

Supporting information

Experimental and theoretical insights into the synthesis of α -aminoalkyl naphthol derivatives catalyzed by manganese complex immobilized on multi-wall carbon nanotubes

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COORDINATES

R1

C	2.868667000	1.940363000	0.405459000
C	1.490673000	2.204023000	-0.037710000
C	0.575158000	0.997067000	-0.140942000
C	1.192933000	-0.345360000	-0.191019000
C	2.556781000	-0.493100000	0.189983000
C	3.344369000	0.682153000	0.532905000
C	0.521564000	-1.483259000	-0.677303000
C	1.140424000	-2.732445000	-0.716255000
C	2.459946000	-2.883182000	-0.272916000
C	3.161339000	-1.763504000	0.165460000
C	-0.750333000	1.321242000	-0.138984000
O	1.100855000	3.344955000	-0.245252000
C	-1.982412000	0.538048000	0.015242000
C	-3.143174000	0.976027000	-0.656916000
C	-4.356561000	0.302198000	-0.512274000
C	-4.446936000	-0.802030000	0.340366000
C	-3.314438000	-1.224875000	1.046729000
C	-2.095734000	-0.567617000	0.884529000
H	3.485287000	2.820380000	0.601248000
H	4.378299000	0.517230000	0.852739000
H	-0.498957000	-1.388397000	-1.046172000
H	0.589149000	-3.594122000	-1.101077000
H	2.942196000	-3.863414000	-0.292179000
H	4.205154000	-1.856894000	0.477803000
H	-0.914678000	2.401928000	-0.236392000
H	-3.081963000	1.852821000	-1.307174000
H	-5.238493000	0.649139000	-1.056608000
H	-5.399120000	-1.323562000	0.466134000
H	-3.383908000	-2.071606000	1.734474000
H	-1.223408000	-0.897654000	1.451122000

R2

N	2.312033000	-0.000001000	-0.051340000
C	0.938789000	0.000002000	-0.007163000
C	0.196761000	-1.199389000	-0.003065000
C	-1.195127000	-1.135752000	0.002710000

N	-1.900413000	0.000000000	0.005752000
C	-1.195129000	1.135749000	0.002740000
C	0.196761000	1.199390000	-0.003075000
H	0.704511000	-2.167934000	-0.006833000
H	-1.772232000	-2.069032000	0.006616000
H	-1.772233000	2.069032000	0.006596000
H	0.704507000	2.167937000	-0.006868000
H	2.800889000	0.854350000	0.183353000
H	2.800885000	-0.854348000	0.183372000

pre-TS

C	1.335096000	3.152952000	0.455087000
C	0.568184000	2.001276000	-0.032049000
C	1.313758000	0.691089000	-0.126136000
C	2.789507000	0.739940000	-0.185057000
C	3.458356000	1.929744000	0.219132000
C	2.680212000	3.099843000	0.591204000
C	3.571573000	-0.308583000	-0.704806000
C	4.962458000	-0.221178000	-0.754154000
C	5.618298000	0.924829000	-0.286809000
C	4.863982000	1.994780000	0.185484000
C	0.501898000	-0.409049000	-0.087793000
O	-0.631698000	2.112037000	-0.283605000
C	0.730599000	-1.843499000	0.104124000
C	1.777245000	-2.386831000	0.880296000
C	1.877410000	-3.763212000	1.073922000
C	0.945367000	-4.631156000	0.491132000
C	-0.109209000	-4.108996000	-0.263674000
C	-0.227307000	-2.729962000	-0.436323000
H	0.762345000	4.058797000	0.665006000
H	3.229286000	3.981769000	0.936085000
H	3.083067000	-1.201780000	-1.093171000
H	5.539334000	-1.052640000	-1.166791000
H	6.708594000	0.988451000	-0.314637000
H	5.358187000	2.912302000	0.516462000
N	-2.896476000	0.479878000	-1.329998000
H	2.500036000	-1.722442000	1.355708000
H	2.686066000	-4.164186000	1.690247000
H	1.032629000	-5.710205000	0.641041000
H	-0.853278000	-4.777278000	-0.704002000
H	-1.071914000	-2.317717000	-0.994887000
C	-4.072479000	0.530575000	-0.619241000
C	-4.137964000	1.150412000	0.647657000
C	-5.342550000	1.137808000	1.345661000
N	-6.472138000	0.572459000	0.901972000
C	-6.408453000	-0.009931000	-0.299513000
C	-5.262363000	-0.061944000	-1.091114000
H	-3.253945000	1.639120000	1.064305000
H	-5.394840000	1.621640000	2.329369000
H	-7.333935000	-0.471080000	-0.667927000
H	-5.287683000	-0.558960000	-2.065292000

