

Supporting information for

Alkoxyacylation of α,β -Unsaturated Amides Catalyzed by Palladium (II) Complexes: A DFT Study of the Mechanism

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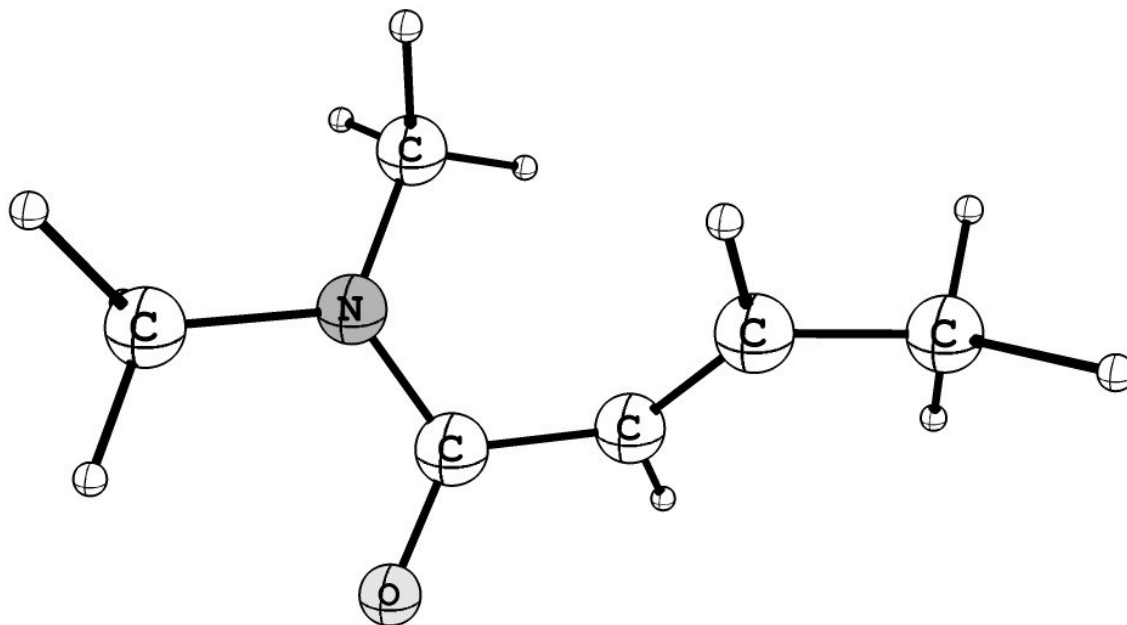
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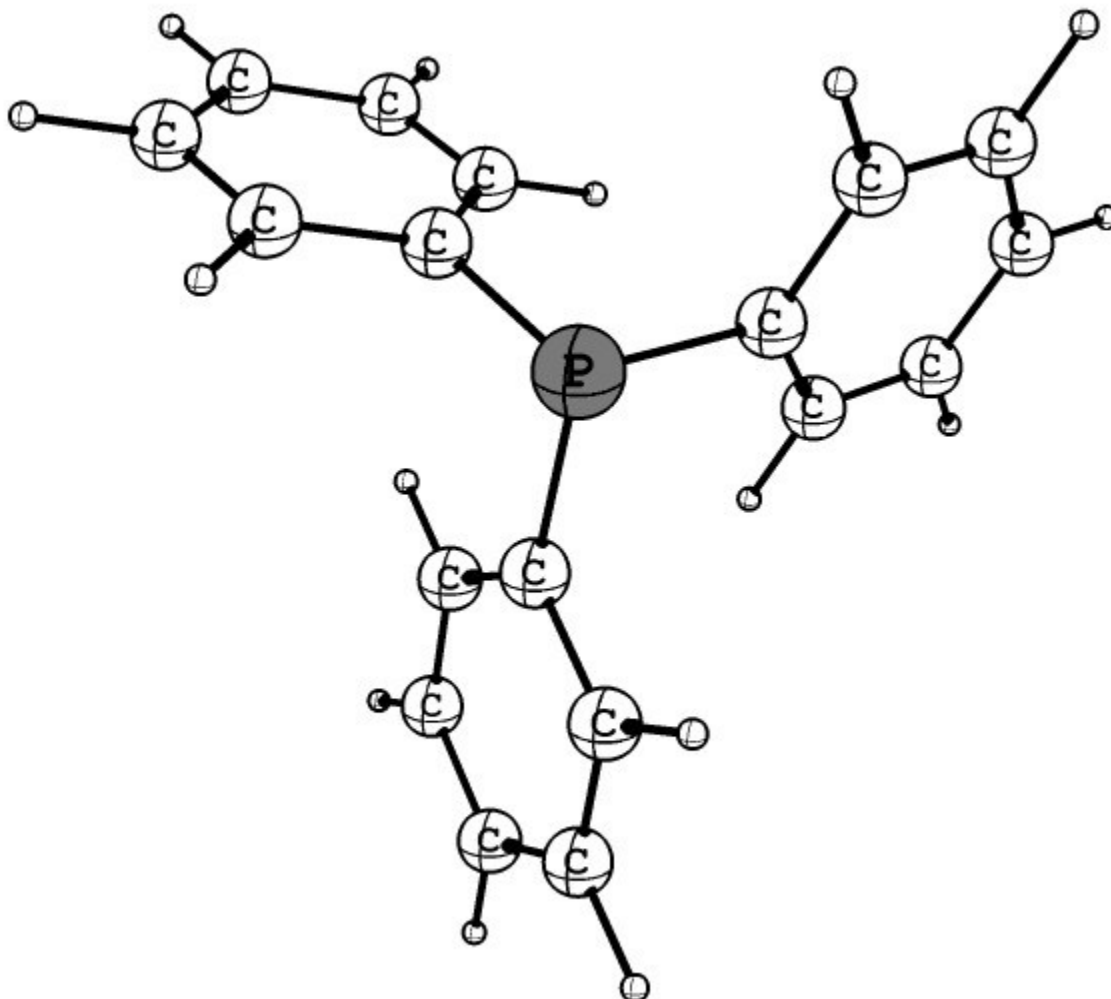
S1. Cartesian coordinates (in Å) of all the B3LYP/ Def2-SVP optimized structures of reactants, intermediates, transition states and products in the hydride cycle in Methanol phase.

α,β -Unsaturated Amide



C	-3.320807000	-0.233302000	0.176325000
C	-1.830388000	-0.215575000	0.300770000
H	-3.675072000	-1.235524000	-0.120827000
H	-3.797263000	-0.013319000	1.147351000
H	-3.679722000	0.498523000	-0.562566000
C	-1.011746000	0.604301000	-0.374406000
H	-1.399962000	-0.924527000	1.018049000
H	-1.427928000	1.359732000	-1.049836000
C	0.455715000	0.761942000	-0.139217000
O	0.912167000	1.903512000	-0.037869000
N	1.241673000	-0.349963000	-0.006541000
C	2.629132000	-0.185937000	0.391899000
H	2.873884000	-0.892538000	1.201987000
H	3.312202000	-0.385049000	-0.453150000
H	2.784775000	0.841013000	0.738285000
C	0.861678000	-1.702997000	-0.376469000
H	1.648144000	-2.139527000	-1.014461000
H	0.747558000	-2.352365000	0.509130000
H	-0.077171000	-1.705381000	-0.938630000

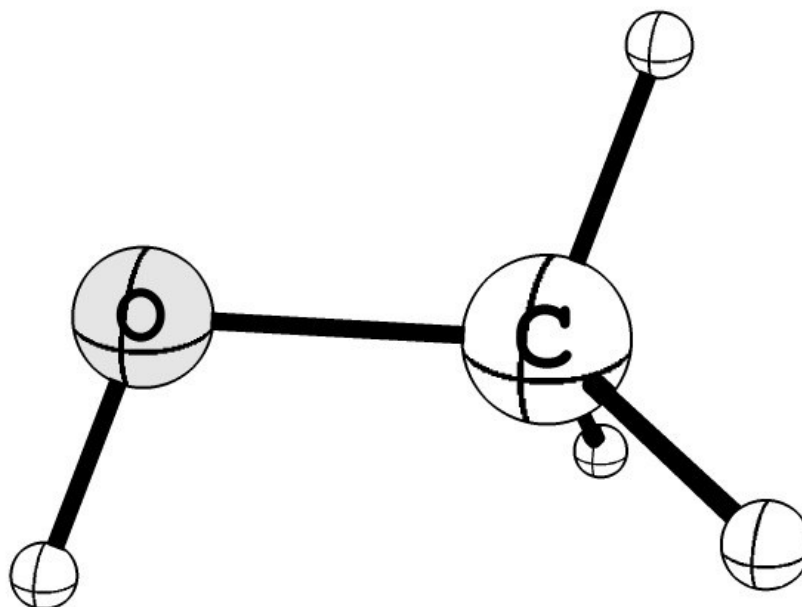
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C	2.301620000	-1.548323000	-0.998282000
C	2.101922000	0.174110000	0.688686000
C	3.499101000	-1.978593000	-0.422520000
H	1.915702000	-2.054418000	-1.887873000
C	3.307195000	-0.249211000	1.257975000
H	1.560049000	1.011168000	1.132275000
C	4.006479000	-1.327313000	0.707278000
H	4.042483000	-2.818885000	-0.861572000
H	3.699094000	0.264529000	2.139366000
H	4.947131000	-1.657416000	1.154491000
C	-1.201623000	-1.135155000	-0.445039000

C	-2.492793000	-1.213801000	-0.996279000
C	-0.898539000	-1.912975000	0.683447000
C	-3.464937000	-2.035105000	-0.421074000
H	-2.739134000	-0.622500000	-1.882937000
C	-1.868575000	-2.744695000	1.252067000
H	0.098665000	-1.866507000	1.124479000
C	-3.153642000	-2.805546000	0.704806000
H	-4.465746000	-2.080787000	-0.857468000
H	-1.618850000	-3.344990000	2.130513000
H	-3.910469000	-3.454642000	1.151680000
C	-0.381421000	1.607874000	-0.444713000
C	-1.215585000	1.735807000	0.676944000
C	0.204338000	2.764152000	-0.989933000
C	-1.452215000	2.992080000	1.244420000
H	-1.679977000	0.849997000	1.113651000
C	-0.021921000	4.016804000	-0.415509000
H	0.846838000	2.680745000	-1.871237000
C	-0.854269000	4.134042000	0.703232000
H	-2.104278000	3.077147000	2.117317000
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H	-1.039077000	5.114249000	1.149131000

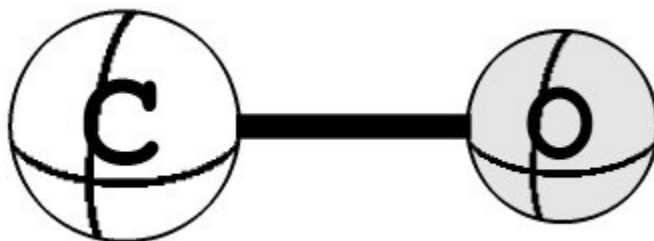
CH₃OH



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H	-0.441934000	1.087689000	-0.895002000

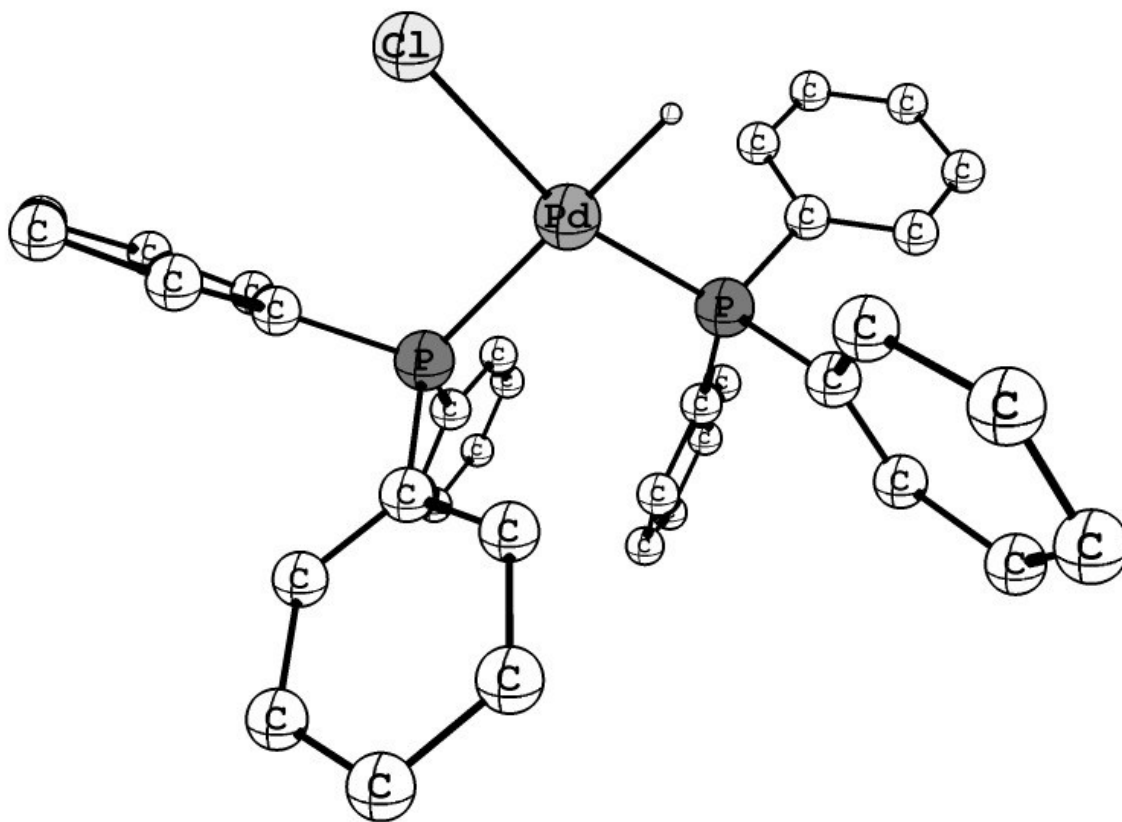
H	1.096002000	0.991787000	0.000000000
O	0.047202000	-0.756148000	0.000000000
H	-0.872967000	-1.051884000	0.000000000

