0.699844000
1	-2.823974000	-1.886400000	-0.776506000
1	-4.019848000	-0.649964000	-1.212033000
6	-3.187928000	-0.470837000	0.781609000
6	-4.435820000	-0.511476000	1.413502000
1	-5.332616000	-0.722156000	0.825822000
6	-2.136417000	0.023137000	2.801358000
1	-1.197647000	0.240038000	3.315311000
7	-2.045756000	-0.195169000	1.468477000
6	-2.208603000	1.331475000	-1.633245000
1	-2.903582000	1.698429000	-0.856905000
1	-2.713332000	1.482488000	-2.608661000
6	-0.943329000	2.181737000	-1.570188000
7	-0.008150000	1.833067000	-0.645229000
6	1.100516000	2.599233000	-0.529246000
1	1.834303000	2.277236000	0.215380000
6	1.324700000	3.734779000	-1.310679000
1	2.239761000	4.313693000	-1.174899000
6	-0.779803000	3.299121000	-2.395884000
1	-1.546632000	3.542803000	-3.135184000
6	0.365693000	4.092852000	-2.263328000
1	0.509136000	4.969073000	-2.899381000
6	-4.519588000	-0.287173000	2.791916000
1	-5.485201000	-0.317274000	3.301260000
6	-3.343794000	-0.018874000	3.500214000
1	-3.355934000	0.163580000	4.576126000
6	1.558857000	-3.698838000	-0.973307000
1	2.313327000	-4.379780000	-0.575634000
6	4.051145000	0.594798000	1.452672000
6	2.936682000	1.053907000	2.261084000
8	4.938469000	1.322157000	1.014587000
8	4.010408000	-0.765659000	1.214650000
6	5.142480000	-1.263859000	0.458092000
1	6.084890000	-1.001202000	0.959647000
1	5.015245000	-2.352301000	0.421998000
1	5.149834000	-0.837184000	-0.556037000
1	2.979158000	2.111267000	2.531648000
6	1.786939000	0.217922000	2.670579000
1	2.076847000	-0.829225000	2.842689000
1	1.287996000	0.618360000	3.565974000

1 0.997909000 0.186895000 1.853047000

[(TPMA)Cu--H--(CH₂CHCOOCH₃)⁺ (TS)
E = -1419.205486
G(MA) = -1418.991005



29	-0.363054000	-0.015691000	-0.342110000
7	-0.218723000	2.037949000	0.202970000
6	0.403898000	3.003359000	-0.504916000
1	0.926053000	2.669106000	-1.404207000
6	-0.307567000	4.704357000	1.038315000
1	-0.348671000	5.745966000	1.364631000
6	-0.957957000	3.706480000	1.773372000
1	-1.513478000	3.951483000	2.681838000
6	-0.885965000	2.380088000	1.332118000
6	-1.494444000	1.232862000	2.122737000
1	-0.717435000	0.829121000	2.795500000
1	-2.319418000	1.596987000	2.765909000
7	-1.923819000	0.130154000	1.235894000
6	-3.188129000	0.418965000	0.527054000
1	-3.194266000	1.498364000	0.293996000
1	-4.076350000	0.220582000	1.158375000
6	-3.282185000	-0.347873000	-0.782289000
6	-4.511057000	-0.743789000	-1.323069000
1	-5.436578000	-0.554185000	-0.774084000
6	-2.136531000	-1.194740000	-2.624359000
1	-1.164016000	-1.357157000	-3.094455000
7	-2.110817000	-0.577802000	-1.424421000
6	-1.924304000	-1.187678000	1.908815000
1	-2.487122000	-1.884005000	1.262461000
1	-2.447943000	-1.157996000	2.884394000
6	-0.512869000	-1.726670000	2.074833000
7	0.365417000	-1.404356000	1.093043000
6	1.617746000	-1.905196000	1.148121000
1	2.291501000	-1.616456000	0.339795000
6	2.046958000	-2.746352000	2.178325000
1	3.071871000	-3.120911000	2.173607000
6	-0.152930000	-2.551906000	3.145643000
1	-0.881485000	-2.783364000	3.926449000
6	1.145749000	-3.074063000	3.196200000
1	1.448201000	-3.721717000	4.022229000
6	-4.533089000	-1.378624000	-2.570164000
1	-5.480408000	-1.694591000	-3.012645000
6	-3.323276000	-1.606246000	-3.235199000
1	-3.293788000	-2.10044000	-4.208000000
6	0.389136000	4.346396000	-0.121155000
1	0.908533000	5.092420000	-0.725090000
6	4.268732000	-0.664696000	-1.239456000
6	3.181878000	-1.188430000	-2.090467000
8	4.860961000	-1.343002000	-0.407848000
8	4.527135000	0.656788000	-1.455723000
6	5.591549000	1.207400000	-0.637819000
1	6.526039000	0.652525000	-0.802895000
1	5.696415000	2.248812000	-0.962828000
1	5.327660000	1.154284000	0.428830000
1	3.121408000	-2.279535000	-2.107354000

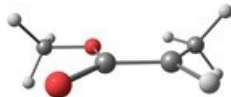
6	2.242601000	-0.418554000	-2.706534000	1	1.503960000	-0.868357000	-3.372181000
1	2.358114000	0.665244000	-2.750869000	1	0.752928000	-0.133992000	-1.466693000

B. Full QM calculations using BP86, LANL2DZ on M and 6-311+G(d,p) on O, N, C, H

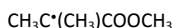
B1. Organic molecules



E = -307.1385561



6	-4.079541000	-0.731228000	1.274461000
6	-2.873237000	-1.180069000	1.943011000
8	-4.878434000	-1.472663000	0.700153000
8	-4.249714000	0.635404000	1.345212000
6	-5.439941000	1.128365000	0.691919000
1	-6.341335000	0.687729000	1.144199000
1	-5.423943000	2.215188000	0.839247000
1	-5.424534000	0.880901000	-0.380346000
1	-2.714804000	-2.260832000	1.901410000
6	-1.890029000	-0.314245000	2.643880000
1	-2.173745000	0.745133000	2.607781000
1	-1.783861000	-0.618522000	3.703170000
1	-0.881338000	-0.427937000	2.201635000

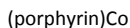


E = -346.468128007

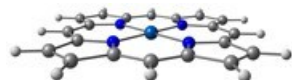


6	0.277679000	-0.347793000	0.000581000
6	-1.097368000	0.132287000	0.000127000
8	0.605090000	-1.536379000	0.000066000
8	1.206532000	0.674742000	0.000070000
6	2.581204000	0.234968000	-0.000292000
1	2.795856000	-0.369451000	-0.894791000
1	3.180940000	1.153632000	-0.000680000
1	2.796435000	-0.369079000	0.894319000
6	-1.453593000	1.582680000	-0.000029000
1	-0.568723000	2.230343000	-0.000002000
1	-2.075192000	1.830600000	-0.882554000
1	-2.075314000	1.830752000	0.882373000
6	-2.174251000	-0.905954000	-0.000202000
1	-2.087096000	-1.571184000	-0.878327000
1	-2.087586000	-1.571225000	0.877938000
1	-3.174331000	-0.448427000	-0.000478000

B2. Co(porphyrin) system



E = -1419.2618864

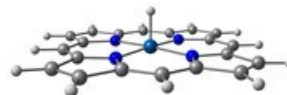


27	0.000003000	0.000004000	-0.000015000
7	-1.521459000	-1.282006000	-0.000138000
7	-1.282008000	1.521455000	-0.000032000
7	1.521452000	1.282005000	-0.000128000
7	1.282004000	-1.521457000	-0.000031000
6	-1.458854000	-2.666379000	0.000529000
6	-2.784228000	-3.239569000	0.000300000
6	-3.664584000	-2.194970000	-0.000609000
6	-2.875176000	-0.985885000	-0.000792000

6	-3.417169000	0.291674000	-0.001216000
6	-2.666381000	1.458855000	-0.000571000
6	-3.239567000	2.784229000	-0.000129000
6	-2.194966000	3.664582000	0.000794000
6	-0.985884000	2.875174000	0.000778000
6	0.291673000	3.417167000	0.001089000
6	1.458855000	2.666380000	0.000555000
6	2.784228000	3.239565000	0.000331000
6	3.664582000	2.194964000	-0.000589000
6	2.875175000	0.985884000	-0.000782000
6	3.417166000	-0.291674000	-0.001204000
6	2.666378000	-1.458855000	-0.000565000
6	3.239567000	-2.784227000	-0.000142000
6	2.194968000	-3.664582000	0.000757000
6	0.985886000	-2.875176000	0.000751000
6	-0.291674000	-3.417167000	0.001052000
1	-2.994351000	-4.307767000	0.000772000
1	-4.752947000	-2.221085000	-0.001003000
1	-4.307763000	2.994353000	-0.000394000
1	-2.221080000	4.752947000	0.001412000
1	2.994356000	4.307761000	0.000815000
1	4.752945000	2.221079000	-0.000985000
1	4.307764000	-2.994354000	-0.000401000
1	2.221083000	-4.752945000	0.001354000
1	-4.505210000	0.384720000	-0.001874000
1	0.384718000	4.505209000	0.001459000
1	4.505207000	-0.384721000	-0.001860000
1	-0.384722000	-4.505208000	0.001401000



E = -1134.4712381



27	0.000012000	0.000005000	0.029179000
7	-0.962114000	1.729506000	-0.026827000
7	1.729518000	0.962093000	-0.026717000
7	0.962112000	-1.729506000	-0.026863000
7	-1.729529000	-0.962095000	-0.026686000
6	-2.333569000	1.937632000	-0.013144000
6	-2.643212000	3.347318000	-0.010567000
6	-1.450044000	4.011032000	-0.011771000
6	-0.415588000	3.004524000	-0.014735000
6	0.939322000	3.294416000	-0.010127000
6	1.937633000	2.333563000	-0.014405000
6	3.347315000	2.643209000	-0.011070000
6	4.011031000	1.450041000	-0.010102000
6	3.004528000	0.415582000	-0.012935000
6	3.294414000	-0.939326000	-0.007498000
6	2.333567000	-1.937634000	-0.013149000
6	2.643206000	-3.347320000	-0.010571000
6	1.450036000	-4.011031000	-0.011769000
6	0.415581000	-3.004521000	-0.014757000
6	-0.939329000	-3.294414000	-0.010113000
6	-1.937640000	-2.333562000	-0.014363000
6	-3.347325000	-2.643211000	-0.011039000
6	-4.011040000	-1.450042000	-0.010091000
6	-3.004533000	-0.415584000	-0.012935000
6	-3.294418000	0.939325000	-0.007508000
1	-3.652009000	3.756565000	-0.010347000
1	-1.266039000	5.084005000	-0.012686000