H	-2.148621000	1.122820000	-1.065301000
H	-0.560410000	-0.160996000	-0.183423000
H	-2.962755000	0.276284000	-2.319957000

TS

C	-2.548105000	-2.932494000	0.091925000
C	-1.288176000	-2.251482000	0.283312000
C	-1.269231000	-0.801715000	0.260970000
C	-2.512775000	-0.063285000	0.085812000
C	-3.724796000	-0.802472000	-0.141446000
C	-3.695844000	-2.236863000	-0.134440000
C	-2.652542000	1.347279000	0.209390000
C	-3.872173000	1.984439000	0.040725000
C	-5.039736000	1.252500000	-0.246889000
C	-4.955696000	-0.125847000	-0.319261000
C	0.057426000	-0.260465000	0.494396000
O	-0.208775000	-2.926784000	0.386184000
C	0.495230000	1.153211000	0.361057000
C	1.177711000	1.762843000	1.426424000
C	1.638171000	3.079287000	1.322759000
C	1.449370000	3.794621000	0.138753000
C	0.794188000	3.189193000	-0.941666000
C	0.319547000	1.883599000	-0.830565000
H	-2.520706000	-4.024087000	0.108917000
H	-4.637168000	-2.769267000	-0.302797000
H	-1.792167000	1.957633000	0.467339000
H	-3.923018000	3.071702000	0.145837000
H	-5.996190000	1.762220000	-0.384634000
H	-5.852841000	-0.724639000	-0.501464000
H	0.575700000	-0.779693000	1.310044000
H	1.342019000	1.201257000	2.349621000
H	2.155931000	3.540695000	2.167120000
H	1.816351000	4.820333000	0.051926000
H	0.647951000	3.742847000	-1.872524000
H	-0.212538000	1.428642000	-1.670120000
N	1.200076000	-1.179615000	-0.771809000
C	2.577642000	-1.067850000	-0.539830000
C	3.397370000	-0.214798000	-1.294773000
C	4.752338000	-0.133904000	-0.969347000
N	5.320869000	-0.813278000	0.030708000
C	4.532910000	-1.620125000	0.747676000
C	3.167434000	-1.789975000	0.512109000
H	5.013692000	-2.177249000	1.560601000
H	5.409874000	0.522265000	-1.552127000
H	2.987767000	0.373821000	-2.118990000
H	2.569806000	-2.479897000	1.111738000
H	0.742912000	-2.105027000	-0.422167000
H	0.894630000	-0.871215000	-1.692629000

[P]

C	-0.029815000	2.534666000	2.248230000
C	-0.030858000	1.133821000	2.002566000

C	0.296406000	0.612170000	0.752788000
C	0.708096000	1.524816000	-0.283504000
C	0.699322000	2.939594000	-0.032957000
C	0.312667000	3.411537000	1.253609000
C	1.145597000	1.095759000	-1.571429000
C	1.518347000	1.998780000	-2.548146000
C	1.479034000	3.390028000	-2.300048000
C	1.081786000	3.844000000	-1.060072000
C	0.136324000	-0.887829000	0.477462000
O	-0.402034000	0.383171000	3.079048000
C	1.447116000	-1.656951000	0.253113000
C	2.673750000	-1.146746000	0.703696000
C	3.850746000	-1.887744000	0.563263000
C	3.821914000	-3.151671000	-0.031711000
C	2.604365000	-3.671402000	-0.479941000
C	1.426853000	-2.932577000	-0.335194000
H	-0.315235000	2.873783000	3.245714000
H	0.303098000	4.488300000	1.441840000
H	1.227869000	0.031944000	-1.791596000
H	1.855607000	1.631179000	-3.520795000
H	1.771302000	4.095065000	-3.081831000
H	1.058532000	4.915763000	-0.844034000
N	-0.824176000	-1.189549000	-0.575840000
H	2.711384000	-0.156067000	1.161147000
H	4.796483000	-1.469304000	0.917072000
H	4.743018000	-3.728800000	-0.145221000
H	2.567441000	-4.661590000	-0.941631000
H	0.478191000	-3.352524000	-0.675814000
C	-2.190595000	-1.049477000	-0.472450000
C	-2.862847000	-0.740416000	0.728574000
C	-4.258128000	-0.677529000	0.722998000
N	-5.026862000	-0.879077000	-0.348839000
C	-4.385764000	-1.156910000	-1.490956000
C	-3.003779000	-1.251856000	-1.611056000
H	-2.327307000	-0.527826000	1.653084000
H	-4.778599000	-0.438448000	1.658956000
H	-5.012531000	-1.317297000	-2.377060000
H	-2.551253000	-1.487305000	-2.578619000
H	-0.458948000	-1.224736000	-1.519085000
H	-0.238111000	-0.554851000	2.922512000
H	-0.300627000	-1.346641000	1.382707000

IM[Cata_{Cu}-R1]

C	0.669938000	2.446900000	-1.993704000
C	0.904285000	1.311067000	-1.103260000
C	2.309895000	1.105942000	-0.625795000
C	3.268089000	2.221610000	-0.776745000
C	2.937841000	3.318245000	-1.622607000
C	1.633843000	3.362941000	-2.252154000
C	4.468265000	2.304076000	-0.042796000
C	5.341578000	3.378483000	-0.197128000
C	5.042811000	4.418709000	-1.088270000
C	3.840097000	4.388703000	-1.784062000
C	2.569781000	-0.149882000	-0.133760000
O	-0.025245000	0.528455000	-0.854937000