CO



C	0.000000000	0.000000000	-0.645784000
O	0.000000000	0.000000000	0.484338000

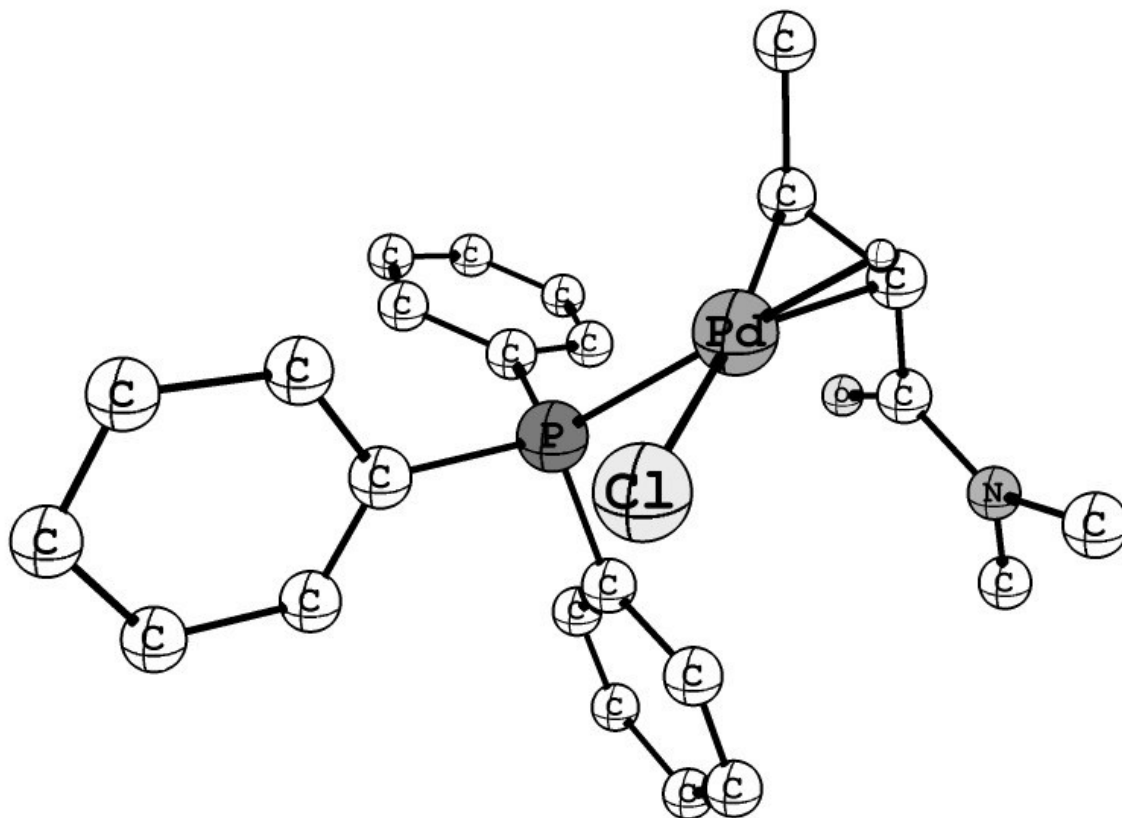
1H



Pd	0.059045000	0.472659000	-1.568695000
H	1.243414000	0.894133000	-2.497742000
P	-1.816431000	-0.037040000	-0.099404000
P	1.893627000	0.096207000	-0.278911000
Cl	-1.389310000	1.107150000	-3.369447000
C	-2.087651000	1.306373000	1.125331000
C	-3.299071000	1.454336000	1.823429000
C	-1.049844000	2.222136000	1.362152000
C	-3.451335000	2.475764000	2.763287000
H	-4.133174000	0.780163000	1.621484000
C	-1.202844000	3.243716000	2.303627000
H	-0.119713000	2.148248000	0.798698000
C	-2.401891000	3.368362000	3.010198000
H	-4.395987000	2.578492000	3.302213000
H	-0.383666000	3.945742000	2.475010000
H	-2.525268000	4.167580000	3.744713000
C	-3.460489000	-0.185312000	-0.904915000
C	-4.056255000	-1.435852000	-1.124381000
C	-4.103308000	0.972486000	-1.374878000
C	-5.281077000	-1.526374000	-1.793786000
H	-3.569032000	-2.344652000	-0.767837000
C	-5.330056000	0.879810000	-2.032942000
H	-3.646928000	1.950928000	-1.217988000
C	-5.922089000	-0.370325000	-2.246321000
H	-5.737165000	-2.506140000	-1.954616000
H	-5.824794000	1.787962000	-2.385465000
H	-6.881881000	-0.441411000	-2.763450000
C	-1.707748000	-1.601232000	0.852646000
C	-0.927154000	-2.632477000	0.309011000
C	-2.399445000	-1.820937000	2.052670000
C	-0.841436000	-3.867146000	0.955173000
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C	-2.310569000	-3.055288000	2.698150000
H	-3.000743000	-1.027295000	2.496565000
C	-1.532539000	-4.080137000	2.150794000
H	-0.220093000	-4.658681000	0.531310000
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H	-1.456369000	-5.042308000	2.662457000
C	1.791694000	-1.040661000	1.157169000
C	2.469612000	-2.268214000	1.166472000
C	0.985257000	-0.693752000	2.253338000
C	2.343793000	-3.132735000	2.257294000
H	3.095539000	-2.557063000	0.322110000
C	0.865513000	-1.556407000	3.341050000
H	0.444645000	0.253291000	2.261011000
C	1.542148000	-2.780306000	3.344482000

H	2.872567000	-4.088505000	2.251576000
H	0.227869000	-1.278240000	4.182368000
H	1.436815000	-3.460797000	4.192242000
C	3.299601000	-0.599169000	-1.230151000
C	4.630076000	-0.339876000	-0.871167000
C	3.026570000	-1.461884000	-2.302662000
C	5.675603000	-0.935547000	-1.582018000
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C	4.073339000	-2.066178000	-3.002500000
H	1.989883000	-1.654998000	-2.589576000
C	5.399611000	-1.801029000	-2.645153000
H	6.709955000	-0.721983000	-1.302958000
H	3.852639000	-2.739474000	-3.833876000
H	6.218658000	-2.266168000	-3.198563000
C	2.523483000	1.660535000	0.447119000
C	2.314687000	2.863623000	-0.247765000
C	3.207277000	1.685041000	1.673469000
C	2.780173000	4.070807000	0.276944000
H	1.772327000	2.850733000	-1.195217000
C	3.670626000	2.895407000	2.195894000
H	3.373544000	0.760310000	2.227413000
C	3.456597000	4.089597000	1.501176000
H	2.606881000	5.000635000	-0.269332000
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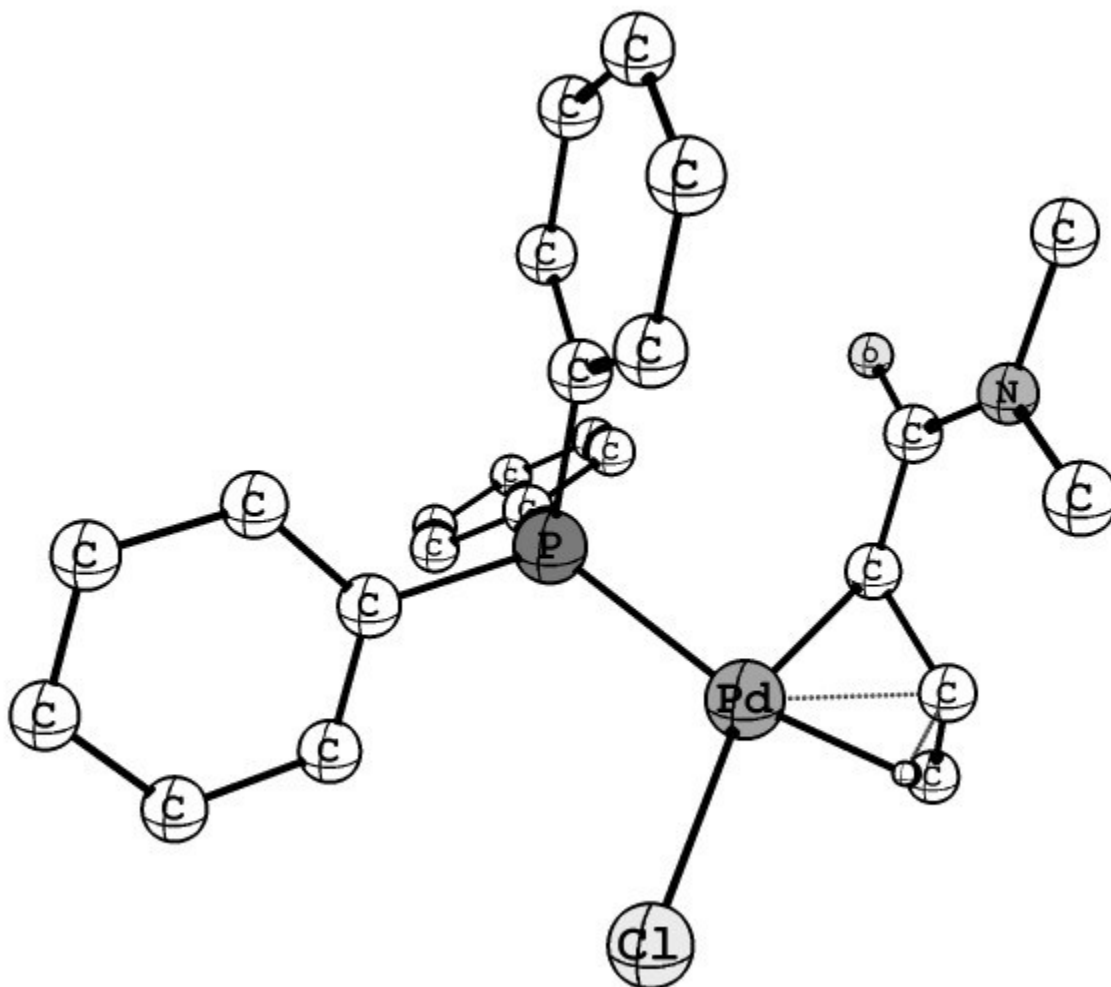
2H



Pd	-0.794429000	-1.271805000	-1.158238000
H	-1.730843000	-2.265941000	-1.888925000
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P	0.797581000	0.144565000	0.093707000
C	-1.449452000	0.421784000	-2.449454000
C	-2.510665000	-0.008735000	-1.677136000
C	-1.255567000	0.062527000	-3.887832000
H	-1.838750000	-0.811264000	-4.174171000
H	-1.564620000	0.908804000	-4.510234000
H	-0.203974000	-0.126595000	-4.107292000
C	-2.915124000	0.733587000	-0.434164000
O	-2.539622000	1.896425000	-0.259404000
N	-3.731226000	0.101909000	0.437506000
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H	-3.506414000	-1.836227000	-0.354269000
H	-3.910906000	-1.759086000	1.353737000
H	-5.160281000	-1.415437000	0.145448000
C	-4.241806000	0.824962000	1.591191000
H	-3.707485000	0.529613000	2.497044000
H	-4.113867000	1.890622000	1.437037000
H	-5.300394000	0.594009000	1.717670000
H	-3.253752000	-0.655246000	-2.122178000

H	-0.898869000	1.283523000	-2.098963000
C	1.370459000	1.754538000	-0.559704000
C	2.669625000	1.928440000	-1.041240000
C	0.472648000	2.825494000	-0.630920000
C	3.063499000	3.147396000	-1.582285000
H	3.382274000	1.118517000	-0.990689000
C	0.872905000	4.042533000	-1.165946000
H	-0.540014000	2.704388000	-0.272732000
C	2.168382000	4.208123000	-1.645457000
H	4.075032000	3.266105000	-1.948573000
H	0.168420000	4.863224000	-1.209334000
H	2.477588000	5.157498000	-2.062942000
C	2.355250000	-0.747394000	0.406413000
C	2.990956000	-0.731106000	1.646235000
C	2.933248000	-1.454954000	-0.649954000
C	4.192786000	-1.407847000	1.825425000
H	2.549517000	-0.196006000	2.475417000
C	4.139535000	-2.117735000	-0.474244000
H	2.431929000	-1.492559000	-1.608420000
C	4.770897000	-2.097424000	0.766006000
H	4.676409000	-1.394140000	2.793557000
H	4.580887000	-2.659942000	-1.300309000
H	5.706361000	-2.623157000	0.906615000
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C	-0.727138000	-0.427448000	2.326307000
C	0.455927000	1.667666000	2.461286000
C	-1.245061000	-0.217407000	3.597027000
H	-0.982009000	-1.326074000	1.780756000
C	-0.072740000	1.880420000	3.728864000
H	1.118677000	2.403418000	2.028048000
C	-0.923192000	0.939522000	4.299033000
H	-1.906250000	-0.953559000	4.035274000
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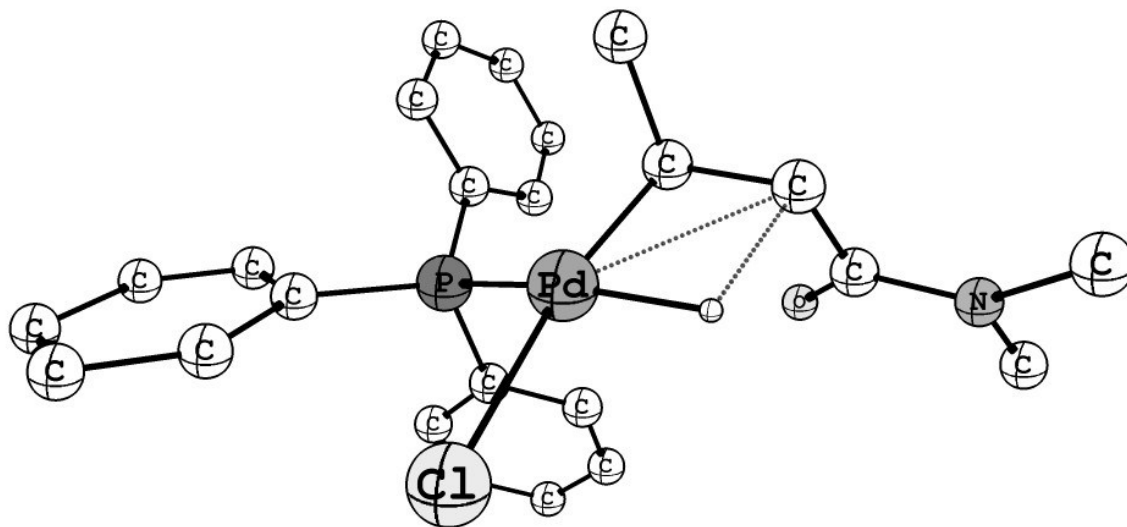
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C	-2.246023000	-0.731040000	1.137127000
C	-2.884562000	0.520028000	0.600362000
O	-2.804551000	1.529517000	1.311750000
N	-3.531069000	0.552045000	-0.599725000
C	-3.560102000	-0.504620000	-1.595059000
H	-3.529345000	-0.046152000	-2.594478000
H	-2.680976000	-1.154193000	-1.518354000
H	-4.475971000	-1.117254000	-1.530770000
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H	-3.728609000	2.268802000	-1.814412000
H	-5.266214000	1.515288000	-1.294193000
H	-4.273880000	2.445169000	-0.121135000
H	-1.780613000	-0.491077000	2.096450000
H	-3.575185000	-2.238719000	0.426138000