1	3.756562000	3.652006000	-0.011718000
1	5.084004000	1.266038000	-0.009816000
1	3.652003000	-3.756570000	-0.010338000
1	1.266026000	-5.084002000	-0.012672000
1	-3.756571000	-3.652008000	-0.011675000
1	-5.084012000	-1.266037000	-0.009818000
1	1.238798000	4.344549000	-0.001352000
1	4.344536000	-1.238801000	0.002473000
1	-1.238802000	-4.344547000	-0.001326000
1	-4.344540000	1.238803000	0.002437000
1	0.000192000	-0.000115000	1.444557000

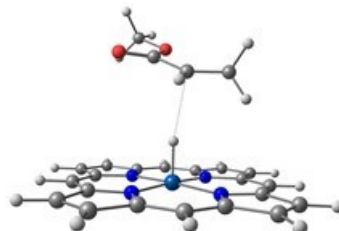
(porphyrin)Co--H--3.00 Å--CHCH₃COOCH₃
E = -1441.6105812



27	-0.715968000	0.109413000	-0.684983000
7	-2.240047000	-0.729252000	0.265230000
7	-1.338903000	1.895222000	-0.103014000
7	0.743931000	0.954641000	-1.719672000
7	-0.164117000	-1.669281000	-1.362975000
6	-2.553159000	-2.079930000	0.343440000
6	-3.714325000	-2.295266000	1.174080000
6	-4.112868000	-1.065830000	1.618262000
6	-3.194998000	-0.103912000	1.055736000
6	-3.280390000	1.262619000	1.276502000
6	-2.409449000	2.192314000	0.728995000
6	-2.509900000	3.614804000	0.957107000
6	-1.483551000	4.195887000	0.268125000
6	-0.759642000	3.126461000	-0.377888000
6	0.365395000	3.324647000	-1.163336000
6	1.066697000	2.302846000	-1.784680000
6	2.240739000	2.516413000	-2.597515000
6	2.648981000	1.285934000	-3.028038000
6	1.723142000	0.325030000	-2.475884000
6	1.812968000	-1.041406000	-2.692294000
6	0.924543000	-1.969135000	-2.170138000
6	1.016407000	-3.389878000	-2.410347000
6	-0.020480000	-3.969944000	-1.735599000
6	-0.741323000	-2.901044000	-1.085291000
6	-1.859292000	-3.100501000	-0.289276000
1	-4.156215000	-3.269838000	1.375258000
1	-4.952711000	-0.812628000	2.263281000
1	-3.275565000	4.088478000	1.569169000
1	-1.222320000	5.250059000	0.192426000
1	2.680462000	3.491397000	-2.800622000
1	3.495799000	1.031521000	-3.663349000
1	1.782029000	-3.863541000	-3.022543000
1	-0.290909000	-5.022782000	-1.673478000
1	-4.085099000	1.629161000	1.917430000
1	0.724850000	4.347274000	-1.295356000
1	2.633084000	-1.409219000	-3.312607000
1	-2.213767000	-4.124143000	-0.150264000
1	0.124770000	0.003048000	0.450959000
6	1.489010000	-0.397041000	3.092696000
1	0.756641000	0.394823000	3.268042000
6	1.057727000	-1.818496000	3.105455000
1	0.239404000	-1.983331000	2.380218000
1	1.884099000	-2.502346000	2.874577000

1	0.638790000	-2.089808000	4.094681000
6	2.843017000	0.079375000	2.887570000
8	3.184576000	1.262862000	2.918686000
8	3.737237000	-0.946015000	2.652336000
6	5.097028000	-0.516894000	2.431550000
1	5.484671000	0.017275000	3.312636000
1	5.668248000	-1.436858000	2.254948000
1	5.156663000	0.150921000	1.558584000

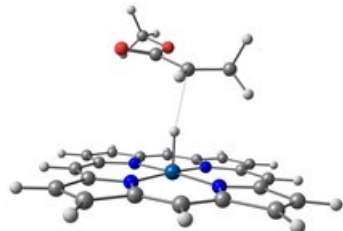
(porphyrin)Co--H--2.40 Å--CHCH₃COOCH₃
E = -1441.6114826



27	-0.447247000	0.091553000	-0.728482000
7	-2.304851000	-0.224428000	-0.108563000
7	-0.717940000	2.043636000	-0.537662000
7	1.362615000	0.414941000	-1.459612000
7	-0.222308000	-1.853535000	-1.032422000
6	-2.951657000	-1.442853000	0.051332000
6	-4.286141000	-1.256910000	0.570496000
6	-4.458146000	0.088718000	0.737693000
6	-3.228094000	0.719342000	0.320764000
6	-3.017068000	2.089995000	0.348879000
6	-1.839577000	2.702265000	-0.052911000
6	-1.627785000	4.130640000	-0.018547000
6	-0.359621000	4.349957000	-0.475903000
6	0.197965000	3.055268000	-0.789273000
6	1.479215000	2.869773000	-1.284623000
6	2.017249000	1.630869000	-1.596984000
6	3.349219000	1.446140000	-2.123139000
6	3.517810000	0.102155000	-2.301386000
6	2.288482000	-0.529113000	-1.881657000
6	2.079886000	-1.899595000	-1.908535000
6	0.902224000	-2.512996000	-1.508628000
6	0.689636000	-3.940720000	-1.545645000
6	-0.575258000	-4.161397000	-1.078147000
6	-1.130330000	-2.867323000	-0.757888000
6	-2.407468000	-2.682872000	-0.249669000
1	-4.989111000	-2.064445000	0.768850000
1	-5.332557000	0.624345000	1.103756000
1	-2.368050000	4.855680000	0.315754000
1	0.168594000	5.294164000	-0.596896000
1	4.049408000	2.254995000	-2.325215000
1	4.386236000	-0.432313000	-2.683082000
1	1.425445000	-4.664784000	-1.891811000
1	-1.103298000	-5.106021000	-0.958260000
1	-3.828047000	2.726041000	0.710117000
1	2.103276000	3.752831000	-1.436364000
1	2.893025000	-2.534838000	-2.266287000
1	-3.023978000	-3.568122000	-0.079205000
1	0.077455000	0.002152000	0.598212000
6	0.390989000	-0.151896000	2.972652000
1	-0.257210000	0.726980000	2.948477000
6	-0.195976000	-1.506724000	3.144263000
1	-1.109236000	-1.620844000	2.538329000
1	0.519939000	-2.298550000	2.886985000
1	-0.498785000	-1.663024000	4.200915000
6	1.811791000	0.157321000	3.008763000
8	2.283751000	1.294263000	3.005556000
8	2.596807000	-0.974813000	3.058590000

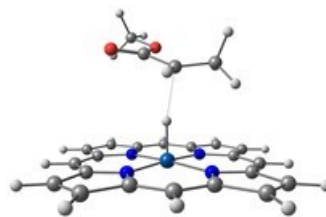
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1	4.288633000	-0.129655000	3.975758000
1	4.491283000	-1.707570000	3.117771000
1	4.328320000	-0.166953000	2.186410000

(porphyrin)Co--H--2.20 Å--CHCH₃COOCH₃
E = -1441.6124889



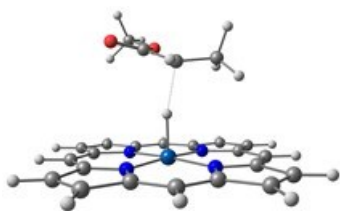
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7	-0.609168000	2.043686000	-0.583199000
7	1.438642000	0.306611000	-1.375386000
7	-0.252528000	-1.883976000	-0.947760000
6	-3.009357000	-1.332346000	-0.003183000
6	-4.354808000	-1.078666000	0.455818000
6	-4.473074000	0.276014000	0.594789000
6	-3.200325000	0.844416000	0.218080000
6	-2.931655000	2.205386000	0.225629000
6	-1.717533000	2.759240000	-0.151971000
6	-1.450139000	4.178823000	-0.151364000
6	-0.162101000	4.335180000	-0.577828000
6	0.353001000	3.010871000	-0.835895000
6	1.641869000	2.760408000	-1.280752000
6	2.143074000	1.492073000	-1.530523000
6	3.485613000	1.239704000	-1.998771000
6	3.609805000	-0.115265000	-2.122776000
6	2.342520000	-0.685480000	-1.728973000
6	2.081411000	-2.047279000	-1.719996000
6	0.863673000	-2.601447000	-1.354353000
6	0.592759000	-4.019812000	-1.365850000
6	-0.701285000	-4.175547000	-0.955514000
6	-1.215350000	-2.851508000	-0.694080000
6	-2.506568000	-2.600874000	-0.253875000
1	-5.100637000	-1.850837000	0.637861000
1	-5.337030000	0.855974000	0.915387000
1	-2.170324000	4.941768000	0.139638000
1	0.406309000	5.254145000	-0.710395000
1	4.222822000	2.014480000	-2.202818000
1	4.470716000	-0.694551000	-2.452710000
1	1.312350000	-4.782688000	-1.658629000
1	-1.274343000	-5.093952000	-0.838742000
1	-3.727116000	2.882957000	0.543294000
1	2.304524000	3.613722000	-1.438938000
1	2.882384000	-2.724751000	-2.023658000
1	-3.168616000	-3.454908000	-0.095233000
1	0.065753000	0.008189000	0.654337000
6	0.248390000	-0.052303000	2.845908000
1	-0.370829000	0.846856000	2.813484000
6	-0.378132000	-1.379857000	3.087205000
1	-1.335602000	-1.468777000	2.551298000
1	0.286857000	-2.204483000	2.797040000
1	-0.603059000	-1.504535000	4.167335000
6	1.679933000	0.215990000	2.915630000
8	2.184797000	1.337627000	2.909984000
8	2.426055000	-0.937964000	3.004040000
6	3.853109000	-0.726850000	3.069007000
1	4.118152000	-0.137751000	3.960261000
1	4.293809000	-1.730008000	3.123300000
1	4.206322000	-0.194861000	2.172925000