C	3.821989000	-0.874714000	0.090101000
C	3.865646000	-1.845873000	1.116041000
C	5.026881000	-2.593590000	1.325505000
C	6.139256000	-2.424624000	0.496504000
C	6.090828000	-1.495380000	-0.551695000
C	4.949248000	-0.723546000	-0.749771000
H	-0.330718000	2.522944000	-2.424216000
H	1.421047000	4.206264000	-2.916946000
H	4.715957000	1.521327000	0.672726000
H	6.262381000	3.409262000	0.390759000
H	5.733833000	5.255481000	-1.214438000
H	3.567874000	5.211916000	-2.450477000
H	1.671298000	-0.738996000	0.084425000
H	2.994811000	-1.998486000	1.764336000
H	5.053016000	-3.323627000	2.138416000
H	7.040232000	-3.023359000	0.655098000
H	6.947971000	-1.377214000	-1.219737000
H	4.915484000	-0.011469000	-1.576186000
C	-3.450551000	1.670793000	0.362801000
N	-2.968958000	0.504099000	-0.062512000
C	-3.469826000	-0.114858000	-1.148916000
C	-4.518907000	0.462949000	-1.874032000
C	-5.041858000	1.686105000	-1.454953000
C	-4.504339000	2.296682000	-0.319524000
C	-2.840108000	-1.418879000	-1.480033000
N	-1.852368000	-1.808134000	-0.651524000
C	-1.209396000	-2.960004000	-0.824401000
C	-1.540099000	-3.816143000	-1.882216000
C	-2.560004000	-3.443631000	-2.761911000
C	-3.217176000	-2.231470000	-2.557617000
Cl	-5.120655000	3.811853000	0.248081000
Cl	-0.688598000	-5.311308000	-2.085435000
Cu	-1.282337000	-0.417247000	0.797445000
O	-1.145991000	0.963474000	2.102878000
O	-0.043354000	-1.643231000	1.597726000
C	0.323860000	-1.704888000	2.845232000
C	-0.645132000	-1.356302000	3.951216000
O	1.420878000	-2.125052000	3.196679000
C	-1.746403000	0.878554000	3.258378000
O	-2.539604000	1.726969000	3.655409000
C	-1.461486000	-0.303968000	4.142089000
H	-2.994998000	2.093267000	1.267289000
H	-4.931614000	-0.027035000	-2.756178000
H	-5.859941000	2.162544000	-1.998164000
H	-0.420409000	-3.184934000	-0.100152000
H	-2.832108000	-4.096716000	-3.592969000
H	-4.015344000	-1.930608000	-3.236563000
H	-0.558811000	-2.072176000	4.776754000
H	-2.012157000	-0.248216000	5.086455000

IM[Cata_{Cu}-R1-R2]

C	-1.534855000	0.055100000	-2.529795000
C	-0.823384000	0.572513000	-1.364567000
C	-1.212707000	1.936719000	-0.895390000

C	-2.531198000	2.457726000	-1.307001000
C	-3.210031000	1.848370000	-2.400108000
C	-2.636633000	0.674194000	-3.023240000
C	-3.202555000	3.479583000	-0.608308000
C	-4.453744000	3.935412000	-1.017781000
C	-5.082619000	3.381486000	-2.142116000
C	-4.464407000	2.336497000	-2.818143000
C	-0.245418000	2.586427000	-0.169347000
O	0.101333000	-0.091692000	-0.858645000
C	-0.048024000	3.986705000	0.204113000
C	0.728873000	4.258305000	1.353983000
C	0.989355000	5.574580000	1.737940000
C	0.524519000	6.640567000	0.962714000
C	-0.205214000	6.384511000	-0.205858000
C	-0.494616000	5.074958000	-0.579332000
H	-1.145891000	-0.867806000	-2.965531000
H	-3.158201000	0.252847000	-3.888683000
H	-2.746399000	3.910511000	0.282160000
H	-4.949165000	4.725721000	-0.448357000
H	-6.058964000	3.748848000	-2.466569000
H	-4.958270000	1.862544000	-3.670944000
H	0.579840000	1.938963000	0.141204000
H	1.123956000	3.426323000	1.944526000
H	1.576467000	5.766396000	2.639379000
H	0.744176000	7.670532000	1.255734000
H	-0.543816000	7.213463000	-0.832561000
H	-1.047083000	4.888321000	-1.501153000
N	3.030334000	0.591192000	-0.049150000
C	4.101677000	1.015629000	-0.779156000
C	4.183565000	0.816322000	-2.177367000
C	5.320650000	1.235911000	-2.862465000
N	6.374954000	1.830934000	-2.292907000
C	6.295514000	2.023745000	-0.969960000
C	5.214283000	1.649052000	-0.177699000
H	7.156261000	2.515718000	-0.498554000
H	5.377953000	1.079533000	-3.947895000
H	3.358856000	0.338891000	-2.714353000
H	5.221133000	1.841535000	0.898232000
H	2.883595000	0.913298000	0.911528000
H	2.178871000	0.313514000	-0.528982000
C	-2.832297000	-2.609165000	0.324412000
N	-1.508453000	-2.737793000	0.240361000
C	-0.934465000	-3.756282000	-0.430824000
C	-1.727920000	-4.712424000	-1.076569000
C	-3.116381000	-4.600824000	-1.011080000
C	-3.677808000	-3.537984000	-0.298507000
C	0.549716000	-3.770891000	-0.403158000
N	1.119983000	-2.789321000	0.325253000
C	2.442131000	-2.685937000	0.443719000
C	3.292694000	-3.604327000	-0.188205000
C	2.734470000	-4.633114000	-0.950446000
C	1.346413000	-4.716857000	-1.058595000
Cl	-5.395266000	-3.358252000	-0.179328000
Cl	5.005964000	-3.447757000	-0.018540000
Cu	-0.178162000	-1.385661000	1.117532000