P	0.862215000	0.150556000	0.026266000
H	-1.912456000	-2.547662000	-0.100300000
C	-2.463846000	-3.038294000	2.131630000
C	1.272016000	0.753463000	1.712943000
C	0.258958000	1.320182000	2.509389000
C	2.563840000	0.612381000	2.243218000
C	0.545142000	1.739765000	3.809928000
H	-0.751988000	1.455257000	2.117915000
C	2.839708000	1.026895000	3.550051000
H	3.362575000	0.181108000	1.639112000
C	1.833032000	1.591571000	4.336601000
H	-0.246996000	2.186152000	4.415870000
H	3.849714000	0.910347000	3.949822000
H	2.050582000	1.918115000	5.356188000
C	2.497177000	-0.083683000	-0.763140000
C	3.109105000	0.937915000	-1.505571000
C	3.168635000	-1.302765000	-0.575830000
C	4.381374000	0.742989000	-2.049595000
H	2.594077000	1.887677000	-1.658555000
C	4.444662000	-1.488800000	-1.112372000
H	2.684546000	-2.107343000	-0.021730000
C	5.051849000	-0.468061000	-1.851172000
H	4.850615000	1.541813000	-2.628502000
H	4.962917000	-2.438415000	-0.960377000
H	6.047178000	-0.618162000	-2.275994000
C	0.136422000	1.586223000	-0.849615000
C	-0.548512000	1.330290000	-2.049228000
C	0.257256000	2.906088000	-0.393204000
C	-1.098457000	2.380832000	-2.784630000
H	-0.647573000	0.303144000	-2.407529000
C	-0.305012000	3.955580000	-1.126142000
H	0.789606000	3.118807000	0.534731000
C	-0.981722000	3.696054000	-2.321126000
H	-1.626623000	2.171635000	-3.717504000
H	-0.210843000	4.980767000	-0.760976000
H	-1.421324000	4.517880000	-2.890873000
H	-1.513869000	-2.866151000	2.657327000
H	-3.288691000	-2.905235000	2.849821000
H	-2.484841000	-4.077892000	1.776379000

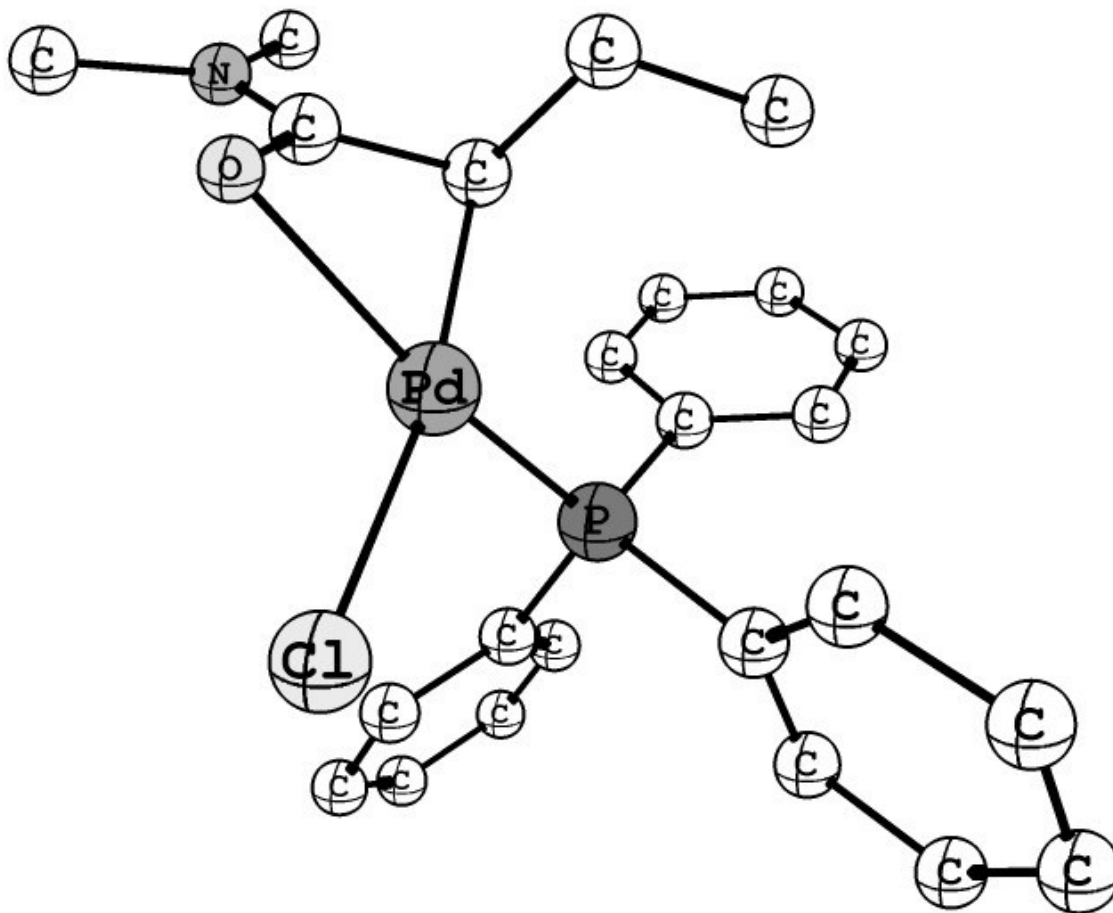
TSH23-b



Pd	-0.746074000	-0.972217000	-0.917914000
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C	-3.182248000	0.340997000	-1.184575000
C	-1.719436000	0.787965000	-1.227426000
C	-1.248483000	1.295930000	-2.579379000
H	-1.474868000	1.423666000	-0.367925000
H	-3.679196000	0.104951000	-2.126198000
P	1.217742000	0.059333000	0.006772000
C	1.357262000	1.867613000	-0.262661000
C	1.960790000	2.342679000	-1.441061000
C	0.754062000	2.783130000	0.612819000
C	1.974404000	3.708381000	-1.726614000
H	2.426092000	1.641753000	-2.137649000
C	0.761924000	4.150569000	0.318811000
H	0.279606000	2.433103000	1.530877000
C	1.372265000	4.616494000	-0.848192000
H	2.453568000	4.064841000	-2.641303000
H	0.290455000	4.852968000	1.009941000
H	1.380201000	5.685123000	-1.074435000
C	1.019262000	-0.111498000	1.827531000
C	2.115635000	-0.269952000	2.688677000
C	-0.280422000	-0.075715000	2.365125000
C	1.916496000	-0.384764000	4.067325000
H	3.128557000	-0.310064000	2.285912000
C	-0.472353000	-0.179686000	3.745117000
H	-1.152575000	0.041110000	1.715968000
C	0.624035000	-0.337369000	4.598752000
H	2.776994000	-0.513008000	4.728134000
H	-1.486210000	-0.143373000	4.150373000

H	0.471371000	-0.427752000	5.676769000
C	2.894746000	-0.582698000	-0.351633000
C	3.021393000	-1.904124000	-0.809214000
C	4.048988000	0.192831000	-0.143594000
C	4.289251000	-2.441150000	-1.051647000
H	2.125823000	-2.511319000	-0.965747000
C	5.311978000	-0.348817000	-0.391127000
H	3.962866000	1.221784000	0.209557000
C	5.434435000	-1.666494000	-0.845517000
H	4.380615000	-3.470153000	-1.407368000
H	6.203728000	0.260694000	-0.227565000
H	6.423690000	-2.087453000	-1.040153000
C	-3.911083000	0.405626000	0.122854000
O	-3.361013000	0.897340000	1.112205000
N	-5.183469000	-0.075005000	0.139788000
H	-1.731739000	2.260058000	-2.816293000
H	-0.164535000	1.461306000	-2.594454000
H	-1.500884000	0.587781000	-3.384658000
C	-5.979775000	0.068380000	1.348702000
H	-6.924329000	0.589111000	1.121919000
H	-6.221790000	-0.920206000	1.773570000
H	-5.409947000	0.646058000	2.083348000
C	-5.823627000	-0.734216000	-0.993114000
H	-6.232209000	-0.011001000	-1.718766000
H	-5.129885000	-1.410759000	-1.508900000
H	-6.655167000	-1.343316000	-0.615473000
H	-2.290401000	-1.305277000	-0.908319000

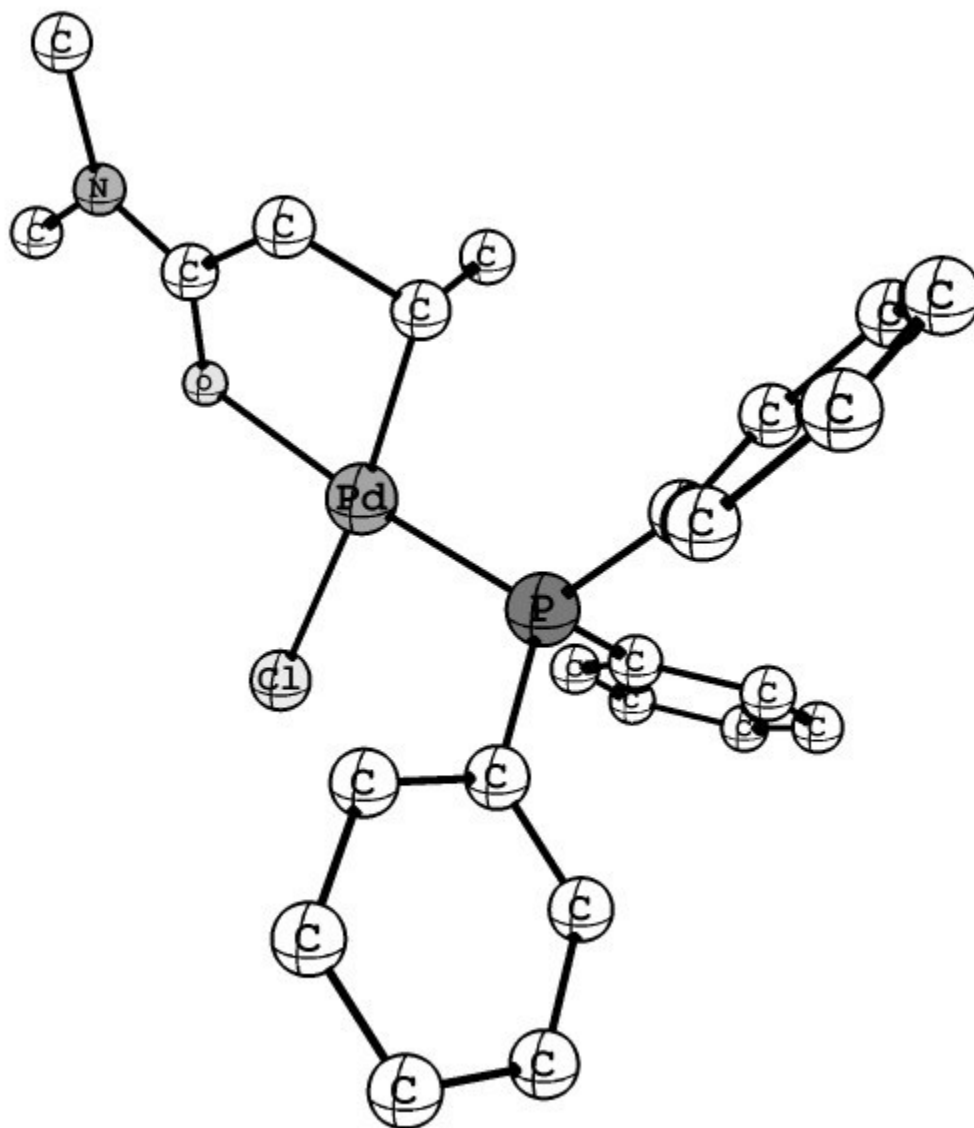
3H-a



Pd	1.033624000	-0.888818000	-0.659576000
Cl	0.050233000	-3.044007000	-1.199222000
C	2.368165000	1.503344000	-1.848485000
C	2.288366000	0.753626000	-0.518574000
C	1.177184000	2.405951000	-2.149173000
H	0.252547000	1.821765000	-2.258864000
H	1.010555000	3.135878000	-1.342765000
H	1.338003000	2.963988000	-3.084944000
C	3.368781000	-0.252558000	-0.335064000
O	3.190429000	-1.310469000	-1.020841000
N	4.374958000	-0.133250000	0.542424000
C	4.634592000	1.089662000	1.287000000
H	4.121752000	1.941064000	0.827040000
H	4.301845000	0.993954000	2.334278000
H	5.716053000	1.293644000	1.284552000
C	5.240050000	-1.266311000	0.840611000
H	5.235454000	-1.463062000	1.924866000
H	4.873552000	-2.149216000	0.306927000