(porphyrin)Co--H--2.00 Å--CHCH₃COOCH₃
E = -1441.6149225



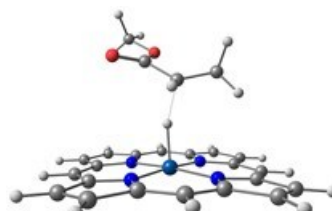
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7	1.480491000	0.259972000	-1.308307000
7	-0.257768000	-1.897589000	-0.894723000
6	-3.035811000	-1.285680000	-0.050950000
6	-4.387421000	-1.003982000	0.372955000
6	-4.478398000	0.352250000	0.518378000
6	-3.184095000	0.893871000	0.176427000
6	-2.888335000	2.249586000	0.186490000
6	-1.660535000	2.779965000	-0.181664000
6	-1.372708000	4.195635000	-0.202303000
6	-0.080649000	4.326648000	-0.625231000
6	0.417930000	2.990679000	-0.855539000
6	1.709078000	2.713466000	-1.278313000
6	2.200641000	1.432968000	-1.483213000
6	3.551178000	1.152150000	-1.910952000
6	3.664287000	-0.207503000	-1.987015000
6	2.381028000	-0.752186000	-1.608720000
6	2.100553000	-2.110060000	-1.575267000
6	0.860819000	-2.639116000	-1.247148000
6	0.563987000	-4.052500000	-1.255856000
6	-0.749969000	-4.179729000	-0.902645000
6	-1.249288000	-2.843727000	-0.674738000
6	-2.551590000	-2.564733000	-0.286320000
1	-5.155069000	-1.759938000	0.530830000
1	-5.337304000	0.949756000	0.819831000
1	-2.083587000	4.973684000	0.071064000
1	0.501143000	5.235243000	-0.770764000
1	4.301342000	1.912429000	-2.122291000
1	4.526728000	-0.805405000	-2.277502000
1	1.280598000	-4.831822000	-1.510127000
1	-1.345078000	-5.086069000	-0.803053000
1	-3.676173000	2.943394000	0.487760000
1	2.384370000	3.554626000	-1.447939000
1	2.901218000	-2.805181000	-1.837053000
1	-3.236753000	-3.404481000	-0.151114000
1	0.072536000	0.008518000	0.715848000
6	0.163747000	-0.020438000	2.713558000
1	-0.448588000	0.884208000	2.724809000
6	-0.466025000	-1.340268000	2.999944000
1	-1.449486000	-1.422446000	2.513633000
1	0.173534000	-2.175264000	2.683687000
1	-0.632653000	-1.449683000	4.091824000
6	1.599571000	0.245138000	2.829658000
8	2.102754000	1.364908000	2.872513000
8	2.339123000	-0.911023000	2.902720000
6	3.765313000	-0.707462000	3.011941000
1	4.007994000	-0.149800000	3.929280000
1	4.201037000	-1.713641000	3.044142000
1	4.142963000	-0.147499000	2.143501000

(porphyrin)Co--H--1.83 Å--CHCH₃COOCH₃
E = -1441.6196424



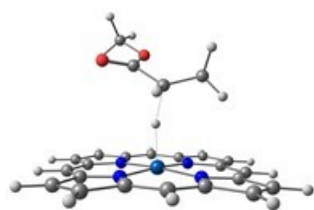
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7	1.428011000	0.533238000	-1.214826000
7	-0.032883000	-1.842828000	-0.915783000
6	-2.866540000	-1.621545000	-0.052549000
6	-4.250501000	-1.526652000	0.345388000
6	-4.530519000	-0.195046000	0.478262000
6	-3.316144000	0.518063000	0.163978000
6	-3.205701000	1.901144000	0.191874000
6	-2.042095000	2.597903000	-0.107730000
6	-1.930056000	4.038028000	-0.062113000
6	-0.642467000	4.341619000	-0.396631000
6	0.028521000	3.088238000	-0.646395000
6	1.360859000	2.989724000	-1.018948000
6	2.007460000	1.792426000	-1.290252000
6	3.382500000	1.699547000	-1.718822000
6	3.647892000	0.371157000	-1.905716000
6	2.435943000	-0.343979000	-1.584918000
6	2.317962000	-1.724829000	-1.643746000
6	1.158670000	-2.421165000	-1.326950000
6	1.042668000	-3.859398000	-1.387486000
6	-0.229420000	-4.166976000	-0.999487000
6	-0.889315000	-2.916104000	-0.709822000
6	-2.210529000	-2.820604000	-0.299819000
1	-4.909730000	-2.379452000	0.491886000
1	-5.469233000	0.279032000	0.757607000
1	-2.744172000	4.712124000	0.194764000
1	-0.170197000	5.318004000	-0.471676000
1	4.041657000	2.553112000	-1.860890000
1	4.571994000	-0.099807000	-2.235344000
1	1.842708000	-4.530392000	-1.691909000
1	-0.699684000	-5.144080000	-0.919160000
1	-4.089182000	2.477979000	0.469367000
1	1.935518000	3.912148000	-1.110863000
1	3.191280000	-2.299070000	-1.955345000
1	-2.775157000	-3.746242000	-0.177788000
1	0.007139000	0.048651000	0.835621000
6	0.233572000	-0.240419000	2.628403000
1	-0.476649000	0.548096000	2.882255000
6	-0.184828000	-1.669029000	2.792204000
1	-1.207713000	-1.824012000	2.418207000
1	0.502549000	-2.356563000	2.282426000
1	-0.182245000	-1.939462000	3.866828000
6	1.636380000	0.195007000	2.729482000
8	2.002845000	1.340369000	2.957997000
8	2.504311000	-0.854661000	2.551192000
6	3.903571000	-0.499130000	2.600291000
1	4.151393000	-0.024772000	3.560668000
1	4.446303000	-1.444397000	2.481370000
1	4.149525000	0.193422000	1.781999000

(porphyrin)Co--H--1.73 Å--CHCH₃COOCH₃
E = -1441.6251880



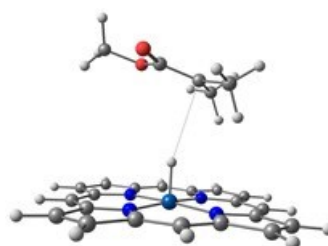
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7	1.528297000	-0.062550000	-1.311305000
7	-0.497412000	-1.933635000	-0.790379000
6	-3.178579000	-0.887692000	-0.053967000
6	-4.477400000	-0.396712000	0.345095000
6	-4.364371000	0.960835000	0.464309000
6	-3.000850000	1.295402000	0.123756000
6	-2.507776000	2.593700000	0.089559000
6	-1.223668000	2.929984000	-0.317230000
6	-0.744884000	4.289687000	-0.425030000
6	0.537365000	4.217928000	-0.890671000
6	0.842137000	2.814748000	-1.052912000
6	2.072619000	2.336034000	-1.480417000
6	2.389095000	0.989271000	-1.588554000
6	3.687219000	0.498501000	-1.988534000
6	3.625405000	-0.866188000	-1.937235000
6	2.285576000	-1.206100000	-1.518098000
6	1.824170000	-2.508208000	-1.383227000
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6	0.018991000	-4.196560000	-1.014140000
6	-1.313630000	-4.117268000	-0.720218000
6	-1.624020000	-2.713861000	-0.573860000
6	-2.882702000	-2.231777000	-0.241811000
1	-5.351459000	-1.024899000	0.509584000
1	-5.126966000	1.685983000	0.743946000
1	-1.332624000	5.172416000	-0.178248000
1	1.231739000	5.028876000	-1.103823000
1	4.526873000	1.133075000	-2.267450000
1	4.402050000	-1.592906000	-2.170357000
1	0.624500000	-5.082369000	-1.199352000
1	-2.036252000	-4.924034000	-0.608310000
1	-3.184284000	3.404655000	0.368150000
1	2.848901000	3.064575000	-1.723312000
1	2.526106000	-3.322294000	-1.576329000
1	-3.686949000	-2.957117000	-0.100465000
1	0.258793000	-0.083070000	0.788387000
6	0.089405000	0.179369000	2.489955000
1	-0.409247000	1.149228000	2.413225000
6	-0.714468000	-0.984299000	2.990107000
1	-1.694758000	-1.024255000	2.493745000
1	-0.190496000	-1.937686000	2.841357000
1	-0.896038000	-0.870850000	4.077177000
6	1.530880000	0.325026000	2.802678000
8	2.138835000	1.387676000	2.820114000
8	2.122228000	-0.880767000	3.078352000
6	3.539538000	-0.809045000	3.356087000
1	3.731344000	-0.169226000	4.230366000
1	3.848973000	-1.842221000	3.555766000
1	4.080370000	-0.401856000	2.488847000

(porphyrin)Co--H--1.63 Å--CHCH₃COOCH₃
E = -1441.633058



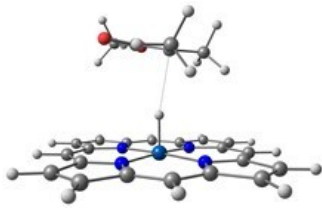
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7	-0.550257000	-1.940008000	-0.769527000
6	-3.198215000	-0.843755000	0.019019000
6	-4.485013000	-0.328252000	0.426206000
6	-4.356258000	1.030759000	0.506660000
6	-2.994033000	1.341566000	0.139328000
6	-2.485164000	2.632722000	0.072565000
6	-1.196571000	2.944713000	-0.340662000
6	-0.695456000	4.295371000	-0.461575000
6	0.588768000	4.197748000	-0.917194000
6	0.871014000	2.788192000	-1.065056000
6	2.091515000	2.285621000	-1.494938000
6	2.380484000	0.933254000	-1.613296000
6	3.661436000	0.418663000	-2.038149000
6	3.569821000	-0.944988000	-2.002945000
6	2.230046000	-1.260673000	-1.565030000
6	1.744328000	-2.554093000	-1.427713000
6	0.438872000	-2.863603000	-1.069831000
6	-0.078932000	-4.210654000	-1.003830000
6	-1.399266000	-4.108643000	-0.664632000
6	-1.682240000	-2.699889000	-0.514445000
6	-2.923847000	-2.194850000	-0.152548000
1	-5.363138000	-0.942201000	0.620129000
1	-5.106911000	1.771147000	0.778532000
1	-1.269966000	5.190155000	-0.227460000
1	1.297644000	4.995087000	-1.133868000
1	4.510638000	1.037713000	-2.322949000
1	4.326644000	-1.685524000	-2.256801000
1	0.505308000	-5.106955000	-1.206013000
1	-2.130603000	-4.903290000	-0.525868000
1	-3.150229000	3.457746000	0.336948000
1	2.880205000	2.999703000	-1.740658000
1	2.425140000	-3.380907000	-1.641229000
1	-3.734351000	-2.906570000	0.018949000
1	0.343470000	-0.168910000	0.828140000
6	0.179503000	0.200513000	2.407235000
1	-0.289147000	1.184024000	2.310437000
6	-0.657662000	-0.893730000	3.016223000
1	-1.646872000	-0.936595000	2.538337000
1	-0.171778000	-1.874670000	2.931654000
1	-0.813852000	-0.688663000	4.092483000
6	1.623668000	0.333678000	2.750869000
8	2.255070000	1.380515000	2.728999000
8	2.180827000	-0.869107000	3.096746000
6	3.593993000	-0.816226000	3.401292000
1	3.783042000	-0.138011000	4.246652000
1	3.874119000	-1.844970000	3.658659000
1	4.162019000	-0.465467000	2.526871000