O	-1.620544000	-0.280933000	1.674190000
O	1.187457000	-0.649640000	2.240720000
C	1.116665000	0.499429000	2.831063000
C	0.102676000	0.707904000	3.925178000
O	1.901989000	1.423792000	2.598095000
C	-2.107439000	-0.108194000	2.875995000
O	-3.274853000	-0.355821000	3.152190000
C	-1.219250000	0.463602000	3.945532000
H	-3.203698000	-1.757889000	0.908076000
H	-1.277736000	-5.542215000	-1.621928000
H	-3.761279000	-5.331909000	-1.501920000
H	2.815498000	-1.846097000	1.035240000
H	3.380997000	-5.354987000	-1.452542000
H	0.898583000	-5.514078000	-1.652254000
H	0.543120000	1.191318000	4.804834000
H	-1.778169000	0.716823000	4.851586000

TS[Cata_{Cu} -R1-R2]

C	0.712307000	-2.257729000	-1.795464000
C	-0.151403000	-1.356919000	-1.078102000
C	-1.475468000	-1.799904000	-0.722323000
C	-1.858815000	-3.183273000	-0.974943000
C	-0.959461000	-4.030936000	-1.707959000
C	0.312287000	-3.521223000	-2.117049000
C	-3.030141000	-3.806316000	-0.459962000
C	-3.333140000	-5.131727000	-0.724073000
C	-2.478430000	-5.930256000	-1.510142000
C	-1.300849000	-5.380114000	-1.977448000
C	-2.285691000	-0.777800000	-0.077543000
O	0.242609000	-0.143932000	-0.857573000
C	-3.735343000	-0.808436000	0.212115000
C	-4.172674000	-0.374667000	1.477455000
C	-5.537986000	-0.362704000	1.783123000
C	-6.478367000	-0.742169000	0.823783000
C	-6.053412000	-1.135771000	-0.453194000
C	-4.694883000	-1.170935000	-0.755537000
H	1.689842000	-1.873131000	-2.092850000
H	0.977888000	-4.183163000	-2.679468000
H	-3.699834000	-3.247466000	0.187004000
H	-4.243412000	-5.563796000	-0.299646000
H	-2.729013000	-6.973119000	-1.718271000
H	-0.594693000	-5.988380000	-2.550028000
H	-1.726161000	-0.187806000	0.654247000
H	-3.436477000	-0.039022000	2.213140000
H	-5.864336000	-0.037475000	2.773918000
H	-7.545138000	-0.720915000	1.061523000
H	-6.787581000	-1.419140000	-1.211644000
H	-4.369278000	-1.494729000	-1.747277000
N	-2.155127000	0.751108000	-1.359920000
C	-2.843460000	1.940675000	-1.066358000
C	-3.892818000	2.389834000	-1.882968000
C	-4.549069000	3.572186000	-1.536749000
N	-4.245912000	4.301760000	-0.460491000
C	-3.259422000	3.852398000	0.322609000
C	-2.525885000	2.689543000	0.077719000

H	-3.032597000	4.449078000	1.213811000
H	-5.364213000	3.943789000	-2.169536000
H	-4.187166000	1.835172000	-2.777936000
H	-1.755938000	2.354835000	0.777893000
H	-1.109784000	0.725949000	-1.212285000
H	-2.399776000	0.344052000	-2.261064000
C	3.856506000	-1.422275000	0.268393000
N	3.338364000	-0.218693000	0.025275000
C	3.896952000	0.625616000	-0.864367000
C	5.039540000	0.248933000	-1.580416000
C	5.599851000	-1.007951000	-1.353377000
C	5.006173000	-1.851689000	-0.411837000
C	3.229937000	1.946768000	-0.985080000
N	2.160174000	2.127984000	-0.186474000
C	1.494050000	3.279974000	-0.167020000
C	1.876763000	4.349025000	-0.986580000
C	2.975001000	4.190862000	-1.836267000
C	3.659675000	2.976897000	-1.832747000
Cl	5.670955000	-3.415337000	-0.080638000
Cl	0.991984000	5.837247000	-0.937098000
Cu	1.520119000	0.445359000	0.864304000
O	1.337169000	-1.175038000	1.856867000
O	0.211489000	1.462372000	1.863669000
C	-0.418931000	0.996882000	2.902350000
C	0.375446000	0.502460000	4.086879000
O	-1.641486000	1.021231000	3.011571000
C	1.830420000	-1.333891000	3.056414000
O	2.703059000	-2.158707000	3.311695000
C	1.293469000	-0.475893000	4.165466000
H	3.356306000	-2.032375000	1.031482000
H	5.498634000	0.920954000	-2.305924000
H	6.491283000	-1.331138000	-1.893923000
H	0.646000000	3.337308000	0.520662000
H	3.287716000	5.010261000	-2.485843000
H	4.522476000	2.842970000	-2.485332000
H	0.062100000	0.985217000	5.020139000
H	1.718161000	-0.725171000	5.142523000