H	6.275519000	-1.053576000	0.529231000
H	2.125479000	1.423940000	0.330306000
H	3.288903000	2.120375000	-1.833079000
P	-0.865274000	0.017751000	0.133476000
H	2.508675000	0.779104000	-2.667634000
C	-0.814075000	1.794349000	0.574507000
C	-1.586428000	2.754134000	-0.091904000
C	0.069198000	2.202967000	1.588773000
C	-1.469754000	4.106541000	0.244603000
H	-2.275116000	2.452373000	-0.882042000
C	0.180768000	3.551976000	1.925211000
H	0.665454000	1.460692000	2.124855000
C	-0.585792000	4.508614000	1.248889000
H	-2.073771000	4.847783000	-0.283527000
H	0.868990000	3.858475000	2.716102000
H	-0.494843000	5.565744000	1.508488000
C	-2.250541000	-0.116547000	-1.055591000
C	-3.586185000	-0.150978000	-0.627258000
C	-1.962613000	-0.142392000	-2.428959000
C	-4.620802000	-0.201016000	-1.564899000
H	-3.821221000	-0.139784000	0.438412000
C	-2.999390000	-0.186104000	-3.363690000
H	-0.923186000	-0.136525000	-2.763352000
C	-4.329539000	-0.215741000	-2.932938000
H	-5.658454000	-0.229930000	-1.224720000
H	-2.766833000	-0.204408000	-4.430782000
H	-5.140362000	-0.255744000	-3.664008000
C	-1.475812000	-0.768212000	1.679041000
C	-1.270506000	-2.141942000	1.887953000
C	-2.181454000	-0.021810000	2.638648000
C	-1.765037000	-2.755492000	3.041612000
H	-0.736992000	-2.726117000	1.135110000
C	-2.672741000	-0.642003000	3.790230000
H	-2.349637000	1.045659000	2.491253000
C	-2.464120000	-2.009026000	3.995369000
H	-1.600331000	-3.824487000	3.196208000
H	-3.219915000	-0.052218000	4.529266000
H	-2.845730000	-2.491579000	4.898244000

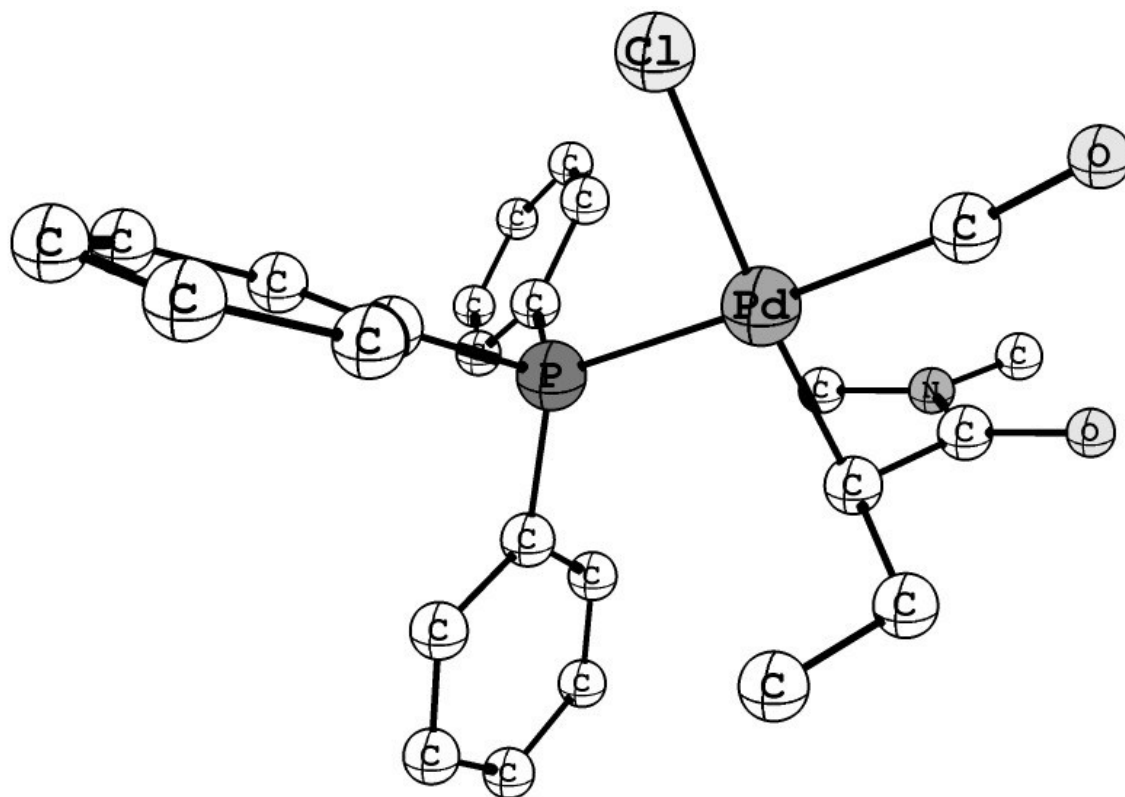
3H-b



Pd	-1.036996000	-0.604987000	-0.190818000
Cl	-0.451415000	-3.006984000	-0.205447000
C	-1.777440000	1.309833000	-0.273422000
C	-3.122687000	1.250654000	0.469972000
C	-1.946898000	1.701639000	-1.737223000
H	-2.588939000	0.988140000	-2.279710000
H	-2.416109000	2.700761000	-1.826636000
H	-0.980977000	1.741240000	-2.261161000
C	-3.877120000	0.007643000	0.058973000
O	-3.196888000	-0.996784000	-0.278945000
N	-5.216314000	-0.041288000	0.059251000
C	-6.072725000	1.048238000	0.510969000

H	-5.534374000	1.729362000	1.177026000
H	-6.475382000	1.618126000	-0.343043000
H	-6.918008000	0.624752000	1.072814000
C	-5.910350000	-1.232847000	-0.415384000
H	-6.672520000	-0.942675000	-1.155098000
H	-5.190808000	-1.914857000	-0.878156000
H	-6.412636000	-1.745360000	0.421311000
H	-2.954779000	1.176272000	1.558750000
H	-1.127551000	2.029848000	0.238032000
H	-3.702372000	2.172372000	0.298715000
P	1.103255000	0.051142000	0.015605000
C	1.887301000	-0.750252000	1.467257000
C	3.246349000	-1.093382000	1.491930000
C	1.092014000	-0.993559000	2.599129000
C	3.803327000	-1.667561000	2.638383000
H	3.873759000	-0.921357000	0.616308000
C	1.653587000	-1.557961000	3.746006000
H	0.029355000	-0.740656000	2.573937000
C	3.010537000	-1.897788000	3.766677000
H	4.861820000	-1.937731000	2.647425000
H	1.028181000	-1.740986000	4.622746000
H	3.448533000	-2.347714000	4.660714000
C	2.183649000	-0.334179000	-1.416041000
C	3.380136000	0.370794000	-1.637505000
C	1.821497000	-1.370012000	-2.291780000
C	4.197699000	0.045632000	-2.722039000
H	3.674520000	1.179563000	-0.966874000
C	2.643793000	-1.690524000	-3.375479000
H	0.908517000	-1.937307000	-2.101239000
C	3.829599000	-0.983527000	-3.594880000
H	5.124476000	0.600268000	-2.885860000
H	2.353889000	-2.497298000	-4.052778000
H	4.468012000	-1.233249000	-4.445647000
C	1.392451000	1.841723000	0.302816000
C	1.551295000	2.350597000	1.600306000
C	1.343922000	2.734095000	-0.781715000
C	1.662189000	3.728812000	1.808293000
H	1.590042000	1.672829000	2.454284000
C	1.457584000	4.108908000	-0.571306000
H	1.223632000	2.353529000	-1.797399000
C	1.615448000	4.610658000	0.725270000
H	1.789252000	4.112493000	2.823236000
H	1.422298000	4.791146000	-1.423734000
H	1.703548000	5.686979000	0.889747000

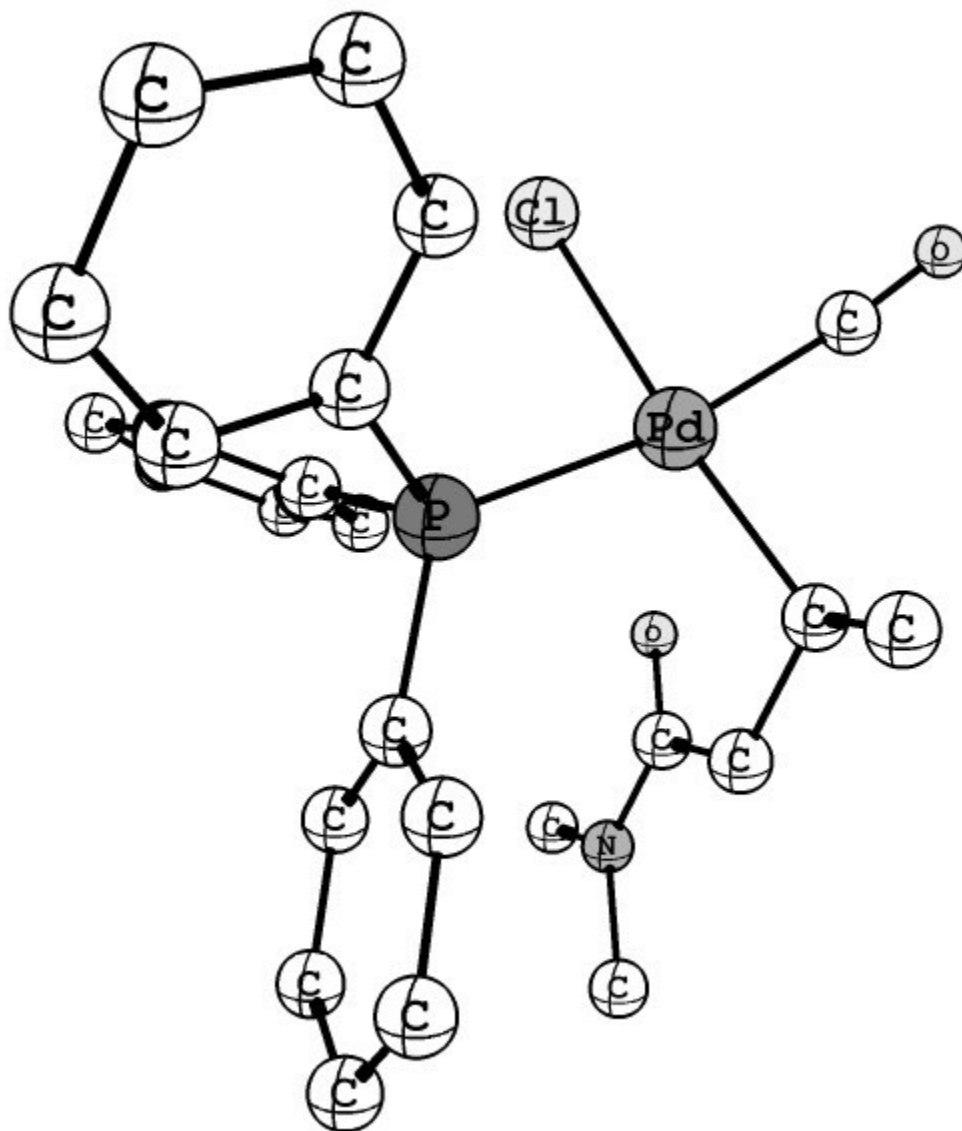
4H-a



Pd	-1.024300000	-1.092254000	-0.271590000
C	-2.293451000	-0.680544000	2.448204000
C	-2.099081000	0.061204000	1.130004000
C	-1.006780000	-1.039487000	3.185482000
H	-0.375770000	-1.714670000	2.585686000
H	-0.407680000	-0.146601000	3.415093000
H	-1.231209000	-1.547762000	4.136434000
C	-3.418832000	0.349638000	0.448960000
O	-4.405488000	-0.362768000	0.669975000
N	-3.487880000	1.396555000	-0.431122000
C	-2.382285000	2.280778000	-0.747415000
H	-1.429351000	1.743251000	-0.742983000
H	-2.519083000	2.673470000	-1.764995000
H	-2.320247000	3.141224000	-0.057254000
C	-4.762375000	1.732212000	-1.043171000
H	-4.683168000	1.703763000	-2.143033000
H	-5.513198000	1.007206000	-0.713415000
H	-5.082183000	2.747064000	-0.749159000
H	-1.522710000	0.974795000	1.300446000
H	-2.911608000	-0.036396000	3.103416000
H	-2.899333000	-1.582380000	2.276884000
C	-2.549539000	-2.310328000	-0.447654000

O	-3.322924000	-3.121839000	-0.622384000
Cl	0.055888000	-2.411491000	-2.028243000
P	0.968883000	0.166525000	-0.030878000
C	1.209411000	1.173011000	1.482767000
C	0.496767000	2.373971000	1.649114000
C	2.036095000	0.722138000	2.523100000
C	0.597763000	3.098268000	2.837830000
H	-0.128377000	2.760984000	0.845075000
C	2.135896000	1.450535000	3.711238000
H	2.600409000	-0.203914000	2.414311000
C	1.413653000	2.635391000	3.875111000
H	0.037625000	4.028918000	2.951102000
H	2.782857000	1.086644000	4.512464000
H	1.491073000	3.201318000	4.806075000
C	2.412206000	-0.957853000	-0.027259000
C	3.620219000	-0.598689000	-0.639670000
C	2.312927000	-2.183748000	0.650005000
C	4.721288000	-1.457431000	-0.570024000
H	3.705317000	0.347683000	-1.175827000
C	3.417648000	-3.032756000	0.726866000
H	1.368491000	-2.476368000	1.113264000
C	4.623259000	-2.671855000	0.114836000
H	5.658633000	-1.174035000	-1.053996000
H	3.334453000	-3.983293000	1.258383000
H	5.485215000	-3.340808000	0.168670000
C	1.235325000	1.335744000	-1.413424000
C	2.014429000	2.493527000	-1.251579000
C	0.669454000	1.050077000	-2.667286000
C	2.215768000	3.358874000	-2.329533000
H	2.463329000	2.724669000	-0.284651000
C	0.875821000	1.918931000	-3.740769000
H	0.083121000	0.139177000	-2.800237000
C	1.644287000	3.075455000	-3.573654000
H	2.821401000	4.257762000	-2.194685000
H	0.430831000	1.691809000	-4.712108000
H	1.798857000	3.756250000	-4.413886000