(porphyrin)Co--H--3.00 Å--C(CH₃)₂COOCH₃
E = -1480.94059717



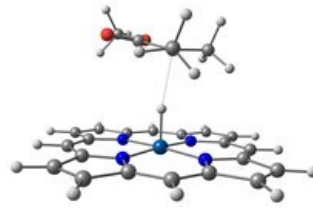
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7	1.451362000	1.736501000	-0.395562000
7	2.028819000	-1.003405000	-0.419934000
7	-0.483926000	-1.522889000	-1.535994000
7	-1.063417000	1.215420000	-1.506920000
6	0.994102000	3.047408000	-0.414975000
6	2.001656000	3.955128000	0.079841000
6	3.087933000	3.194239000	0.409851000
6	2.736997000	1.823500000	0.122259000
6	3.582923000	0.748223000	0.349768000
6	3.241867000	-0.572951000	0.101728000
6	4.116166000	-1.690422000	0.369306000
6	3.427706000	-2.819166000	0.023177000
6	2.138450000	-2.386734000	-0.461727000
6	1.160342000	-3.253310000	-0.925744000
6	-0.061437000	-2.841186000	-1.434470000
6	-1.058365000	-3.746781000	-1.955516000
6	-2.104894000	-2.977369000	-2.377411000
6	-1.747211000	-1.604951000	-2.104681000
6	-2.576550000	-0.526536000	-2.371457000
6	-2.254269000	0.790023000	-2.078713000
6	-3.137604000	1.905185000	-2.326611000
6	-2.489266000	3.024624000	-1.887049000
6	-1.208721000	2.590184000	-1.380614000
6	-0.253325000	3.452593000	-0.865251000
1	1.877845000	5.034562000	0.150217000
1	4.048302000	3.513778000	0.811254000
1	5.124830000	-1.602145000	0.769679000
1	3.749103000	-3.858019000	0.076994000
1	-0.950539000	-4.829621000	-1.987609000
1	-3.043939000	-3.291450000	-2.829955000
1	-4.124269000	1.821112000	-2.779278000
1	-2.826910000	4.059607000	-1.902863000
1	4.573863000	0.953572000	0.760370000
1	1.370874000	-4.324524000	-0.901598000
1	-3.549583000	-0.727942000	-2.824474000
1	-0.491741000	4.517590000	-0.825786000
1	-0.104963000	-0.031936000	0.382718000
6	-0.525742000	-0.310535000	3.339966000
6	-0.078329000	1.113773000	3.405732000
1	0.669779000	1.321683000	2.617707000
1	-0.910418000	1.818754000	3.294642000
1	0.430361000	1.314018000	4.369275000
6	-1.925575000	-0.693484000	3.195907000
8	-2.348363000	-1.851919000	3.171677000
8	-2.767879000	0.396319000	3.090305000
6	-4.161599000	0.061166000	2.932722000
1	-4.526298000	-0.509600000	3.800721000
1	-4.685352000	1.022196000	2.854224000
1	-4.316059000	-0.540067000	2.023876000
6	0.489812000	-1.398311000	3.456581000
1	0.015023000	-2.388106000	3.453110000
1	1.213062000	-1.346419000	2.620585000
1	1.083545000	-1.282938000	4.383602000

(porphyrin)Co--H--2.40 Å--C(CH₃)₂COOCH₃
E = -1480.94107192



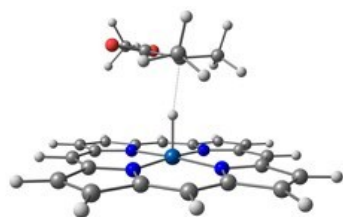
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7	-1.512846000	-0.213881000	-1.379522000
7	0.146315000	1.989491000	-0.895456000
6	2.958703000	1.453229000	-0.125725000
6	4.335608000	1.207403000	0.232939000
6	4.505920000	-0.148725000	0.230198000
6	3.231662000	-0.726134000	-0.127447000
6	3.006067000	-2.090986000	-0.230979000
6	1.783489000	-2.651885000	-0.567703000
6	1.554297000	-4.074921000	-0.662107000
6	0.239141000	-4.238816000	-0.992024000
6	-0.328898000	-2.915649000	-1.102110000
6	-1.653782000	-2.673322000	-1.429747000
6	-2.200228000	-1.405776000	-1.560853000
6	-3.574993000	-1.160503000	-1.928550000
6	-3.734339000	0.196108000	-1.968555000
6	-2.457388000	0.773967000	-1.620238000
6	-2.226001000	2.139089000	-1.544182000
6	-1.005324000	2.700985000	-1.201856000
6	-0.773459000	4.123898000	-1.118712000
6	0.530741000	4.287911000	-0.745706000
6	1.091268000	2.964323000	-0.605651000
6	2.406875000	2.720782000	-0.240146000
1	5.065428000	1.986278000	0.448037000
1	5.405682000	-0.723800000	0.443022000
1	2.315463000	-4.834624000	-0.492057000
1	-0.314845000	-5.162348000	-1.151334000
1	-4.306805000	-1.940420000	-2.132619000
1	-4.625757000	0.771807000	-2.212664000
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1	1.082399000	5.212017000	-0.580800000
1	3.841308000	-2.765324000	-0.029958000
1	-2.305863000	-3.532852000	-1.598091000
1	-3.056962000	2.813095000	-1.763267000
1	3.050651000	3.579988000	-0.039632000
1	-0.012271000	-0.020853000	0.568569000
6	-0.194958000	0.006929000	2.961445000
6	0.169363000	1.453355000	3.065763000
1	1.159481000	1.641616000	2.619956000
1	-0.574677000	2.104842000	2.590893000
1	0.238778000	1.752483000	4.132647000
6	-1.586896000	-0.434566000	2.856633000
8	-1.965353000	-1.606242000	2.890970000
8	-2.463815000	0.620394000	2.725196000
6	-3.848500000	0.236085000	2.593299000
1	-4.177349000	-0.343801000	3.469206000
1	-4.406130000	1.178251000	2.520983000
1	-3.995900000	-0.371016000	1.687311000
6	0.846978000	-1.032758000	3.210710000
1	1.208095000	-0.970030000	4.257747000
1	0.450333000	-2.042676000	3.044731000
1	1.728539000	-0.868588000	2.567637000

(porphyrin)Co-H--2.20 Å—C(CH₃)₂COOCH₃
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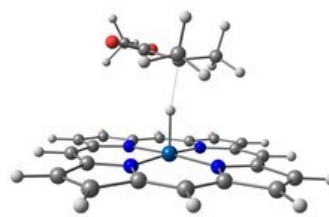
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7	-1.520718000	-0.242849000	-1.323133000
7	0.112052000	1.987114000	-0.867890000
6	2.941223000	1.494560000	-0.129834000
6	4.327472000	1.270755000	0.207139000
6	4.519432000	-0.082535000	0.200897000
6	3.248669000	-0.680202000	-0.135935000
6	3.042275000	-2.048705000	-0.233670000
6	1.822477000	-2.629328000	-0.546959000
6	1.612965000	-4.056115000	-0.632415000
6	0.294819000	-4.240780000	-0.939094000
6	-0.294449000	-2.926442000	-1.045029000
6	-1.627017000	-2.704447000	-1.356258000
6	-2.192735000	-1.445461000	-1.489737000
6	-3.574045000	-1.222055000	-1.847157000
6	-3.752230000	0.132001000	-1.897182000
6	-2.480290000	0.730067000	-1.564423000
6	-2.266861000	2.098920000	-1.500100000
6	-1.051729000	2.680222000	-1.170001000
6	-0.839591000	4.106877000	-1.096153000
6	0.464793000	4.291480000	-0.733293000
6	1.045357000	2.976634000	-0.591220000
6	2.368406000	2.753439000	-0.239111000
1	5.048208000	2.061182000	0.410496000
1	5.431628000	-0.643152000	0.398940000
1	2.388189000	-4.803853000	-0.473001000
1	-0.247884000	-5.173050000	-1.085991000
1	-4.296762000	-2.013539000	-2.038848000
1	-4.653362000	0.693378000	-2.139086000
1	-1.603349000	4.855291000	-1.301362000
1	1.004393000	5.224299000	-0.577712000
1	3.891328000	-2.709686000	-0.046473000
1	-2.268991000	-3.574002000	-1.511529000
1	-3.108588000	2.759912000	-1.717911000
1	3.001741000	3.622678000	-0.048662000
1	-0.001234000	-0.020688000	0.622224000
6	-0.172697000	0.001542000	2.815419000
6	0.185691000	1.445404000	2.974943000
1	1.196078000	1.644529000	2.584888000
1	-0.534902000	2.108734000	2.480428000
1	0.196599000	1.714916000	4.051884000
6	-1.572810000	-0.435911000	2.741919000
8	-1.952233000	-1.605494000	2.788938000
8	-2.445933000	0.621431000	2.629061000
6	-3.835462000	0.243978000	2.523199000
1	-4.148638000	-0.339326000	3.402418000
1	-4.389769000	1.189115000	2.467409000
1	-4.002894000	-0.356801000	1.616496000
6	0.858341000	-1.045905000	3.082455000
1	1.103831000	-1.068136000	4.164737000
1	0.496242000	-2.043687000	2.802456000
1	1.796383000	-0.822609000	2.549283000