[Cata_{Cu}-P]

C	0.326050000	-2.515027000	-1.658194000
C	-0.450788000	-1.441125000	-1.161610000
C	-1.811470000	-1.570274000	-0.848109000
C	-2.398293000	-2.890136000	-0.966557000
C	-1.597765000	-3.973109000	-1.490914000
C	-0.238619000	-3.748743000	-1.833150000
C	-3.725671000	-3.236487000	-0.564731000
C	-4.229435000	-4.513989000	-0.708849000
C	-3.448036000	-5.550212000	-1.266426000
C	-2.152684000	-5.274229000	-1.640720000
C	-2.503539000	-0.289766000	-0.311387000
O	0.223983000	-0.258546000	-1.010981000
C	-4.008225000	-0.271550000	-0.062800000
C	-4.489078000	-0.254161000	1.254958000
C	-5.864847000	-0.205427000	1.505958000

C	-6.773960000	-0.157833000	0.446290000
C	-6.300554000	-0.150982000	-0.870949000
C	-4.928616000	-0.202673000	-1.121213000
H	1.372836000	-2.319694000	-1.895316000
H	0.353637000	-4.580506000	-2.223108000
H	-4.365525000	-2.491238000	-0.109499000
H	-5.249822000	-4.721653000	-0.376119000
H	-3.860782000	-6.555508000	-1.380810000
H	-1.513615000	-6.061088000	-2.051149000
H	-2.026779000	-0.073594000	0.657236000
H	-3.775819000	-0.271565000	2.083132000
H	-6.224801000	-0.195140000	2.538014000
H	-7.848398000	-0.116926000	0.643195000
H	-7.004472000	-0.107727000	-1.706198000
H	-4.577106000	-0.210319000	-2.157070000
N	-2.124179000	0.840132000	-1.214603000
C	-2.413015000	2.176679000	-0.887944000
C	-2.617353000	3.116055000	-1.914928000
C	-2.833071000	4.452395000	-1.580154000
N	-2.867308000	4.910946000	-0.326351000
C	-2.679232000	4.010711000	0.644261000
C	-2.449573000	2.648364000	0.436240000
H	-2.711174000	4.390040000	1.672796000
H	-2.992728000	5.188522000	-2.378016000
H	-2.610626000	2.806397000	-2.964285000
H	-2.287142000	1.984353000	1.288396000
H	-0.471055000	0.454007000	-1.049975000
H	-2.346112000	0.629866000	-2.186117000
C	4.061772000	-1.545231000	-0.063866000
N	3.491850000	-0.341252000	-0.113690000
C	4.034525000	0.671596000	-0.818332000
C	5.218146000	0.477190000	-1.540478000
C	5.832438000	-0.774469000	-1.514927000
C	5.251187000	-1.798436000	-0.762562000
C	3.300577000	1.959454000	-0.736328000
N	2.196444000	1.944042000	0.038033000
C	1.456985000	3.036782000	0.218886000
C	1.799381000	4.248995000	-0.395962000
C	2.935477000	4.296872000	-1.208925000
C	3.694009000	3.139720000	-1.379689000
Cl	5.978863000	-3.366433000	-0.686934000
Cl	0.820106000	5.650882000	-0.145405000
Cu	1.691622000	0.098804000	0.858764000
O	1.565512000	-1.682504000	1.498604000
O	0.299978000	0.871678000	1.920393000
C	-0.417978000	0.286568000	2.830527000
C	0.246131000	-0.510468000	3.924362000
O	-1.638917000	0.424096000	2.901005000
C	1.893400000	-2.076065000	2.701918000
O	2.752767000	-2.926230000	2.903267000
C	1.173909000	-1.482968000	3.879989000
H	3.561482000	-2.297871000	0.558360000
H	5.666009000	1.286956000	-2.116896000
H	6.756197000	-0.957254000	-2.066744000
H	0.581007000	2.927437000	0.865064000

H	3.218783000	5.230608000	-1.697989000
H	4.583971000	3.166138000	-2.008810000
H	-0.192798000	-0.280977000	4.902109000
H	1.467991000	-1.957368000	4.821264000

IM[Cata_{Mn}-R1]