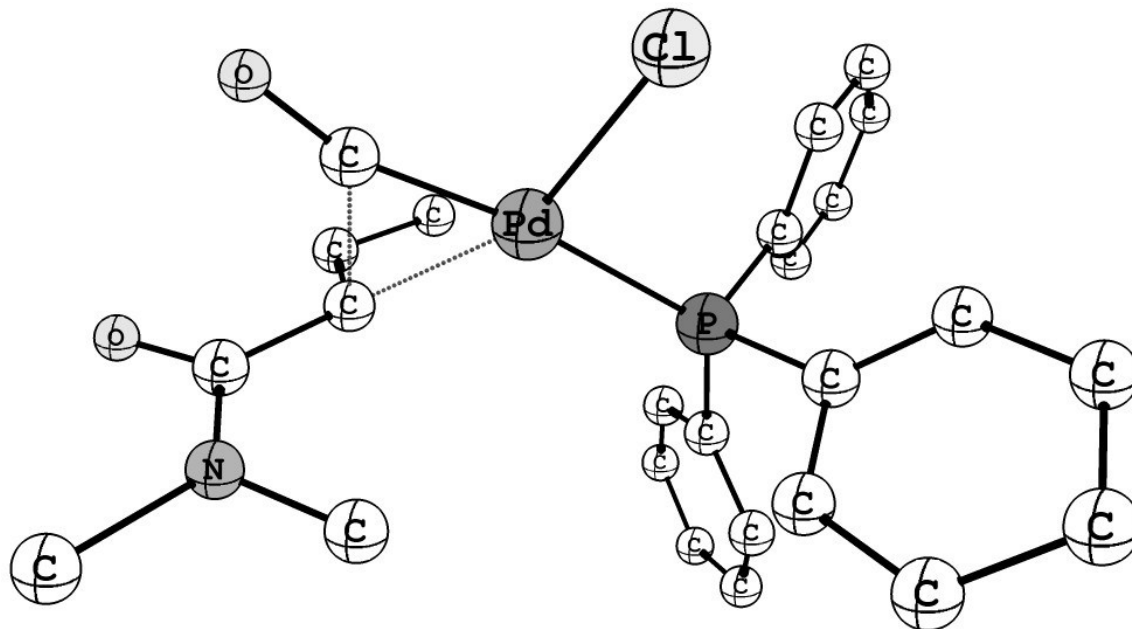
4H-b



Pd	0.338167000	1.859313000	-0.130855000
C	-1.135079000	1.923283000	-1.627848000
C	-2.304576000	0.972843000	-1.417063000
C	-0.505255000	1.755625000	-3.003465000
H	-0.037942000	0.766670000	-3.122587000
H	-1.270285000	1.850270000	-3.798231000
H	0.267081000	2.515261000	-3.194348000
C	-2.860747000	0.926333000	-0.002767000
O	-2.361102000	1.598561000	0.907381000
N	-3.912629000	0.092369000	0.224402000
C	-4.607692000	-0.654956000	-0.809912000
H	-3.962698000	-0.851138000	-1.670800000

H	-4.918359000	-1.628348000	-0.403320000
H	-5.511867000	-0.121269000	-1.153265000
C	-4.499334000	0.013384000	1.552195000
H	-4.438011000	-1.018174000	1.937430000
H	-3.956573000	0.685541000	2.224209000
H	-5.562006000	0.308059000	1.522993000
H	-3.119684000	1.271304000	-2.103812000
H	-1.522233000	2.946945000	-1.527321000
H	-2.036269000	-0.046687000	-1.722741000
C	0.558138000	3.775337000	-0.329366000
O	0.801503000	4.882992000	-0.411671000
Cl	2.050579000	2.017378000	1.649633000
P	0.624127000	-0.506484000	-0.004258000
C	2.270623000	-0.998789000	-0.649843000
C	3.251090000	-0.023685000	-0.888918000
C	2.566735000	-2.349607000	-0.907145000
C	4.507408000	-0.394923000	-1.376163000
H	3.033685000	1.022191000	-0.672239000
C	3.824200000	-2.716011000	-1.390103000
H	1.812316000	-3.119529000	-0.738129000
C	4.796685000	-1.738826000	-1.627496000
H	5.262479000	0.372548000	-1.561176000
H	4.043279000	-3.768357000	-1.584566000
H	5.778672000	-2.026182000	-2.010547000
C	-0.491615000	-1.714036000	-0.826176000
C	-1.507085000	-2.372962000	-0.117380000
C	-0.365728000	-1.937297000	-2.208984000
C	-2.379251000	-3.241088000	-0.780484000
H	-1.621637000	-2.214063000	0.954921000
C	-1.241851000	-2.799970000	-2.868325000
H	0.426821000	-1.443020000	-2.773635000
C	-2.252732000	-3.454290000	-2.155135000
H	-3.162425000	-3.751373000	-0.215763000
H	-1.132408000	-2.964672000	-3.942505000
H	-2.937461000	-4.131078000	-2.670912000
C	0.571900000	-1.031123000	1.753515000
C	1.477219000	-1.957306000	2.288021000
C	-0.436141000	-0.493412000	2.572180000
C	1.369127000	-2.351766000	3.625082000
H	2.275091000	-2.369796000	1.669782000
C	-0.546750000	-0.901279000	3.903104000
H	-1.128820000	0.249883000	2.170294000
C	0.355341000	-1.829968000	4.433366000
H	2.083306000	-3.069797000	4.034964000
H	-1.336384000	-0.482595000	4.531556000
H	0.272282000	-2.141249000	5.477334000

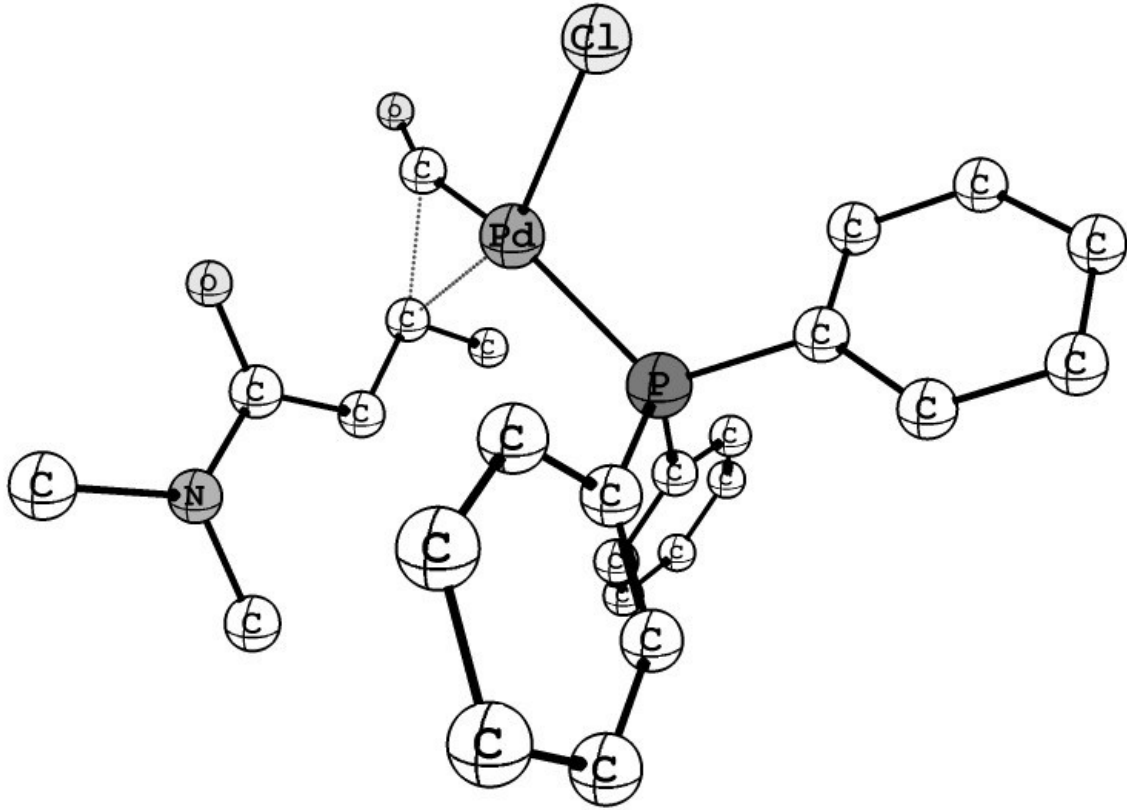
TSH45-a



Pd	1.049280000	-0.912381000	0.438436000
C	3.089843000	-1.113752000	-2.229349000
C	2.895808000	-0.246763000	-0.991962000
C	4.168516000	0.430563000	-0.512877000
O	5.245651000	0.055486000	-0.970795000
N	4.074048000	1.421567000	0.417338000
C	2.828189000	2.041345000	0.840073000
H	2.035846000	1.302775000	0.957688000
H	2.984610000	2.506180000	1.813805000
H	2.494163000	2.815663000	0.139457000
C	5.290451000	2.117674000	0.819625000
H	5.306143000	2.225618000	1.906355000
H	6.151311000	1.541686000	0.494756000
H	5.336747000	3.114607000	0.367879000
H	2.101840000	0.486374000	-1.152161000
H	3.563358000	-0.476320000	-2.982255000
H	3.817546000	-1.896159000	-2.012663000
C	2.801529000	-1.569293000	0.441737000
O	3.708727000	-2.239771000	0.685847000
Cl	0.020076000	-2.127083000	2.216160000
P	-1.126027000	0.142710000	-0.053711000
C	1.789855000	-1.715406000	-2.794392000
C	-1.520097000	1.490025000	-1.223172000
C	-1.408347000	1.132543000	-2.570123000
C	-1.931075000	2.782368000	-0.887467000
C	-1.658179000	2.059753000	-3.573211000

H	-1.123783000	0.114291000	-2.829384000
C	-2.190232000	3.706474000	-1.897368000
H	-2.098790000	3.066551000	0.151787000
C	-2.043482000	3.354059000	-3.235183000
H	-1.559239000	1.772857000	-4.617865000
H	-2.517136000	4.710326000	-1.633980000
H	-2.243945000	4.084305000	-4.016250000
C	-2.417686000	-1.058375000	-0.566086000
C	-2.606990000	-2.191102000	0.229975000
C	-3.189763000	-0.904726000	-1.724082000
C	-3.570587000	-3.136795000	-0.103325000
H	-1.996707000	-2.332302000	1.117706000
C	-4.150800000	-1.855547000	-2.053997000
H	-3.035203000	-0.064832000	-2.393105000
C	-4.348944000	-2.968642000	-1.243870000
H	-3.710594000	-4.010931000	0.529334000
H	-4.743863000	-1.727239000	-2.957193000
H	-5.100817000	-3.709596000	-1.507516000
C	-1.822060000	0.856555000	1.451174000
C	-2.889467000	0.316487000	2.158185000
C	-1.178814000	2.010454000	1.904373000
C	-3.316324000	0.938388000	3.329883000
H	-3.382354000	-0.582727000	1.796255000
C	-1.603776000	2.625264000	3.076086000
H	-0.360886000	2.426334000	1.312472000
C	-2.672793000	2.085498000	3.788995000
H	-4.151408000	0.524109000	3.890898000
H	-1.108851000	3.526370000	3.432004000
H	-3.008992000	2.564360000	4.706255000
H	0.954651000	-1.495523000	-2.141712000
H	1.577275000	-1.306381000	-3.773170000
H	1.879314000	-2.790097000	-2.880105000

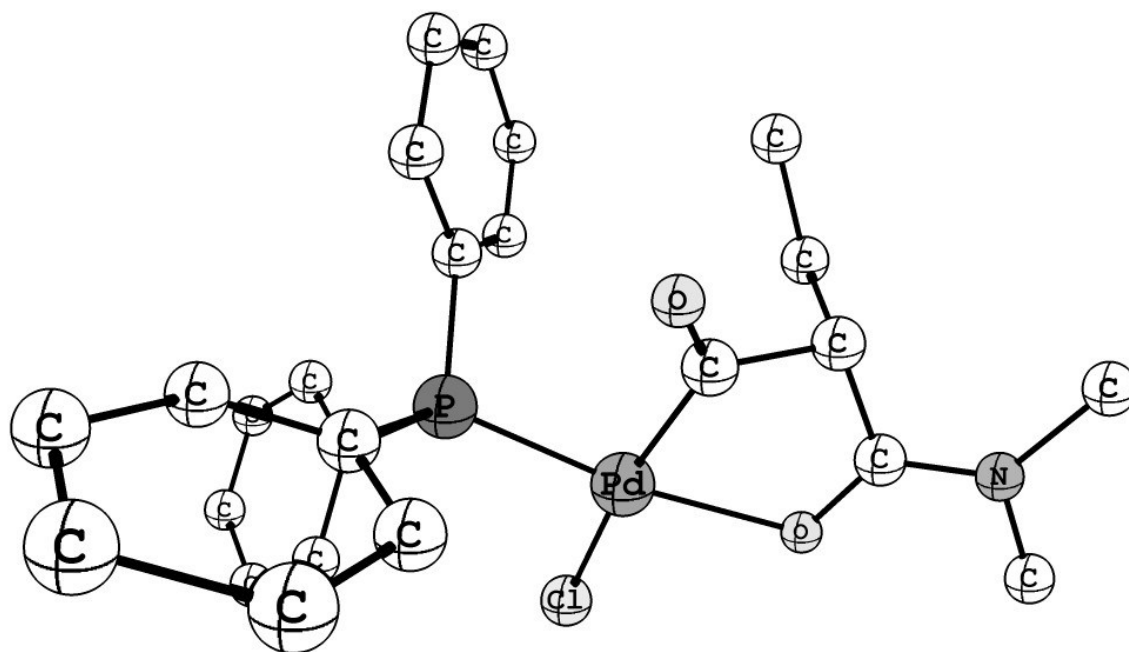
TSH45-b



Pd	-0.536981000	-1.522129000	-0.573958000
C	-2.149782000	-1.807734000	1.162540000
C	-2.623163000	-0.361074000	1.196917000
C	-3.392295000	0.084212000	-0.036745000
O	-3.692063000	-0.723689000	-0.918757000
N	-3.754508000	1.384432000	-0.106612000
C	-3.382038000	2.388892000	0.879555000
H	-3.138065000	1.936625000	1.834165000
H	-2.529206000	2.980204000	0.540124000
H	-4.226237000	3.059307000	1.039276000
C	-4.436029000	1.853431000	-1.304360000
H	-5.128069000	2.646952000	-1.029705000
H	-3.724546000	2.254221000	-2.035233000
H	-4.975338000	1.032757000	-1.761977000
H	-3.309057000	-0.284316000	2.051234000
H	-3.043375000	-2.425852000	1.181765000
C	-1.699551000	-2.944846000	-0.361854000
O	-2.113931000	-4.018362000	-0.445108000
Cl	0.547394000	-2.098779000	-2.630908000
P	1.031619000	0.252623000	0.043025000
H	-1.802006000	0.316725000	1.412200000