(porphyrin)Co-H--2.00 Å—C(CH₃)₂COOCH₃
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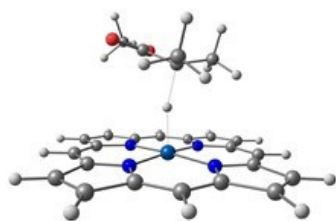
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7	-1.518338000	-0.298137000	-1.261435000
7	0.047250000	1.986518000	-0.834888000
6	2.897777000	1.588044000	-0.120826000
6	4.297402000	1.411628000	0.188919000
6	4.538712000	0.066396000	0.162532000
6	3.283871000	-0.573985000	-0.155947000
6	3.123013000	-1.948666000	-0.257430000
6	1.915740000	-2.571027000	-0.539443000
6	1.751038000	-4.004529000	-0.613340000
6	0.430776000	-4.234092000	-0.879051000
6	-0.203992000	-2.940141000	-0.975130000
6	-1.549861000	-2.762156000	-1.257571000
6	-2.155475000	-1.522661000	-1.400871000
6	-3.545534000	-1.346169000	-1.750966000
6	-3.762622000	0.001194000	-1.828318000
6	-2.506313000	0.642175000	-1.515512000
6	-2.333030000	2.017868000	-1.471555000
6	-1.137023000	2.639855000	-1.144657000
6	-0.971251000	4.073119000	-1.076171000
6	0.324787000	4.301264000	-0.707753000
6	0.947585000	3.006240000	-0.560354000
6	2.279306000	2.826753000	-0.214781000
1	4.992707000	2.225696000	0.387648000
1	5.474530000	-0.462308000	0.336831000
1	2.554817000	-4.725729000	-0.474093000
1	-0.084970000	-5.184470000	-1.005999000
1	-4.246539000	-2.161650000	-1.921685000
1	-4.680918000	0.531339000	-2.076274000
1	-1.757763000	4.795763000	-1.287859000
1	0.833198000	5.251764000	-0.553942000
1	3.998959000	-2.580279000	-0.094119000
1	-2.167977000	-3.652616000	-1.389330000
1	-3.194218000	2.650498000	-1.697595000
1	2.883925000	3.716520000	-0.025585000
1	0.011677000	-0.021218000	0.691622000
6	-0.165149000	-0.044301000	2.683657000
6	0.205338000	1.384351000	2.943029000
1	1.231070000	1.590605000	2.601070000
1	-0.488169000	2.086753000	2.464430000
1	0.179396000	1.583849000	4.034507000
6	-1.580351000	-0.456940000	2.605246000
8	-1.977036000	-1.619223000	2.638953000
8	-2.430750000	0.615753000	2.503680000
6	-3.827471000	0.266863000	2.381132000
1	-4.154756000	-0.335579000	3.241861000
1	-4.363666000	1.223389000	2.350292000
1	-3.999689000	-0.303363000	1.455717000
6	0.831548000	-1.119643000	2.981042000
1	0.965222000	-1.211304000	4.078968000
1	0.492360000	-2.094743000	2.608144000
1	1.816586000	-0.874790000	2.554934000

(porphyrin)Co--H--1.80 Å—C(CH₃)₂COOCH₃
E = -1480.94879541



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7	0.716478000	-1.926292000	-0.749211000
7	-1.518752000	-0.304007000	-1.243361000
7	0.048405000	1.985076000	-0.820197000
6	2.906832000	1.587022000	-0.127775000
6	4.307657000	1.411457000	0.178508000
6	4.545122000	0.065178000	0.172383000
6	3.287361000	-0.576609000	-0.132927000
6	3.123684000	-1.952339000	-0.221483000
6	1.917467000	-2.576323000	-0.506801000
6	1.754528000	-4.010105000	-0.584358000
6	0.437486000	-4.240349000	-0.865770000
6	-0.197840000	-2.946594000	-0.965069000
6	-1.541682000	-2.768505000	-1.259388000
6	-2.150239000	-1.529275000	-1.397524000
6	-3.539929000	-1.353445000	-1.750404000
6	-3.761619000	-0.005847000	-1.812869000
6	-2.507838000	0.636142000	-1.491162000
6	-2.336547000	2.012319000	-1.439874000
6	-1.138634000	2.636228000	-1.121727000
6	-0.971065000	4.070019000	-1.064073000
6	0.330306000	4.299543000	-0.715195000
6	0.953921000	3.004809000	-0.566083000
6	2.289437000	2.825916000	-0.233019000
1	5.006107000	2.226382000	0.362232000
1	5.480333000	-0.463133000	0.351182000
1	2.557365000	-4.731086000	-0.438546000
1	-0.075445000	-5.191118000	-1.001061000
1	-4.237840000	-2.169168000	-1.932450000
1	-4.681054000	0.523582000	-2.058249000
1	-1.759339000	4.792168000	-1.270949000
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1	3.998678000	-2.583657000	-0.051872000
1	-2.156757000	-3.659337000	-1.402684000
1	-3.199593000	2.644279000	-1.660785000
1	2.897469000	3.716668000	-0.059993000
1	-0.018645000	-0.029355000	0.773262000
6	-0.164429000	-0.022453000	2.567335000
6	0.184579000	1.407689000	2.872039000
1	1.221960000	1.625089000	2.577448000
1	-0.490996000	2.114661000	2.375210000
1	0.106737000	1.581297000	3.964520000
6	-1.591409000	-0.446230000	2.552921000
8	-1.977274000	-1.606236000	2.640376000
8	-2.445030000	0.617722000	2.440321000
6	-3.845382000	0.263815000	2.367289000
1	-4.144597000	-0.319691000	3.250662000
1	-4.383758000	1.218749000	2.331149000
1	-4.042412000	-0.326289000	1.459658000
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1	0.880139000	-1.171456000	4.042141000
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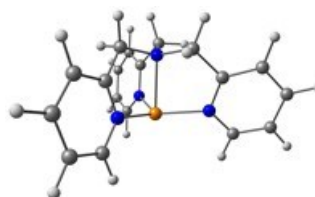
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7	-1.509748000	-0.232718000	-1.298013000
7	0.137102000	1.997030000	-0.819372000
6	2.966638000	1.481958000	-0.072526000
6	4.352865000	1.250134000	0.262461000
6	4.538339000	-0.104474000	0.252452000
6	3.263666000	-0.695848000	-0.084076000
6	3.049456000	-2.063965000	-0.190989000
6	1.827354000	-2.640728000	-0.509145000
6	1.613811000	-4.066517000	-0.611239000
6	0.296176000	-4.244436000	-0.926456000
6	-0.289778000	-2.926926000	-1.021510000
6	-1.618473000	-2.694802000	-1.348979000
6	-2.179184000	-1.432199000	-1.486230000
6	-3.551774000	-1.199729000	-1.872762000
6	-3.722113000	0.155995000	-1.922024000
6	-2.454573000	0.747474000	-1.559530000
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6	-1.017864000	2.692995000	-1.141064000
6	-0.795955000	4.119150000	-1.071308000
6	0.506912000	4.296442000	-0.697690000
6	1.077934000	2.977868000	-0.544581000
6	2.399095000	2.744628000	-0.186197000
1	5.078399000	2.035924000	0.466921000
1	5.448615000	-0.669089000	0.448118000
1	2.385888000	-4.818771000	-0.457621000
1	-0.246809000	-5.174240000	-1.087616000
1	-4.274427000	-1.986139000	-2.084865000
1	-4.615212000	0.721664000	-2.183197000
1	-1.551695000	4.872693000	-1.287389000
1	1.050880000	5.226810000	-0.542399000
1	3.896710000	-2.729268000	-0.010832000
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1	-3.065163000	2.782140000	-1.723578000
1	3.037776000	3.610431000	0.002255000
1	-0.147110000	-0.033422000	0.887436000
6	-0.207650000	-0.000540000	2.485952000
6	0.123359000	1.434658000	2.831357000
1	1.154693000	1.672376000	2.532749000
1	-0.562742000	2.144103000	2.352956000
1	0.048648000	1.575396000	3.926918000
6	-1.642372000	-0.437548000	2.612934000
8	-2.006386000	-1.586790000	2.814886000
8	-2.510774000	0.606999000	2.474506000
6	-3.910570000	0.242827000	2.528377000
1	-4.147585000	-0.240883000	3.487538000
1	-4.459092000	1.186536000	2.422508000
1	-4.158194000	-0.444395000	1.706069000
6	0.792616000	-1.046340000	2.916228000
1	0.826297000	-1.089511000	4.021770000
1	0.513354000	-2.043603000	2.553337000
1	1.799234000	-0.790045000	2.556052000

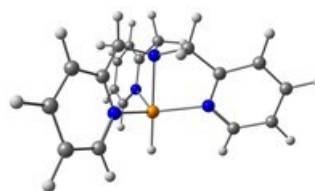
B3. [Cu(TPMA)]⁺ system

[Cu(TPMA)]⁺
E = -1112.11632825



29	0.000003000	-0.000520000	-0.837267000
7	1.789385000	-0.950714000	-0.580917000
6	2.763661000	-1.158926000	-1.497381000
1	2.519693000	-0.886656000	-2.526930000
6	4.279288000	-2.006458000	0.163813000
1	5.249345000	-2.411942000	0.459719000
6	3.278593000	-1.791281000	1.117870000
1	3.451040000	-2.027193000	2.170983000
6	2.042184000	-1.273361000	0.716902000
6	0.897351000	-1.120535000	1.717349000
1	0.293707000	-2.044818000	1.674976000
1	1.308797000	-1.060659000	2.745001000
7	0.000714000	-0.000860000	1.397061000
6	0.522134000	1.335161000	1.718470000
1	1.624496000	1.274419000	1.679486000
1	0.261913000	1.661636000	2.745419000
6	0.084042000	2.403786000	0.717609000
6	-0.083955000	3.733569000	1.118555000
1	0.035470000	4.001016000	2.171496000
6	-0.381108000	2.971492000	-1.495701000
1	-0.498972000	2.623732000	-2.524653000
7	-0.071992000	2.023611000	-0.579943000
6	-1.416794000	-0.217895000	1.719774000
1	-1.916007000	0.767072000	1.682347000
1	-1.568655000	-0.607222000	2.746610000
6	-2.123852000	-1.130661000	0.718391000
7	-1.718607000	-1.073190000	-0.579442000
6	-2.387316000	-1.811546000	-1.496085000
1	-2.029125000	-1.736996000	-2.525521000
6	-3.471640000	-2.627603000	-1.170479000
1	-3.975864000	-3.199117000	-1.951762000
6	-3.191070000	-1.941914000	1.119436000
1	-3.480127000	-1.974806000	2.172893000
6	-3.879717000	-2.698852000	0.165155000
1	-4.716701000	-3.335201000	0.461023000
6	-0.398689000	4.708041000	0.165097000
1	-0.530517000	5.750976000	0.461565000
6	-0.545705000	4.318683000	-1.169866000
1	-0.792239000	5.040642000	-1.950376000
6	4.013570000	-1.687630000	-1.171602000
1	4.761295000	-1.836144000	-1.952700000