C	-0.329258000	-2.518320000	-1.182881000
C	-0.848332000	-1.243103000	-0.747588000
C	-2.320182000	-1.067573000	-0.618600000
C	-3.187329000	-2.235379000	-0.884921000
C	-2.599079000	-3.442092000	-1.369129000
C	-1.165129000	-3.535616000	-1.516326000
C	-4.567549000	-2.263682000	-0.596507000
C	-5.344197000	-3.392349000	-0.846321000
C	-4.769341000	-4.549912000	-1.389409000
C	-3.402774000	-4.571234000	-1.632728000
C	-2.692608000	0.190570000	-0.194159000
O	-0.065834000	-0.276058000	-0.549963000
C	-3.957182000	0.919010000	-0.147761000
C	-4.148364000	1.834595000	0.913606000
C	-5.310756000	2.603650000	0.978569000
C	-6.275308000	2.513221000	-0.030451000
C	-6.075381000	1.643427000	-1.110519000
C	-4.933455000	0.847547000	-1.166995000
H	0.754175000	-2.614246000	-1.262850000
H	-0.752581000	-4.482086000	-1.878477000
H	-5.044757000	-1.394672000	-0.149908000
H	-6.410251000	-3.371159000	-0.606454000
H	-5.382423000	-5.430802000	-1.593573000
H	-2.924675000	-5.477792000	-2.013665000
H	-1.846995000	0.784335000	0.166793000
H	-3.378706000	1.909069000	1.688466000
H	-5.457438000	3.289150000	1.816989000
H	-7.177453000	3.128941000	0.015206000
H	-6.813633000	1.590469000	-1.914836000
H	-4.776811000	0.184104000	-2.019839000
C	3.576825000	-1.537491000	-0.028553000
N	3.020407000	-0.327525000	-0.234936000
C	3.564578000	0.534181000	-1.140623000
C	4.697979000	0.168222000	-1.884310000
C	5.273760000	-1.080119000	-1.691756000
C	4.702144000	-1.942401000	-0.741243000
C	2.883234000	1.822866000	-1.216708000
N	1.837202000	1.946388000	-0.350268000
C	1.137074000	3.095403000	-0.298247000
C	1.452213000	4.173332000	-1.118053000
C	2.521334000	4.071001000	-2.024605000
C	3.238802000	2.883301000	-2.065585000
Cl	5.390384000	-3.509229000	-0.452199000
Cl	0.523357000	5.637175000	-1.014448000

Mn	1.353205000	0.322700000	0.729340000
O	1.274282000	-1.258856000	1.763017000
O	0.290489000	1.381436000	1.901840000
C	-0.466965000	1.054291000	2.918091000
C	0.141969000	0.314804000	4.079355000
O	-1.640683000	1.385434000	3.011126000
C	1.605633000	-1.527833000	3.004522000
O	2.399477000	-2.412345000	3.291135000
C	0.968639000	-0.745519000	4.117090000
H	3.107069000	-2.161840000	0.738317000
H	5.130621000	0.860118000	-2.607713000
H	6.155066000	-1.390575000	-2.255011000
H	0.323456000	3.124484000	0.430105000
H	2.774387000	4.909864000	-2.674380000
H	4.075517000	2.778141000	-2.757018000
H	-0.247822000	0.681809000	5.035390000
H	1.238426000	-1.149631000	5.097613000

IM[Cata_{Mn}-R1-R2]

C	0.522995000	-2.278417000	1.560503000
C	0.982610000	-1.172208000	0.765657000
C	2.436188000	-0.907393000	0.657055000
C	3.364077000	-1.796115000	1.388524000
C	2.826440000	-2.827483000	2.216513000
C	1.400134000	-3.030812000	2.278034000
C	4.766517000	-1.754742000	1.242495000
C	5.599748000	-2.631053000	1.932441000
C	5.064348000	-3.597947000	2.795505000
C	3.686149000	-3.698090000	2.920363000
C	2.754867000	0.120389000	-0.210960000
O	0.142317000	-0.385582000	0.224281000
C	3.959089000	0.910420000	-0.446327000
C	4.222601000	1.337239000	-1.769392000
C	5.324688000	2.148895000	-2.039580000
C	6.151204000	2.587781000	-0.999609000
C	5.874105000	2.208058000	0.320455000
C	4.795311000	1.371041000	0.596610000
H	-0.550915000	-2.460956000	1.595639000
H	1.028333000	-3.841660000	2.911194000
H	5.220062000	-1.037436000	0.563260000
H	6.681113000	-2.563934000	1.789317000
H	5.721316000	-4.278005000	3.342590000
H	3.244227000	-4.471356000	3.554399000
H	1.918922000	0.417233000	-0.852215000
H	3.560413000	0.996088000	-2.571445000
H	5.532559000	2.451022000	-3.069046000
H	7.005134000	3.235956000	-1.213163000
H	6.502499000	2.570403000	1.138012000
H	4.576877000	1.089321000	1.628866000
N	0.296348000	2.446926000	1.244075000