C	-1.257825000	-2.174776000	2.340303000
C	1.259635000	0.385014000	1.847553000
C	2.141102000	-0.496384000	2.479522000
C	0.447565000	1.205875000	2.634617000
C	2.214046000	-0.548005000	3.865030000
H	2.776592000	-1.140676000	1.887220000
C	0.521505000	1.152668000	4.020734000
H	-0.239283000	1.898292000	2.169636000
C	1.402889000	0.274522000	4.640099000
H	2.907048000	-1.230363000	4.339495000
H	-0.113263000	1.797073000	4.614800000
H	1.460225000	0.232884000	5.719713000
C	2.745121000	0.155507000	-0.588766000
C	3.527435000	1.290304000	-0.806068000
C	3.296671000	-1.103726000	-0.834165000
C	4.837215000	1.168216000	-1.251621000
H	3.117262000	2.274804000	-0.641359000
C	4.610840000	-1.225750000	-1.268969000
H	2.691753000	-1.988591000	-0.703313000
C	5.383449000	-0.090186000	-1.481074000
H	5.429362000	2.057778000	-1.422736000
H	5.024793000	-2.208226000	-1.454405000
H	6.403323000	-0.183501000	-1.830878000
C	0.430924000	1.877948000	-0.527881000
C	-0.355445000	1.886713000	-1.683876000
C	0.731077000	3.093671000	0.092741000
C	-0.803099000	3.084667000	-2.225834000
H	-0.615289000	0.951705000	-2.161673000
C	0.260497000	4.288305000	-0.435665000
H	1.335699000	3.117044000	0.987330000
C	-0.502536000	4.287487000	-1.598675000
H	-1.400887000	3.075584000	-3.127439000
H	0.496228000	5.221448000	0.058710000
H	-0.869003000	5.219738000	-2.007646000
H	-1.809741000	-2.021396000	3.273625000
H	-0.959162000	-3.222017000	2.302495000
H	-0.358354000	-1.564711000	2.379581000

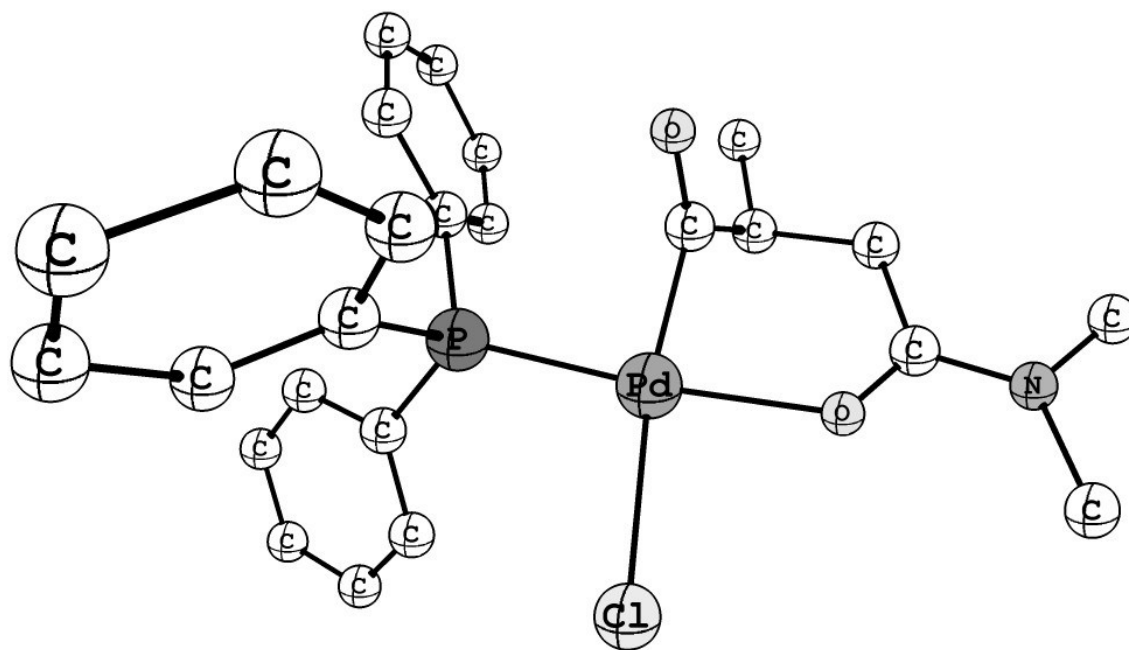
5H-a



Pd	0.795240000	-0.967119000	-0.073934000
C	3.111781000	1.562263000	-0.937856000
C	3.078171000	0.754607000	0.387734000
C	2.665274000	3.010522000	-0.766745000
H	1.638075000	3.074910000	-0.383037000
H	3.324875000	3.545436000	-0.064524000
H	2.694855000	3.537093000	-1.732175000
H	4.137821000	1.529272000	-1.337725000
H	3.593031000	1.324897000	1.174472000
C	1.600555000	0.600475000	0.834996000
O	1.133508000	1.390740000	1.618126000
H	2.473291000	1.044115000	-1.672635000
Cl	0.152920000	-3.016291000	-1.260752000
P	-1.240599000	0.017467000	0.029200000
C	3.678833000	-0.621206000	0.193102000
O	2.901560000	-1.576553000	-0.061759000
N	5.002243000	-0.809757000	0.265245000
C	5.566811000	-2.138106000	0.049352000
H	4.759152000	-2.869937000	-0.041036000
H	6.173329000	-2.145289000	-0.870584000
H	6.216041000	-2.403696000	0.897764000
C	5.984319000	0.242638000	0.490532000
H	6.630725000	0.350067000	-0.395224000
H	5.507190000	1.204425000	0.694295000
H	6.617962000	-0.022707000	1.350980000

C	-2.617048000	-0.759567000	-0.899277000
C	-2.982799000	-2.068622000	-0.541171000
C	-3.326924000	-0.095951000	-1.908975000
C	-4.048924000	-2.698785000	-1.181102000
H	-2.427218000	-2.593625000	0.236851000
C	-4.390845000	-0.735975000	-2.554971000
H	-3.060809000	0.922645000	-2.192150000
C	-4.753636000	-2.034885000	-2.193015000
H	-4.328211000	-3.715432000	-0.894893000
H	-4.938919000	-0.210737000	-3.340599000
H	-5.585793000	-2.532021000	-2.697016000
C	-1.127815000	1.719269000	-0.634130000
C	-1.459525000	2.856118000	0.111864000
C	-0.618009000	1.868205000	-1.936101000
C	-1.302342000	4.129014000	-0.447191000
H	-1.828287000	2.754439000	1.132644000
C	-0.478039000	3.137860000	-2.495506000
H	-0.320612000	0.985963000	-2.508622000
C	-0.821565000	4.272287000	-1.750924000
H	-1.557377000	5.012164000	0.142964000
H	-0.085869000	3.243601000	-3.509317000
H	-0.702095000	5.267814000	-2.184329000
C	-1.939217000	0.129292000	1.715682000
C	-3.236997000	0.633401000	1.906142000
C	-1.206538000	-0.334117000	2.816903000
C	-3.785305000	0.689661000	3.188467000
H	-3.823379000	0.974038000	1.050006000
C	-1.761385000	-0.282567000	4.098470000
H	-0.204830000	-0.738460000	2.664563000
C	-3.047259000	0.232524000	4.286280000
H	-4.793744000	1.084661000	3.330638000
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H	-3.479478000	0.272051000	5.288881000

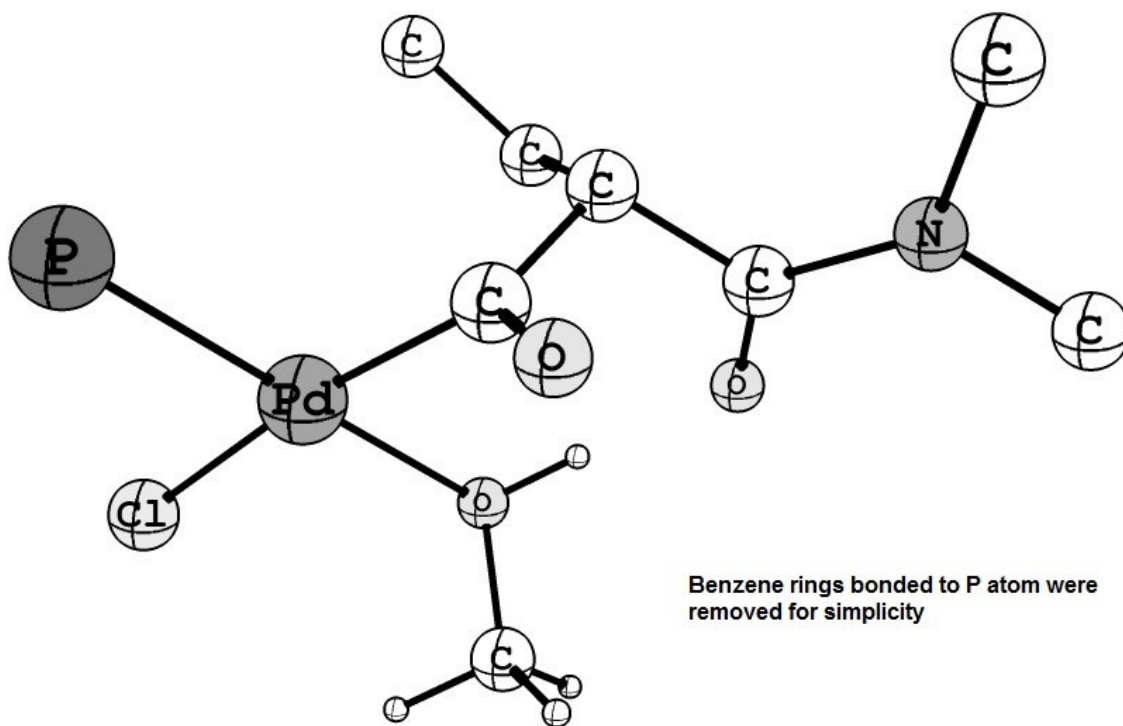
5H-b



Pd	0.904133000	-0.654349000	-0.048571000
C	2.434299000	1.778708000	-0.561278000
C	3.848314000	1.298583000	-0.194914000
C	2.371452000	3.307634000	-0.553353000
H	2.601134000	3.696389000	0.449506000
H	3.097675000	3.726461000	-1.266339000
H	1.367732000	3.656740000	-0.831676000
H	4.558626000	1.723249000	-0.918958000
H	2.185461000	1.394522000	-1.562802000
H	4.128531000	1.714392000	0.789027000
C	1.430821000	1.174119000	0.434746000
O	1.168339000	1.711686000	1.483793000
Cl	0.598557000	-3.100173000	-0.361652000
P	-1.295249000	-0.061420000	-0.023095000
C	4.031790000	-0.206941000	-0.129978000
O	3.062441000	-0.996226000	-0.091482000
N	5.288727000	-0.681066000	-0.097270000
C	5.536345000	-2.119007000	-0.084931000
H	6.164818000	-2.397375000	-0.945561000
H	6.060744000	-2.406486000	0.840175000
H	4.582744000	-2.652135000	-0.142383000
C	6.464858000	0.183537000	-0.123411000
H	6.335632000	1.059309000	0.524656000
H	7.322379000	-0.387263000	0.254106000
H	6.698639000	0.523810000	-1.145795000

C	-2.397843000	-0.677593000	-1.354382000
C	-2.077145000	-1.836533000	-2.076668000
C	-3.593760000	0.007203000	-1.637313000
C	-2.944690000	-2.301447000	-3.070038000
H	-1.158134000	-2.379156000	-1.843342000
C	-4.456017000	-0.464221000	-2.628522000
H	-3.852829000	0.911311000	-1.083792000
C	-4.131693000	-1.618828000	-3.349238000
H	-2.687903000	-3.204094000	-3.629689000
H	-5.382945000	0.073860000	-2.839960000
H	-4.805078000	-1.984237000	-4.128238000
C	-1.595889000	1.747499000	-0.092337000
C	-2.153688000	2.472659000	0.966240000
C	-1.204988000	2.419245000	-1.262851000
C	-2.315587000	3.858606000	0.856681000
H	-2.460470000	1.962347000	1.880056000
C	-1.377808000	3.798525000	-1.373483000
H	-0.760757000	1.859413000	-2.090256000
C	-1.930043000	4.523033000	-0.309678000
H	-2.747622000	4.418699000	1.689182000
H	-1.074274000	4.312007000	-2.288593000
H	-2.058550000	5.604613000	-0.392708000
C	-2.058230000	-0.610930000	1.547278000
C	-3.303667000	-1.251368000	1.600942000
C	-1.338150000	-0.385928000	2.734683000
C	-3.827491000	-1.658205000	2.832524000
H	-3.865746000	-1.437751000	0.684697000
C	-1.870848000	-0.785253000	3.960950000
H	-0.367635000	0.113722000	2.688749000
C	-3.115579000	-1.424415000	4.011844000
H	-4.796722000	-2.161005000	2.867397000
H	-1.310266000	-0.602372000	4.880582000
H	-3.527942000	-1.742975000	4.972053000