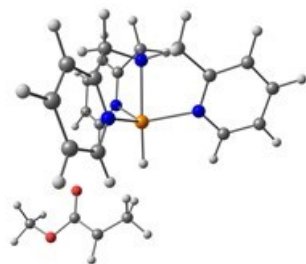
[(TPMA)Cu-H]⁺
E = -1112.66691346



29	-0.001339000	-0.001484000	-0.947732000
7	0.571524000	2.005863000	-0.548413000
6	0.560048000	3.023251000	-1.433849000
1	0.292875000	2.755907000	-2.459137000
6	1.193942000	4.602771000	0.265335000
1	1.433648000	5.618695000	0.587485000

6	1.201409000	3.549169000	1.187014000
1	1.446251000	3.724738000	2.237441000
6	0.893577000	2.258546000	0.742622000
6	0.966887000	1.046391000	1.656140000
1	1.977270000	0.609796000	1.567934000
1	0.834359000	1.343044000	2.714591000
7	-0.000346000	-0.000408000	1.249493000
6	-1.390804000	0.315815000	1.653385000
1	-1.517405000	1.408764000	1.558128000
1	-1.582811000	0.058373000	2.712876000
6	-2.404028000	-0.356513000	0.741892000
6	-3.677055000	-0.730334000	1.186536000
1	-3.952028000	-0.601533000	2.236269000
6	-2.899858000	-1.032842000	-1.432871000
1	-2.534896000	-1.133434000	-2.457924000
7	-2.023631000	-0.514235000	-0.548314000
6	0.422222000	-1.361626000	1.655286000
1	-0.460299000	-2.019046000	1.564680000
1	0.744223000	-1.396311000	2.713984000
6	1.510557000	-1.902697000	0.742311000
7	1.454410000	-1.496731000	-0.548661000
6	2.343099000	-1.994044000	-1.432952000
1	2.245268000	-1.629316000	-2.458373000
6	3.324784000	-2.918369000	-1.067400000
1	4.022398000	-3.297530000	-1.816277000
6	2.474463000	-2.813974000	1.187653000
1	2.502310000	-3.115059000	2.237769000
6	3.393301000	-3.332080000	0.267276000
1	4.153924000	-4.046594000	0.590189000
1	-0.001501000	-0.001805000	-2.504354000
6	-4.586565000	-1.263956000	0.265891000
1	-5.587308000	-1.560675000	0.588086000
6	-4.193292000	-1.414578000	-1.068240000
1	-4.871623000	-1.826667000	-1.817448000
6	0.871727000	4.335409000	-1.069533000
1	0.853974000	5.128248000	-1.819398000

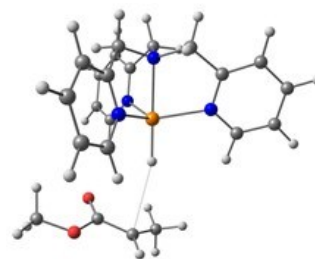
[(TPMA)Cu--H--4.00 Å--CH(CH₃)COOCH₃]⁺
E = -1112.66691346



29	-0.636174000	-0.022823000	-0.384732000
7	-0.940226000	2.079547000	-0.284515000
6	-0.544180000	2.987734000	-1.200674000
1	0.046922000	2.595281000	-2.031930000
6	-1.631835000	4.774005000	-0.012349000
1	-1.908118000	5.825594000	0.094106000
6	-2.047714000	3.833720000	0.938149000
1	-2.651232000	4.134963000	1.798052000
6	-1.676039000	2.493765000	0.776131000
6	-2.011628000	1.430420000	1.809585000
1	-1.162296000	1.355129000	2.511239000
1	-2.897071000	1.728321000	2.404623000
7	-2.181679000	0.099866000	1.184645000
6	-3.476817000	-0.051575000	0.486364000
1	-3.729638000	0.929428000	0.046456000
1	-4.297461000	-0.314354000	1.182200000
6	-3.387626000	-1.065431000	-0.643048000

6	-4.491224000	-1.824892000	-1.049310000
1	-5.439239000	-1.743913000	-0.511712000
6	-2.066657000	-1.978161000	-2.332992000
1	-1.080036000	-2.002782000	-2.801808000
7	-2.191086000	-1.148692000	-1.275231000
6	-1.885142000	-1.019077000	2.107399000
1	-2.270472000	-1.940493000	1.635912000
1	-2.409245000	-0.908574000	3.076884000
6	-0.389313000	-1.180646000	2.322216000
7	0.402092000	-0.874709000	1.262845000
6	1.735070000	-1.058758000	1.369587000
1	2.350752000	-0.800763000	0.503652000
6	2.332170000	-1.558970000	2.531316000
1	3.415214000	-1.689345000	2.555608000
6	0.137511000	-1.669150000	3.522416000
1	-0.527192000	-1.893116000	4.360620000
6	1.520872000	-1.866670000	3.627443000
1	1.954034000	-2.250321000	4.554295000
1	0.427185000	-0.113218000	-1.533083000
6	-4.360097000	-2.680476000	-2.149632000
1	-5.208111000	-3.281443000	-2.486015000
6	-3.126328000	-2.756288000	-2.805951000
1	-2.979807000	-3.411114000	-3.666874000
6	-0.862541000	4.344708000	-1.099723000
1	-0.517993000	5.044248000	-1.863547000
6	5.059789000	-0.204720000	-1.073374000
6	4.346710000	-0.113371000	-2.331273000
8	4.637432000	-0.768143000	-0.054843000
8	6.275375000	0.420853000	-1.134821000
6	7.071299000	0.351466000	0.070977000
1	7.254049000	-0.696600000	0.351649000
1	6.558649000	0.862410000	0.900023000
1	8.011934000	0.858187000	-0.173090000
1	4.747107000	0.548807000	-3.102162000
6	3.069294000	-0.786160000	-2.497525000
1	2.787705000	-0.914550000	-3.552367000
1	3.033352000	-1.743200000	-1.953793000
1	2.120463000	-0.239315000	-2.033019000

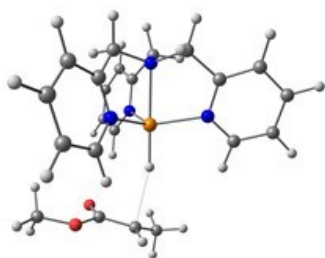
[(TPMA)Cu--H--3.04 Å--CH(CH₃)COOCH₃]⁺
E = -1419.8094096



29	0.322111000	-0.089766000	0.259373000
7	0.163157000	2.029404000	0.257564000
6	-0.556647000	2.770445000	1.125736000
1	-1.167370000	2.207413000	1.835789000
6	0.280277000	4.819321000	0.181697000
1	0.332432000	5.910209000	0.153434000
6	1.029623000	4.052199000	-0.719059000
1	1.673951000	4.529415000	-1.461699000
6	0.940451000	2.656477000	-0.658555000
6	1.650804000	1.752744000	-1.653275000
1	0.955278000	1.541793000	-2.484631000
1	2.530443000	2.264242000	-2.090091000
7	2.011263000	0.452328000	-1.041550000
6	3.198081000	0.543389000	-0.160368000
1	3.161664000	1.527461000	0.339497000
1	4.144449000	0.507738000	-0.734368000

6	3.179079000	-0.532783000	0.912904000
6	4.353918000	-1.060332000	1.461768000
1	5.327882000	-0.745857000	1.078615000
6	1.863976000	-1.806919000	2.354810000
1	0.849717000	-2.068825000	2.665254000
7	1.953235000	-0.908815000	1.351620000
6	2.115406000	-0.644042000	-2.033474000
1	2.630292000	-1.484545000	-1.535619000
1	2.734045000	-0.356099000	-2.905648000
6	0.743831000	-1.122237000	-2.479240000
7	-0.234936000	-1.070330000	-1.541601000
6	-1.463332000	-1.544887000	-1.846741000
1	-2.227238000	-1.474185000	-1.066545000
6	-1.757640000	-2.093128000	-3.099863000
1	-2.764241000	-2.464589000	-3.299974000
6	0.517732000	-1.641666000	-3.758239000
1	1.325218000	-1.658262000	-4.494542000
6	-0.753749000	-2.139168000	-4.072258000
1	-0.954980000	-2.551394000	-5.063904000
1	-0.863302000	-0.460565000	1.207234000
6	4.257946000	-1.988710000	2.505442000
1	5.160506000	-2.412966000	2.951386000
6	2.990507000	-2.366413000	2.963342000
1	2.871302000	-3.087477000	3.774095000
6	-0.530177000	4.167792000	1.118260000
1	-1.129556000	4.728166000	1.838148000
6	-4.065978000	-0.616734000	1.080666000
6	-3.588915000	-1.251506000	2.296755000
8	-4.155777000	-1.153466000	-0.027840000
8	-4.435252000	0.686811000	1.307281000
6	-4.991667000	1.372009000	0.161613000
1	-5.874870000	0.836426000	-0.216564000
1	-4.247004000	1.446379000	-0.645654000
1	-5.271232000	2.367772000	0.525577000
1	-3.530755000	-0.635836000	3.197803000
6	-3.349073000	-2.713454000	2.366361000
1	-4.208252000	-3.217593000	2.855628000
1	-3.239293000	-3.151177000	1.364308000
1	-2.467835000	-2.953669000	2.983196000

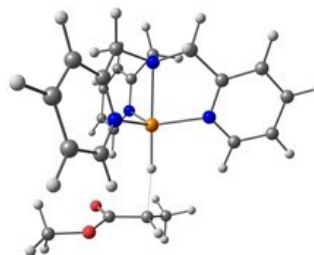
[(TPMA)Cu--H--2.44 Å--CH(CH₃)COOCH₃]⁺
E = -1419.8178372



29	-0.305741000	-0.086754000	-0.244920000
7	0.232614000	1.918082000	0.086104000
6	1.079947000	2.647622000	-0.670836000
1	1.610659000	2.097897000	-1.452004000
6	0.572380000	4.649414000	0.565413000
1	0.697210000	5.718874000	0.750460000
6	-0.304079000	3.893126000	1.353729000
1	-0.871956000	4.357029000	2.164129000
6	-0.443451000	2.525039000	1.093377000
6	-1.300959000	1.619230000	1.964745000
1	-0.652880000	1.182053000	2.744853000
1	-2.081662000	2.205690000	2.487174000
7	-1.871868000	0.495689000	1.188635000
6	-3.032791000	0.890690000	0.362449000
1	-2.855336000	1.926868000	0.023520000