C	-0.355448000	2.655187000	2.427935000
C	-1.231331000	1.685522000	2.968252000
C	-1.903394000	1.964403000	4.155214000
N	-1.785817000	3.104501000	4.846189000
C	-0.950539000	4.017439000	4.337947000
C	-0.222913000	3.855006000	3.161102000
H	-0.846908000	4.951735000	4.904506000
H	-2.580490000	1.209077000	4.575090000
H	-1.369036000	0.729237000	2.458313000
H	0.439954000	4.650468000	2.808973000
H	0.301743000	1.514320000	0.834014000
H	1.052682000	3.066584000	0.985355000
C	-3.273399000	-2.146288000	0.065228000
N	-2.867150000	-0.917438000	-0.307238000
C	-3.606788000	0.179070000	0.019061000
C	-4.788386000	0.048769000	0.764953000
C	-5.212113000	-1.210983000	1.168121000
C	-4.440619000	-2.325858000	0.803672000
C	-3.066181000	1.436071000	-0.495400000
N	-1.921146000	1.290584000	-1.219666000
C	-1.334847000	2.366929000	-1.773828000
C	-1.868331000	3.642403000	-1.621656000
C	-3.041411000	3.821152000	-0.873030000
C	-3.641687000	2.702119000	-0.311106000
Cl	-4.928575000	-3.924140000	1.269352000
Cl	-1.069723000	5.000743000	-2.351120000
Mn	-1.148422000	-0.570785000	-1.338589000
O	-0.809398000	-2.424526000	-1.494762000
O	0.043293000	-0.020075000	-2.716635000
C	0.910103000	-0.670972000	-3.449966000
C	0.474664000	-1.908023000	-4.189225000
O	2.055454000	-0.280932000	-3.629707000
C	-0.919134000	-3.278194000	-2.487559000
O	-1.534603000	-4.327692000	-2.378269000
C	-0.249518000	-2.971790000	-3.797182000
H	-2.647312000	-2.981990000	-0.262857000
H	-5.374365000	0.929352000	1.029175000
H	-6.125628000	-1.341201000	1.750203000
H	-0.427592000	2.172426000	-2.350070000
H	-3.464336000	4.817786000	-0.739778000
H	-4.553721000	2.813529000	0.275590000
H	0.923535000	-1.950172000	-5.187875000
H	-0.378373000	-3.791165000	-4.510968000

TS[Cata_{Mn}-R1-R2]

C	0.883932000	-2.403444000	-1.220055000
C	-0.083275000	-1.497970000	-0.675153000
C	-1.457613000	-1.906315000	-0.564710000
C	-1.828382000	-3.264144000	-0.951170000
C	-0.825782000	-4.117993000	-1.525769000

C	0.516750000	-3.644779000	-1.651237000
C	-3.100097000	-3.856646000	-0.718497000
C	-3.384413000	-5.158057000	-1.098779000
C	-2.411776000	-5.960987000	-1.726555000
C	-1.146687000	-5.441867000	-1.918815000
C	-2.324753000	-0.891410000	0.009980000
O	0.270345000	-0.279213000	-0.371804000
C	-3.793104000	-0.903321000	0.185061000
C	-4.301618000	-0.587539000	1.459119000
C	-5.682277000	-0.560980000	1.680398000
C	-6.567402000	-0.804300000	0.628300000
C	-6.070561000	-1.077838000	-0.653636000
C	-4.696301000	-1.130764000	-0.872607000
H	1.913043000	-2.055518000	-1.302120000
H	1.263589000	-4.314710000	-2.087150000
H	-3.873072000	-3.295999000	-0.202941000
H	-4.377218000	-5.566854000	-0.892783000
H	-2.647298000	-6.984047000	-2.028820000
H	-0.357937000	-6.055357000	-2.363195000
H	-1.832536000	-0.328242000	0.808637000
H	-3.602234000	-0.360524000	2.267994000
H	-6.064983000	-0.330562000	2.677547000
H	-7.646368000	-0.769311000	0.799343000
H	-6.760950000	-1.252749000	-1.482540000
H	-4.315972000	-1.359406000	-1.871417000
N	-2.056088000	0.683000000	-1.213151000
C	-2.783118000	1.865645000	-0.967830000
C	-3.673974000	2.376344000	-1.922818000
C	-4.369898000	3.549507000	-1.624174000
N	-4.243132000	4.213520000	-0.473424000
C	-3.407220000	3.705525000	0.437673000
C	-2.658989000	2.539924000	0.256451000
H	-3.323199000	4.253417000	1.383216000
H	-5.063511000	3.970362000	-2.362075000
H	-3.812973000	1.880095000	-2.887185000
H	-2.031870000	2.145274000	1.061715000
H	-1.047922000	0.679306000	-0.944764000
H	-2.170021000	0.318202000	-2.157884000
C	4.181624000	-1.051677000	-0.022011000
N	3.431964000	0.063325000	-0.167395000
C	3.816566000	1.035857000	-1.049142000
C	4.969949000	0.871674000	-1.836869000
C	5.734338000	-0.277610000	-1.710771000
C	5.331120000	-1.250548000	-0.775760000
C	2.962961000	2.210813000	-1.033712000
N	1.951766000	2.143776000	-0.112852000
C	1.119094000	3.195935000	0.041972000
C	1.245439000	4.345118000	-0.724881000
C	2.267765000	4.433326000	-1.690277000
C	3.129244000	3.356364000	-1.832153000

Cl	6.264880000	-2.699967000	-0.563342000
Cl	0.139085000	5.665403000	-0.490089000
Mn	1.734925000	0.417608000	0.865644000
O	1.926194000	-1.203366000	1.826730000
O	0.580694000	1.225981000	2.167729000
C	-0.259843000	0.603199000	2.942117000
C	0.270374000	-0.167775000	4.115609000
O	-1.480397000	0.663636000	2.790038000
C	2.209630000	-1.510911000	3.071201000
O	3.175347000	-2.193476000	3.376545000
C	1.282508000	-1.051087000	4.162317000
H	3.837634000	-1.766002000	0.731690000
H	5.269910000	1.649564000	-2.540001000
H	6.634716000	-0.429232000	-2.307760000
H	0.353328000	3.089438000	0.811729000
H	2.373524000	5.331318000	-2.300295000
H	3.936217000	3.399977000	-2.564525000
H	-0.326980000	-0.019784000	5.022040000
H	1.498256000	-1.542705000	5.115737000