6H-a



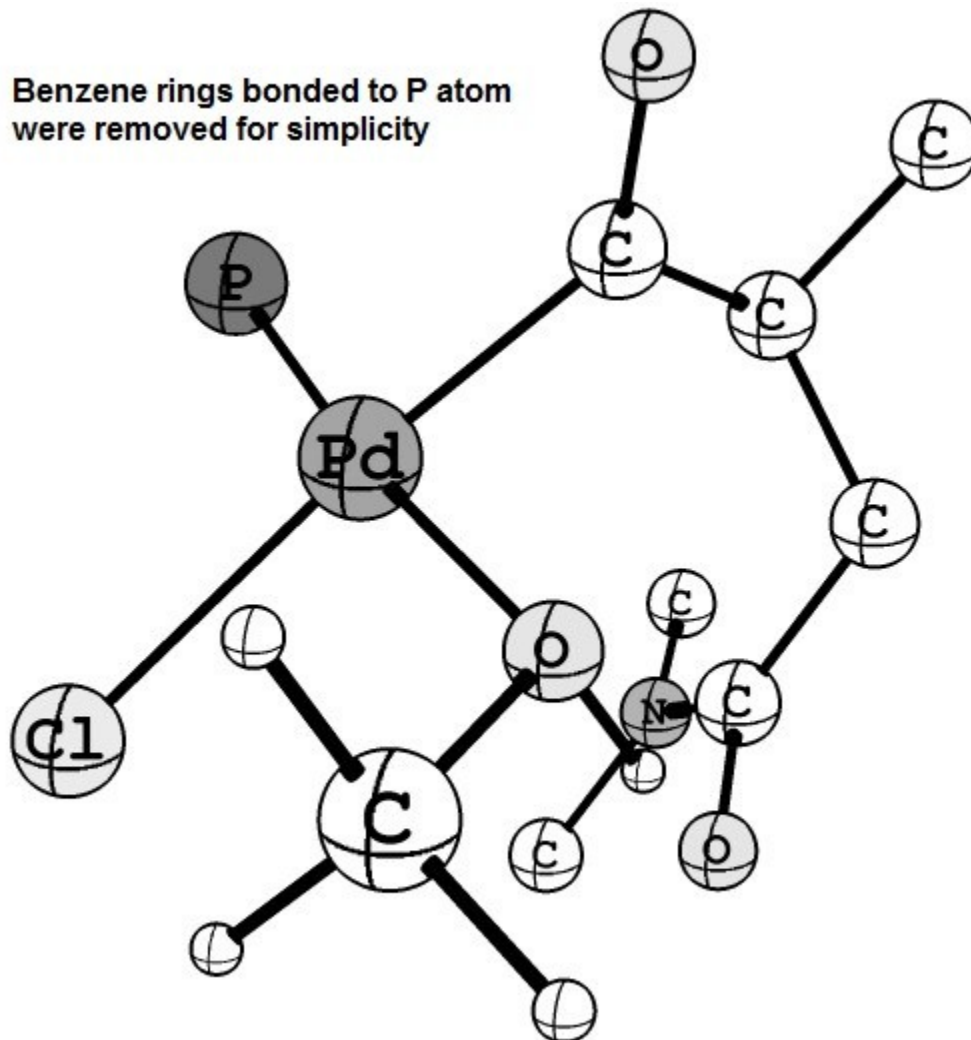
Benzene rings bonded to P atom were removed for simplicity

Pd	-0.328663000	-1.271484000	0.158402000
C	-2.470000000	0.030243000	2.215576000
C	-2.725638000	0.489607000	0.770752000
C	-1.335924000	0.775056000	2.914252000
H	-0.370917000	0.595368000	2.421548000
H	-1.518512000	1.861710000	2.931795000
H	-1.235709000	0.435470000	3.956396000
H	-3.404235000	0.183465000	2.780066000
H	-2.728237000	1.586655000	0.746214000
C	-1.688456000	0.075130000	-0.316367000
O	-1.864239000	0.455284000	-1.451249000
H	-2.276448000	-1.052141000	2.239297000
Cl	1.177227000	-3.153910000	0.648705000
P	1.345874000	0.247452000	-0.090166000
C	-4.049481000	-0.073494000	0.259795000
O	-4.261458000	-1.296342000	0.380815000
N	-4.933737000	0.754226000	-0.321948000
C	-6.205792000	0.229943000	-0.806067000
H	-6.282351000	-0.827494000	-0.535342000
H	-7.040325000	0.787565000	-0.353021000
H	-6.269428000	0.331147000	-1.901556000
C	-4.669230000	2.174030000	-0.555929000
H	-5.442061000	2.560281000	-1.231533000
H	-4.708217000	2.758526000	0.376782000

H	-3.693738000	2.314245000	-1.039860000
C	2.261714000	0.647840000	1.443875000
C	2.401845000	-0.342809000	2.430249000
C	2.846742000	1.909909000	1.640125000
C	3.112118000	-0.066757000	3.600481000
H	1.964114000	-1.330328000	2.266349000
C	3.554845000	2.179225000	2.814033000
H	2.749286000	2.686045000	0.879827000
C	3.685797000	1.193654000	3.796961000
H	3.215291000	-0.840846000	4.364418000
H	4.004397000	3.164043000	2.959846000
H	4.235671000	1.408291000	4.716280000
C	0.831786000	1.871386000	-0.764522000
C	1.022642000	2.188581000	-2.115240000
C	0.110953000	2.756504000	0.055801000
C	0.496244000	3.373712000	-2.640067000
H	1.575538000	1.509597000	-2.765536000
C	-0.409042000	3.938799000	-0.469041000
H	-0.048033000	2.521788000	1.108807000
C	-0.221966000	4.248407000	-1.821873000
H	0.648871000	3.610396000	-3.695500000
H	-0.965043000	4.619990000	0.179059000
H	-0.633947000	5.172194000	-2.234315000
C	2.599081000	-0.360095000	-1.276296000
C	3.946554000	0.014727000	-1.174284000
C	2.184751000	-1.184116000	-2.334607000
C	4.869348000	-0.429963000	-2.124951000
H	4.279799000	0.649774000	-0.351755000
C	3.108418000	-1.619195000	-3.286934000
H	1.137890000	-1.486684000	-2.407279000
C	4.452176000	-1.244469000	-3.182185000
H	5.918601000	-0.138997000	-2.037343000
H	2.779124000	-2.258717000	-4.108937000
H	5.175906000	-1.591401000	-3.923349000
O	-2.046311000	-2.673147000	0.278745000
C	-2.167832000	-3.530142000	-0.853982000
H	-2.387908000	-2.955306000	-1.769676000
H	-1.212378000	-4.055487000	-0.978847000
H	-2.968304000	-4.269824000	-0.689182000
H	-2.918866000	-2.196581000	0.404173000

6H-b

Benzene rings bonded to P atom
were removed for simplicity

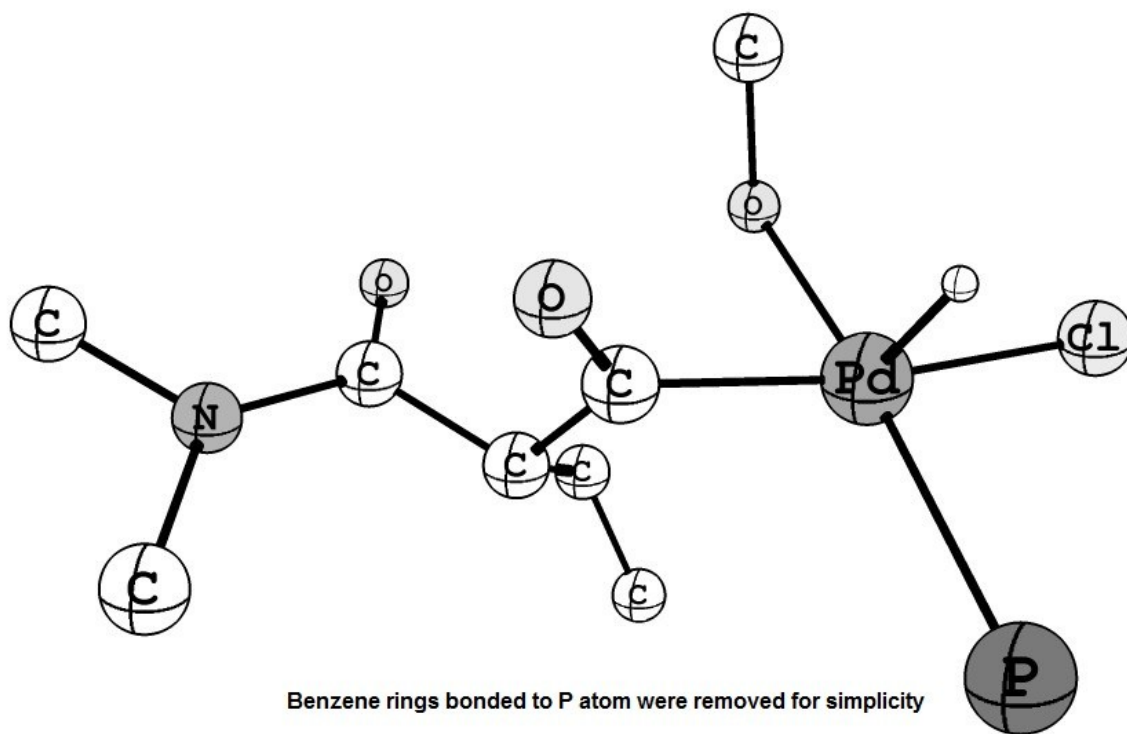


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C	-2.032626000	1.795131000	-1.010895000
C	-3.423487000	1.243745000	-0.616730000
C	-2.173750000	3.070121000	-1.842066000
H	-2.760354000	2.879295000	-2.753200000
H	-2.682688000	3.852216000	-1.258322000
H	-1.187316000	3.446362000	-2.145005000
H	-4.028909000	2.093067000	-0.262722000
H	-1.476684000	2.019256000	-0.090542000
H	-3.929348000	0.849100000	-1.508094000
C	-1.180414000	0.744815000	-1.747397000
O	-0.858244000	0.883830000	-2.901069000
Cl	-0.422058000	-3.046711000	0.460689000
P	1.108889000	0.079031000	0.128739000
C	-3.486239000	0.139261000	0.428175000

O	-3.913909000	-0.991404000	0.119034000
N	-3.111715000	0.387881000	1.699033000
C	-3.150269000	-0.729328000	2.639256000
H	-2.636846000	-0.432480000	3.560570000
H	-4.188476000	-1.009924000	2.878952000
H	-2.644298000	-1.602919000	2.206365000
C	-2.716948000	1.685469000	2.226244000
H	-3.275883000	1.893139000	3.151335000
H	-1.640680000	1.702329000	2.461731000
H	-2.938532000	2.488424000	1.517159000
C	1.101612000	0.356444000	1.937991000
C	0.312383000	-0.481487000	2.741690000
C	1.892278000	1.349740000	2.541967000
C	0.303598000	-0.315337000	4.128602000
H	-0.271479000	-1.275867000	2.274055000
C	1.873623000	1.514806000	3.928862000
H	2.522481000	1.999615000	1.933745000
C	1.075623000	0.686475000	4.724338000
H	-0.311829000	-0.972722000	4.747121000
H	2.486739000	2.293325000	4.388284000
H	1.059816000	0.819627000	5.808504000
C	1.563863000	1.699231000	-0.604723000
C	2.352802000	1.739489000	-1.765269000
C	1.019583000	2.895907000	-0.107912000
C	2.590634000	2.951941000	-2.416036000
H	2.781201000	0.820679000	-2.167920000
C	1.262961000	4.107098000	-0.758516000
H	0.407447000	2.892767000	0.794948000
C	2.045745000	4.138565000	-1.916442000
H	3.206350000	2.967824000	-3.318153000
H	0.835404000	5.029006000	-0.358395000
H	2.232704000	5.086044000	-2.426687000
C	2.565501000	-0.982941000	-0.203375000
C	3.671690000	-1.008917000	0.658142000
C	2.575380000	-1.767641000	-1.367889000
C	4.776883000	-1.808402000	0.354183000
H	3.672630000	-0.413031000	1.572183000
C	3.685615000	-2.557804000	-1.672834000
H	1.707108000	-1.763033000	-2.030982000
C	4.787078000	-2.581176000	-0.811074000
H	5.632210000	-1.828475000	1.033415000
H	3.686007000	-3.164054000	-2.581461000
H	5.651546000	-3.206858000	-1.044906000
O	-2.475173000	-1.726250000	-1.886422000
C	-2.459276000	-3.076481000	-2.336115000
H	-2.189706000	-3.767576000	-1.523249000