1	-3.976590000	0.899015000	0.942111000
6	-3.170951000	0.013589000	-0.872402000
6	-4.412240000	-0.238850000	-1.468179000
1	-5.327194000	0.142994000	-1.008486000
6	-2.064862000	-1.172748000	-2.548359000
1	-1.102659000	-1.522296000	-2.929381000
7	-2.014911000	-0.456361000	-1.404767000
6	-2.114109000	-0.719274000	2.000139000
1	-2.759505000	-1.385781000	1.400978000
1	-2.661806000	-0.494672000	2.936193000
6	-0.818507000	-1.457612000	2.300465000
7	0.131559000	-1.411564000	1.332231000
6	1.283311000	-2.098970000	1.507356000
1	2.027758000	-2.018695000	0.710296000
6	1.525804000	-2.863631000	2.653092000
1	2.470553000	-3.401354000	2.750918000
6	-0.637956000	-2.190450000	3.478357000
1	-1.418649000	-2.199126000	4.243137000
6	0.551611000	-2.909144000	3.655390000
1	0.714468000	-3.490236000	4.566153000
1	0.796796000	-0.479050000	-1.286626000
6	-4.459838000	-0.978088000	-2.656117000
1	-5.417271000	-1.184557000	-3.139954000
6	-3.264024000	-1.449997000	-3.209042000
1	-3.255566000	-2.030848000	-4.133128000
6	1.281227000	4.014744000	-0.460454000
1	1.976560000	4.566199000	-1.095952000
6	3.638312000	-0.697490000	-1.287034000
6	2.854438000	-1.054070000	-2.465210000
8	3.984944000	-1.469441000	-0.391096000
8	3.997660000	0.631874000	-1.300327000
6	4.841582000	1.040782000	-0.197767000
1	5.762364000	0.440158000	-0.173231000
1	4.313640000	0.921995000	0.760863000
1	5.075441000	2.095638000	-0.384815000
1	2.695233000	-0.269045000	-3.207970000
6	2.700744000	-2.480767000	-2.853984000
1	3.584761000	-2.792745000	-3.450868000
1	2.664601000	-3.142618000	-1.977642000
1	1.821380000	-2.646774000	-3.492863000

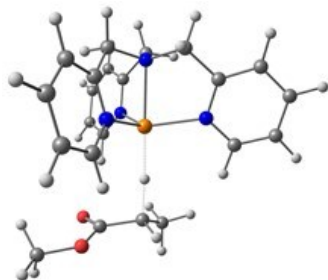
[(TPMA)Cu--H--1.94 Å--CH(CH₃)COOCH₃]⁺
E = -1419.8432314



29	-0.239943000	-0.061177000	-0.199530000
7	0.315254000	1.901293000	0.278425000
6	1.187545000	2.678084000	-0.401486000
1	1.744579000	2.183165000	-1.200987000
6	0.648654000	4.597567000	0.946174000
1	0.770747000	5.651922000	1.204926000
6	-0.253167000	3.794515000	1.655109000
1	-0.844657000	4.206681000	2.476485000
6	-0.390593000	2.447037000	1.301976000
6	-1.286078000	1.499657000	2.089260000
1	-0.664071000	0.999900000	2.852930000
1	-2.064120000	2.069622000	2.634429000
7	-1.858478000	0.444221000	1.229472000
6	-2.979395000	0.909182000	0.390104000

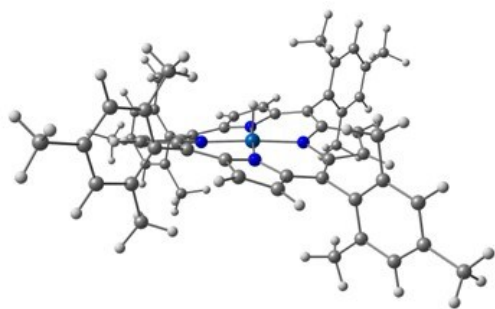
1	-2.787880000	1.969252000	0.145406000	29	0.225260000	-0.041944000	0.186952000
1	-3.950375000	0.874134000	0.922500000	7	-0.405580000	1.811670000	-0.517115000
6	-3.067934000	0.140453000	-0.920955000	6	-1.323784000	2.632058000	0.043941000
6	-4.288272000	-0.046977000	-1.581254000	1	-1.881742000	2.220864000	0.888864000
1	-5.215983000	0.303052000	-1.121732000	6	-0.829719000	4.399511000	-1.511233000
6	-1.912701000	-0.904130000	-2.655486000	1	-0.986911000	5.409193000	-1.897558000
1	-0.941318000	-1.228315000	-3.035207000	6	0.121420000	3.555765000	-2.096456000
7	-1.895299000	-0.292602000	-1.450593000	1	0.718484000	3.891818000	-2.947914000
6	-2.129934000	-0.824246000	1.937059000	6	0.305823000	2.266446000	-1.583308000
1	-2.772294000	-1.434019000	1.276879000	6	1.272070000	1.287007000	-2.241762000
1	-2.692940000	-0.670154000	2.878834000	1	0.694738000	0.667741000	-2.951385000
6	-0.851661000	-1.606152000	2.206362000	1	2.020815000	1.842800000	-2.841505000
7	0.128785000	-1.504332000	1.271688000	7	1.887427000	0.374119000	-1.266451000
6	1.261726000	-2.227706000	1.431538000	6	2.938146000	0.982760000	-0.437973000
1	2.034042000	-2.103585000	0.666841000	1	2.691004000	2.054124000	-0.328692000
6	1.454498000	-3.083121000	2.520607000	1	3.939661000	0.935914000	-0.911362000
1	2.385811000	-3.646153000	2.604222000	6	2.998426000	0.378636000	0.960469000
6	-0.719696000	-2.430507000	3.329162000	6	4.204837000	0.318299000	1.668509000
1	-1.524202000	-2.479659000	4.067310000	1	5.130474000	0.648320000	1.190200000
6	0.449348000	-3.185434000	3.487434000	6	1.838379000	-0.499069000	2.779112000
1	0.572801000	-3.837082000	4.355613000	1	0.873849000	-0.818584000	3.179491000
1	0.917218000	-0.414039000	-1.264657000	7	1.824662000	-0.035756000	1.508185000
6	-4.300120000	-0.678629000	-2.830222000	6	2.215758000	-0.960968000	-1.792147000
1	-5.241161000	-0.832448000	-3.363263000	1	2.863873000	-1.454497000	-1.045890000
6	-3.088318000	-1.111100000	-3.380228000	1	2.794081000	-0.918960000	-2.737248000
1	-3.049833000	-1.607914000	-4.351349000	6	0.974500000	-1.825452000	-1.983424000
6	1.385947000	4.027594000	-0.097136000	7	-0.040044000	-1.657804000	-1.092961000
1	2.101499000	4.615670000	-0.674735000	6	-1.134461000	-2.448781000	-1.203494000
6	3.446945000	-0.677112000	-1.371682000	1	-1.942029000	-2.270129000	-0.487585000
6	2.410357000	-0.944884000	-2.383736000	6	-1.254472000	-3.436386000	-2.185245000
8	3.865595000	-1.485196000	-0.546494000	1	-2.158784000	-4.046186000	-2.227617000
8	3.917597000	0.608404000	-1.457669000	6	0.913694000	-2.783601000	-3.001540000
6	4.973376000	0.935087000	-0.517742000	1	1.744160000	-2.880277000	-3.705558000
1	5.828556000	0.257675000	-0.651954000	6	-0.213422000	-3.607833000	-3.102618000
1	4.609578000	0.852894000	0.517338000	1	-0.278237000	-4.363129000	-3.889299000
1	5.259812000	1.967538000	-0.749986000	1	-1.099142000	-0.394458000	1.384238000
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6	2.168993000	-2.367915000	-2.788888000	1	5.140724000	-0.212426000	3.551477000
1	2.988093000	-2.702758000	-3.456056000	6	2.999100000	-0.572625000	3.551596000
1	2.165318000	-3.044997000	-1.923846000	1	2.950045000	-0.953674000	4.573280000
1	1.231630000	-2.486011000	-3.351021000	6	-1.568899000	3.926171000	-0.422124000
				1	-2.320771000	4.547185000	0.068335000
				6	-3.382087000	-0.594362000	1.367741000
				6	-2.188351000	-0.716648000	2.269346000
				8	-3.786131000	-1.468387000	0.613745000
				8	-3.965850000	0.632848000	1.473034000
				6	-5.142677000	0.831644000	0.640013000
				1	-5.911260000	0.086355000	0.887004000
				1	-4.879591000	0.742888000	-0.423797000
				1	-5.494148000	1.842777000	0.874677000
				1	-2.148524000	0.093641000	3.007947000
				6	-1.966791000	-2.107803000	2.840661000
				1	-2.772596000	-2.355377000	3.552591000
				1	-1.976029000	-2.873682000	2.053124000
				1	-1.014052000	-2.175021000	3.385784000

[(TPMA)Cu--H--1.44 Å--CH(CH₃)COOCH₃]⁺
E = -1419.8857709



C. QM/MM calculations using BP86/UFF, LANL2DZ on M and 6-311+G(d,p) on O, N, C, H

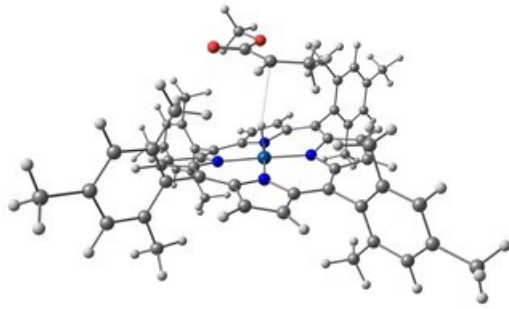
(TMP)Co(H)
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6	-2.83801800	0.94786900	-0.31541500
6	-3.64477200	2.14800900	-0.21628300
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6	3.15270000	2.82058500	-0.22096900
6	2.59672600	1.48554000	-0.31821300
6	3.35255800	0.33018200	-0.54789800
6	2.83479300	-0.95316800	-0.34055000
6	3.63764900	-2.15804900	-0.26812200
6	2.81925400	-3.15941100	0.15803900
6	1.48709200	-2.60058400	0.26816400
6	0.33169800	-3.35371200	0.50315300
1	-2.20523400	-4.72332600	0.33672900
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1	0.00096200	-0.00650600	1.43791300
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1	-7.90508600	-0.80553600	0.42777400
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6	-0.73854600	7.47490200	1.70089400
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6	4.78583100	0.47335900	-0.93980500
6	5.14036800	0.52176400	-2.30805300
6	5.79382000	0.56057000	0.05063900
6	6.48941000	0.65570300	-2.67025500
6	7.13533800	0.69407100	-0.33842100