[Cata_{Mn}-P]

C	0.423583000	-2.586768000	-1.429815000
C	-0.351661000	-1.489204000	-0.990732000
C	-1.723618000	-1.578325000	-0.727855000
C	-2.325413000	-2.894887000	-0.803538000
C	-1.528472000	-4.007704000	-1.265262000
C	-0.158524000	-3.815785000	-1.583145000
C	-3.661843000	-3.206093000	-0.404132000
C	-4.178892000	-4.482672000	-0.500928000
C	-3.403053000	-5.549342000	-1.006747000
C	-2.098616000	-5.306598000	-1.372244000
C	-2.429480000	-0.268428000	-0.296355000
O	0.336608000	-0.300457000	-0.848495000
C	-3.949619000	-0.213689000	-0.207334000
C	-4.559419000	-0.057135000	1.046267000
C	-5.951562000	0.038481000	1.149345000
C	-6.747314000	-0.008066000	0.002089000
C	-6.144745000	-0.146509000	-1.253691000
C	-4.756477000	-0.245023000	-1.355978000
H	1.479696000	-2.419504000	-1.642522000
H	0.430133000	-4.668432000	-1.930468000
H	-4.296026000	-2.435292000	0.016229000
H	-5.204612000	-4.665857000	-0.170566000
H	-3.827246000	-6.553226000	-1.085713000
H	-1.463951000	-6.118380000	-1.738074000
H	-2.047530000	-0.026760000	0.707104000
H	-3.933161000	-0.014769000	1.941423000
H	-6.413735000	0.157552000	2.132660000
H	-7.834619000	0.069136000	0.082815000
H	-6.760644000	-0.181932000	-2.156056000

H	-4.302605000	-0.371405000	-2.343463000
N	-1.940179000	0.827841000	-1.196144000
C	-2.262265000	2.177261000	-0.926876000
C	-2.454647000	3.072468000	-1.992066000
C	-2.714172000	4.414140000	-1.710781000
N	-2.800522000	4.911770000	-0.475188000
C	-2.618787000	4.052692000	0.532322000
C	-2.348528000	2.690397000	0.377777000
H	-2.690409000	4.467373000	1.544878000
H	-2.866987000	5.118854000	-2.537541000
H	-2.408177000	2.727352000	-3.029122000
H	-2.197663000	2.057573000	1.255661000
H	-0.358365000	0.421722000	-0.970308000
H	-2.123870000	0.596585000	-2.172003000
C	3.985694000	-1.540068000	-0.204800000
N	3.415223000	-0.319282000	-0.173251000
C	3.981626000	0.719363000	-0.849609000
C	5.152725000	0.531010000	-1.601080000
C	5.743161000	-0.724300000	-1.653012000
C	5.147338000	-1.774355000	-0.935373000
C	3.281032000	1.988673000	-0.680742000
N	2.179492000	1.913003000	0.122937000
C	1.465030000	3.025957000	0.384786000
C	1.819413000	4.262321000	-0.146137000
C	2.944846000	4.362998000	-0.980960000
C	3.675939000	3.212579000	-1.243334000
Cl	5.848333000	-3.361096000	-0.954600000
Cl	0.871725000	5.665146000	0.225818000
Mn	1.711539000	0.091911000	0.838094000
O	1.658098000	-1.659786000	1.531771000
O	0.364105000	0.806236000	1.981499000
C	-0.434850000	0.246764000	2.846747000
C	0.129814000	-0.628700000	3.930311000
O	-1.645343000	0.457506000	2.861011000
C	1.808707000	-2.190765000	2.723332000
O	2.548703000	-3.139759000	2.927596000
C	1.029402000	-1.627279000	3.879238000
H	3.492531000	-2.315904000	0.388730000
H	5.602000000	1.364659000	-2.141603000
H	6.652580000	-0.899302000	-2.229728000
H	0.599548000	2.897743000	1.037788000
H	3.230706000	5.326622000	-1.404928000
H	4.557154000	3.264381000	-1.883460000
H	-0.372139000	-0.452852000	4.888263000
H	1.234346000	-2.176246000	4.803322000

Table S1. The calculated values of Zero-point Energies of all structure studied in this work at the B3LYP/SVP level of theory (in kcal/mol).

Structure	Without catalyst	With catalyst	
		Cu	Mn
R1	-729.483681	-	-
R2	-303.322191	-	-
Cata	-	-3508.341059	-3018.857286
Pre-TS	-1032.817699	-	-
TS	-1032.786159	-	-
P	-1032.823644	-	-
IM[Cata-R1]	-	-4237.847208	-3748.410276
IM[Cata-R-	-	-4541.184584	-4051.740839
$\tilde{\text{T}}\tilde{\text{S}}[\text{Cata-R-}$	-	-4541.154634	-4051.720544
$\tilde{\text{C}}[\text{Cata-P}]$	-	-4541.184108	-4051.742045