6	7.48733500	0.74188800	-1.69161500
1	6.76431000	0.69297100	-3.71768800
1	7.91342200	0.76144100	0.41311000
6	0.47268200	-4.77830100	0.92346100
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6	0.63769300	-6.43651400	2.70107900
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1	-6.34518300	-0.67002300	2.16362200
1	-4.76146900	-1.41525000	1.76052100
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1	-4.55247600	-0.40066700	-4.39580500
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1	-9.23054300	0.01295900	-2.69126200
1	-9.04909400	-1.78637000	-2.71655300
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1	3.54449000	-0.53171100	-3.29635200
1	3.37049000	1.27029200	-3.27790000
1	4.53494200	0.48473100	-4.40084600
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6	8.93059000	0.88495900	-2.07765500
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1	9.51092900	0.02820300	-1.67499600
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(TMP)Co--H--3.00 Å--CHCH₃COOCH₃
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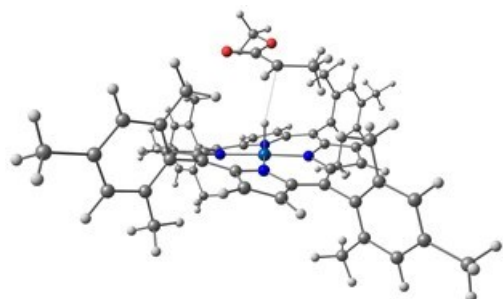


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7	-1.576110000	1.266842000	-0.511606000
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6	3.092796000	2.902477000	-0.599678000
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6	-2.647726000	-1.485447000	-0.680820000
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8	1.037264000	-1.042278000	4.147124000
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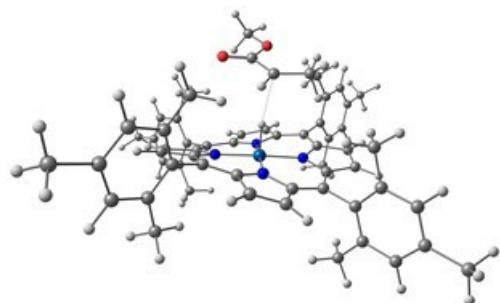


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6	2.807837000	-0.795847000	-0.887376000
6	3.647010000	-1.977505000	-0.916842000
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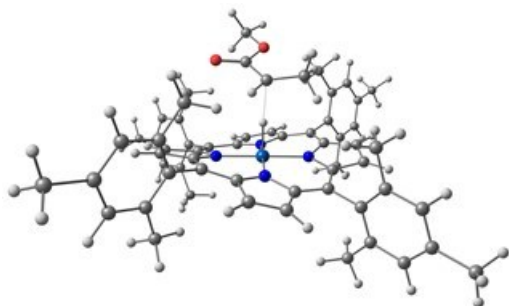
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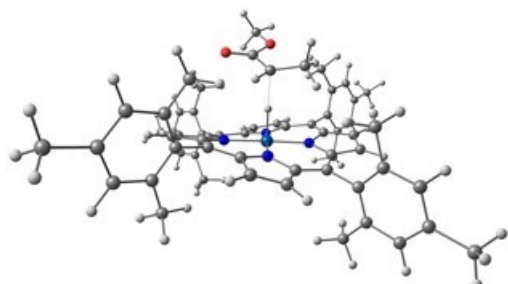


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1	-3.977798000	-0.361238000	-3.438255000
1	-3.517563000	-2.106058000	-3.291695000
1	-4.893730000	-1.618019000	-4.341394000

6	-5.224516000	-1.211253000	1.624213000
1	-6.043487000	-1.353884000	2.360685000
1	-4.411595000	-1.924597000	1.872562000
1	-4.845178000	-0.173448000	1.729211000
6	-8.928648000	-2.444488000	-1.527197000
1	-9.156122000	-2.595285000	-2.603967000
1	-9.137850000	-3.392460000	-0.988170000
1	-9.597218000	-1.649283000	-1.135251000
6	-1.433314000	4.110204000	2.834410000
1	-2.163750000	3.282953000	2.714964000
1	-0.402653000	3.697263000	2.831226000
1	-1.610666000	4.585911000	3.822216000
6	-1.359843000	5.297980000	-2.138761000
1	-0.547783000	5.925753000	-2.562266000
1	-1.092129000	4.236285000	-2.306945000
1	-2.299033000	5.502921000	-2.694490000
6	-2.482479000	8.774529000	1.265272000
1	-2.605262000	8.940558000	2.356728000
1	-1.691434000	9.459074000	0.892961000
1	-3.441401000	9.021075000	0.762640000
6	-1.288741000	-0.986399000	3.290676000
1	-2.055869000	-1.097004000	2.509496000
1	-0.701651000	-1.910548000	3.363449000
1	-1.827501000	-0.858769000	4.252536000
6	-0.432146000	0.204238000	3.031368000
1	-0.901195000	1.145990000	2.743082000
6	0.944065000	0.356605000	3.507196000
1	1.564348000	1.416678000	3.528761000
8	1.479309000	-0.831558000	3.944437000
6	2.849452000	-0.747096000	4.393166000
1	2.936254000	-0.061730000	5.249871000
1	3.123513000	-1.768526000	4.684342000
1	3.498945000	-0.386861000	3.581849000

(TMP)Co--H--1.90 Å--CHCH₃COOCH₃
E = -1441.61348816



27	-0.091899000	0.009010000	-0.343453000
7	0.898034000	1.714078000	-0.398136000
7	1.591941000	-0.989298000	-0.555043000
7	-1.093051000	-1.693294000	-0.344381000
7	-1.797578000	1.012293000	-0.350156000
6	0.403571000	2.976632000	-0.090950000
1	1.474617000	3.953732000	-0.115831000
6	2.603792000	3.296865000	-0.489673000
6	2.252758000	1.897716000	-0.639927000
6	3.171991000	0.885198000	-0.932415000
6	2.845459000	-0.473265000	-0.864900000
6	3.814500000	-1.546740000	-0.967117000
6	3.170414000	-2.699263000	-0.639007000
6	1.784639000	-2.356326000	-0.392651000
6	0.785265000	-3.288961000	-0.096590000
6	-0.574777000	-2.962332000	-0.111364000
6	-1.646106000	-3.936389000	-0.049285000
6	-2.803985000	-3.271995000	-0.313476000
6	-2.465237000	-1.871361000	-0.470512000
6	-3.405173000	-0.851269000	-0.658313000

6	-3.073750000	0.505156000	-0.571025000
6	-4.047407000	1.579425000	-0.553478000
6	-3.375257000	2.722339000	-0.247705000
6	-1.973036000	2.373906000	-0.137281000
6	-0.946431000	3.301731000	0.075281000
1	1.369919000	5.016288000	0.097332000
1	3.596972000	3.720684000	-0.629504000
1	4.864858000	-1.430149000	-1.229942000
1	3.592899000	-3.702012000	-0.596030000
1	-1.524218000	-5.004061000	0.127291000
1	-3.806021000	-3.693631000	-0.377399000
1	-5.117426000	1.468888000	-0.723222000
1	-3.791576000	3.722191000	-0.134580000
1	0.062411000	-0.046379000	1.141019000
6	4.584694000	1.267214000	-1.227915000
6	5.524660000	1.386472000	-0.176038000
6	4.987238000	1.512814000	-2.560905000
6	6.848481000	1.748096000	-0.469178000
6	6.316981000	1.872445000	-2.827172000
6	7.247929000	1.991111000	-1.789386000
1	7.571269000	1.840464000	0.332748000
1	6.633333000	2.061946000	-3.846369000
6	1.183768000	-4.698414000	0.191141000
6	1.257232000	-5.641388000	-0.863551000
6	1.491357000	-5.102107000	1.514496000
6	1.622402000	-6.967125000	-0.584168000
6	1.851299000	-6.433885000	1.763687000
6	1.917169000	-7.367202000	0.724417000
1	1.677939000	-7.691141000	-1.388397000
1	2.084131000	-6.746535000	2.775494000
6	-4.831287000	-1.226342000	-0.892288000
6	-5.305877000	-1.408867000	-2.211907000
6	-5.713521000	-1.395649000	0.201662000
6	-6.649228000	-1.754731000	-2.423438000
6	-7.052294000	-1.740960000	-0.037146000
6	-7.523639000	-1.920674000	-1.342167000
1	-7.016262000	-1.894869000	-3.433235000
1	-7.734650000	-1.872572000	0.794608000
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6	-1.462564000	5.138410000	1.715693000
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6	5.127092000	1.130540000	1.255650000
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1	4.318358000	1.829715000	1.554461000
6	4.009222000	1.393188000	-3.700517000
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1	3.172288000	2.107762000	-3.553140000
6	8.663677000	2.377178000	-2.104096000
1	9.286847000	2.432633000	-1.186212000
1	9.111865000	1.625660000	-2.787696000
1	8.677920000	3.371280000	-2.598568000
6	0.955041000	-5.244876000	-2.286512000
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1	1.182875000	-3.119401000	2.400076000

6	2.305836000	-8.785310000	1.024865000	1	-0.555729000	5.900298000	-2.594590000
1	2.316364000	-9.410509000	0.106738000	1	-1.105419000	4.219965000	-2.295475000
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1	-3.986759000	-0.201946000	-3.410514000	1	-1.539994000	9.494743000	0.843850000
1	-3.547360000	-1.956214000	-3.326024000	1	-3.298181000	9.075212000	0.780506000
1	-4.918582000	-1.415067000	-4.355994000	6	-1.324379000	-0.893563000	3.261141000
6	-5.238522000	-1.215114000	1.620703000	1	-2.136440000	-0.949830000	2.521733000
1	-6.058466000	-1.373947000	2.352818000	1	-0.794833000	-1.854098000	3.298716000
1	-4.433556000	-1.945857000	1.843304000	1	-1.797323000	-0.738305000	4.252592000
1	-4.847282000	-0.185922000	1.761088000	6	-0.407041000	0.243782000	2.959101000
6	-8.960870000	-2.289727000	-1.567085000	1	-0.836911000	1.208564000	2.686431000
1	-9.191453000	-2.398734000	-2.648233000	6	0.967591000	0.346165000	3.467224000
1	-9.181709000	-3.253699000	-1.062176000	8	1.627565000	1.380263000	3.497803000
1	-9.618724000	-1.500615000	-1.145791000	8	1.444387000	-0.859520000	3.919672000
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1	-2.027101000	3.355964000	2.775388000	1	2.907488000	-0.139956000	5.247055000
1	-0.255922000	3.741470000	2.823238000	1	3.031650000	-1.858921000	4.701465000
1	-1.413152000	4.665199000	3.842078000	1	3.488519000	-0.506464000	3.593592000
6	-1.358174000	5.286359000	-2.134134000				