H	-3.443173000	-3.346861000	-2.753643000
H	-1.705485000	-3.158143000	-3.132281000
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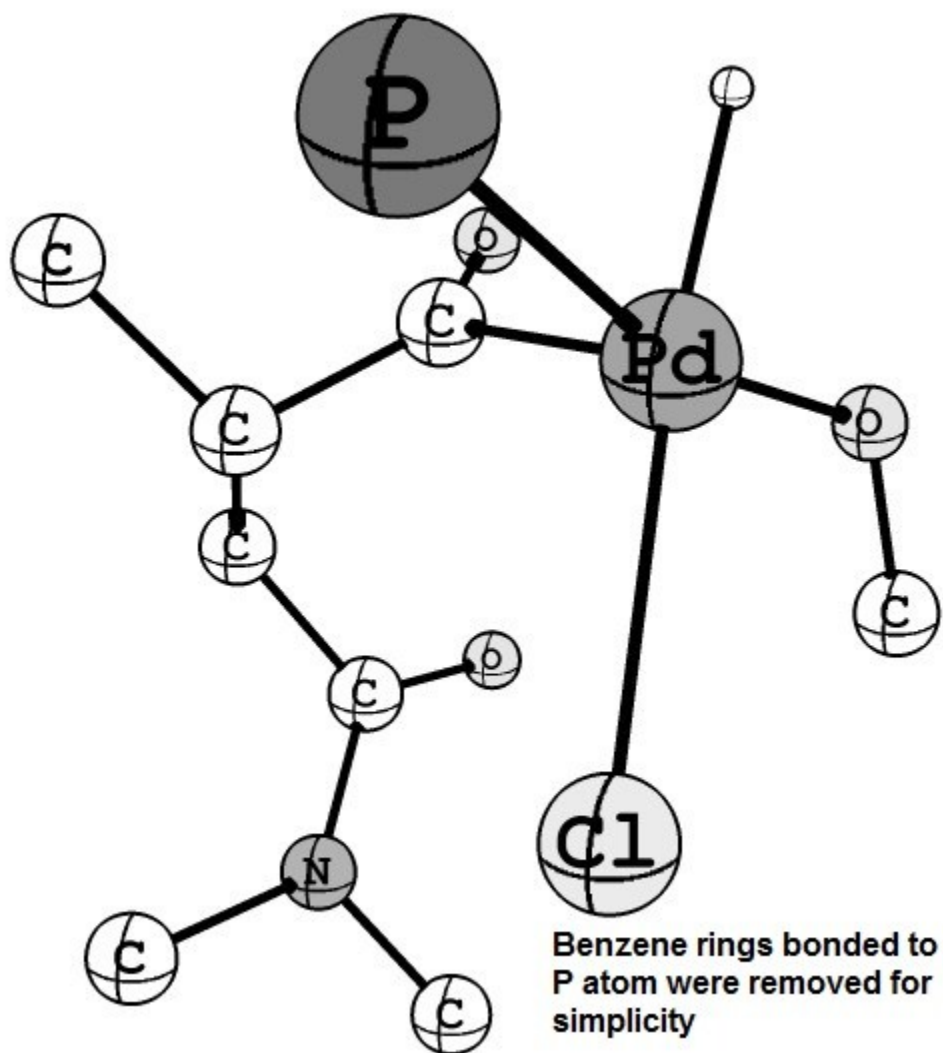
7H-a



Pd	-0.170240000	-1.542661000	-0.134747000
C	-2.478957000	-0.725508000	2.055152000
C	-2.684182000	0.001621000	0.708466000
C	-1.505343000	-0.039225000	3.012383000
H	-0.473594000	-0.000951000	2.637429000
H	-1.816411000	0.997954000	3.217687000
H	-1.472067000	-0.576160000	3.972948000
H	-3.463396000	-0.786267000	2.538994000
H	-2.372505000	1.052103000	0.822430000
C	-1.860739000	-0.463166000	-0.508988000
O	-2.205332000	-0.236283000	-1.631772000
H	-2.191899000	-1.769088000	1.863915000
Cl	1.625077000	-3.188524000	0.372461000
P	1.338020000	0.264469000	-0.079358000
C	-4.167413000	-0.080281000	0.277757000
O	-4.789578000	-1.120184000	0.474563000
N	-4.719219000	1.019709000	-0.294858000
C	-6.117547000	0.982327000	-0.698724000

H	-6.550572000	0.027786000	-0.382918000
H	-6.674785000	1.809648000	-0.230239000
H	-6.210087000	1.076919000	-1.793740000
C	-3.981565000	2.246078000	-0.570453000
H	-4.609205000	2.899859000	-1.188785000
H	-3.725412000	2.798361000	0.348249000
H	-3.062674000	2.042969000	-1.133021000
C	2.350405000	0.398680000	1.438819000
C	2.180980000	-0.476370000	2.520845000
C	3.302300000	1.430700000	1.521440000
C	2.946685000	-0.309936000	3.679089000
H	1.471561000	-1.299848000	2.462767000
C	4.064899000	1.589399000	2.678131000
H	3.448882000	2.116081000	0.685047000
C	3.885726000	0.720351000	3.760743000
H	2.807527000	-0.994560000	4.518454000
H	4.800743000	2.394437000	2.734435000
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C	0.201524000	2.625635000	0.958690000
C	-0.807737000	3.453194000	-1.515625000
H	0.083956000	1.665549000	-2.321177000
C	-0.543509000	3.804601000	0.864501000
H	0.596462000	2.313617000	1.926155000
C	-1.041507000	4.224382000	-0.371524000
H	-1.201994000	3.772296000	-2.482605000
H	-0.727907000	4.398566000	1.762021000
H	-1.618068000	5.148951000	-0.444350000
C	2.527031000	0.276116000	-1.470139000
C	3.003403000	1.484016000	-2.007712000
C	3.019509000	-0.945505000	-1.957719000
C	3.959205000	1.466094000	-3.025765000
H	2.627822000	2.441102000	-1.643625000
C	3.975518000	-0.953652000	-2.976249000
H	2.667409000	-1.883513000	-1.523772000
C	4.445455000	0.248827000	-3.512579000
H	4.322301000	2.408912000	-3.440589000
H	4.354218000	-1.906988000	-3.351533000
H	5.190756000	0.238452000	-4.311141000
O	-1.635405000	-2.942192000	-0.199790000
C	-2.042962000	-3.480283000	-1.419203000
H	-2.396490000	-2.712672000	-2.139133000
H	-1.247816000	-4.066907000	-1.925495000
H	-2.893583000	-4.168022000	-1.241064000
H	0.088015000	-1.429098000	-1.593870000

7H-b

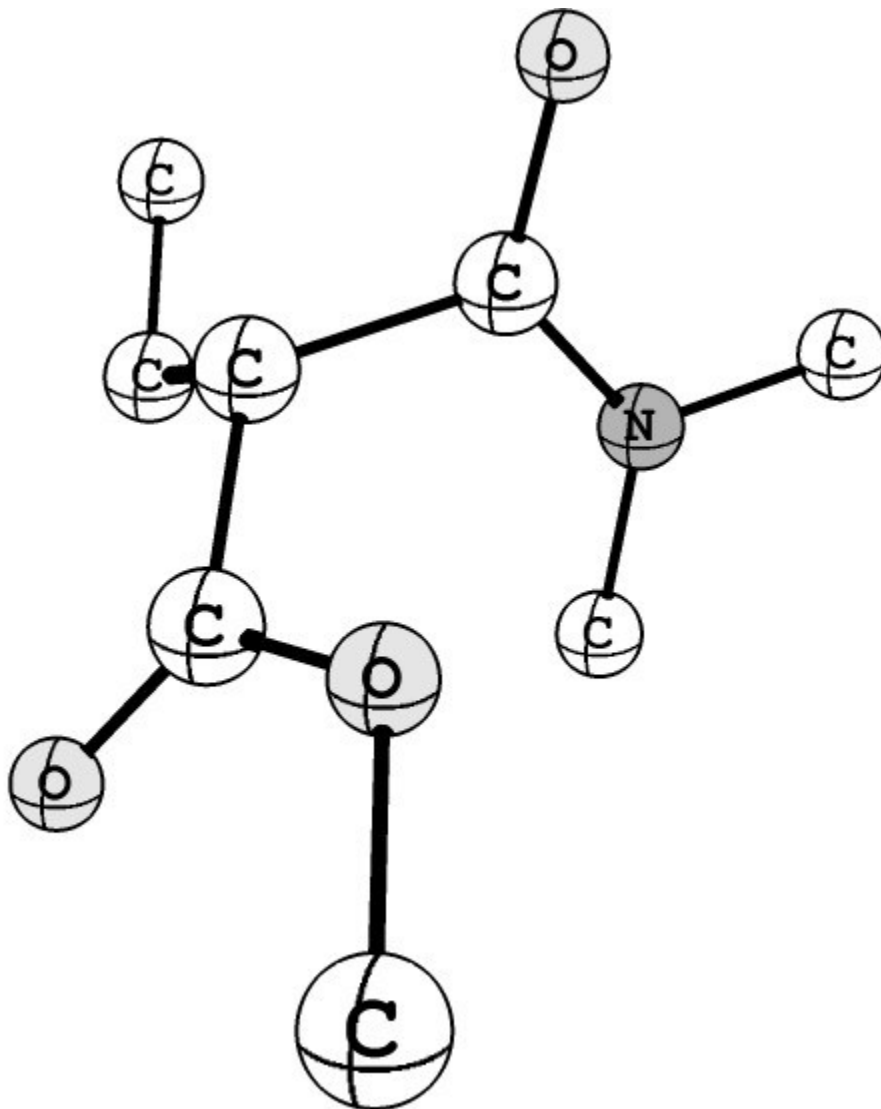


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H	-1.337430000	3.392908000	-1.796709000
H	-1.141914000	3.580882000	-0.024841000
H	0.080379000	2.704970000	-0.965634000
H	-3.516139000	2.738182000	-0.031388000
H	-1.525560000	1.180371000	0.338197000
H	-3.591653000	2.157193000	-1.704883000
C	-1.399999000	0.624226000	-1.731673000
O	-1.604062000	0.756232000	-2.886177000
Cl	-1.542082000	-1.515938000	1.143051000

P	1.402599000	-0.007705000	0.081461000
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O	-4.586428000	-0.056668000	-1.221685000
N	-4.407724000	0.418009000	0.994066000
C	-5.137170000	-0.788665000	1.350290000
H	-4.432198000	-1.588093000	1.635313000
H	-5.804708000	-0.579062000	2.199941000
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C	-3.790673000	1.106999000	2.113971000
H	-4.557525000	1.372572000	2.859180000
H	-3.043723000	0.453429000	2.593321000
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C	0.153729000	1.264882000	2.241070000
C	1.895460000	2.556782000	1.146928000
C	-0.084376000	2.329933000	3.110527000
H	-0.433814000	0.347837000	2.314103000
C	1.650547000	3.618574000	2.021433000
H	2.665329000	2.657647000	0.381725000
C	0.659127000	3.510110000	3.000255000
H	-0.858421000	2.237639000	3.875674000
H	2.236684000	4.535656000	1.931829000
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C	4.069370000	0.477412000	-0.649901000
C	2.396789000	1.160881000	-2.270279000
C	5.074112000	0.972332000	-1.483614000
H	4.333045000	0.019138000	0.304983000
C	3.404925000	1.661210000	-3.097619000
H	1.356729000	1.228145000	-2.592363000
C	4.743718000	1.565757000	-2.706394000
H	6.119190000	0.892810000	-1.176605000
H	3.142137000	2.119379000	-4.053318000
H	5.531939000	1.950511000	-3.357302000
C	2.160972000	-1.365188000	1.041360000
C	2.434808000	-1.251175000	2.410912000
C	2.457111000	-2.563872000	0.367705000
C	2.998461000	-2.328543000	3.101265000
H	2.211738000	-0.325339000	2.941892000
C	3.021774000	-3.633792000	1.061991000
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C	3.290526000	-3.519019000	2.430944000
H	3.210182000	-2.233092000	4.168489000
H	3.250239000	-4.561629000	0.533184000
H	3.728568000	-4.359404000	2.974026000
H	0.420733000	-0.859901000	-2.263573000

O	-1.573623000	-2.214200000	-2.161136000
C	-2.711307000	-2.827874000	-1.629111000
H	-3.132637000	-3.497937000	-2.408190000
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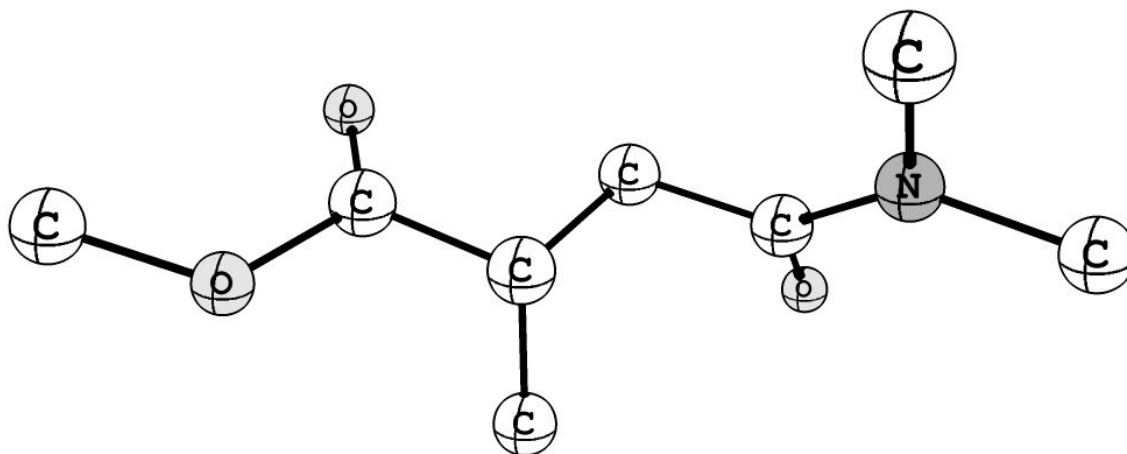
Branch (*alpha*) ester



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C	-2.151452000	2.341892000	0.050992000
H	-2.135858000	2.743547000	-0.974976000
H	-2.839799000	1.482384000	0.059472000

H	-2.573956000	3.114554000	0.711183000
C	-0.911986000	-0.345368000	-0.632903000
O	-1.520125000	-0.478093000	-1.692237000
N	-1.013925000	-1.248876000	0.384506000
C	-1.812653000	-2.447522000	0.183230000
H	-2.384407000	-2.342445000	-0.744105000
H	-1.167077000	-3.340594000	0.111542000
H	-2.501798000	-2.588767000	1.031293000
C	-0.229769000	-1.240200000	1.606111000
H	0.590084000	-1.978057000	1.557844000
H	0.201045000	-0.257077000	1.812846000
H	-0.875147000	-1.501385000	2.459230000
H	-0.028021000	1.358805000	-1.423801000
H	-0.793867000	1.556695000	1.542200000
C	1.377191000	0.665799000	-0.040446000
O	2.041338000	1.350232000	0.703799000
O	1.853803000	-0.412951000	-0.674746000
H	-0.099598000	2.835116000	0.555350000
C	3.222451000	-0.757180000	-0.429065000
H	3.418331000	-1.661336000	-1.016168000
H	3.888497000	0.057480000	-0.747571000
H	3.381835000	-0.954020000	0.640939000

Linear (*beta*) ester



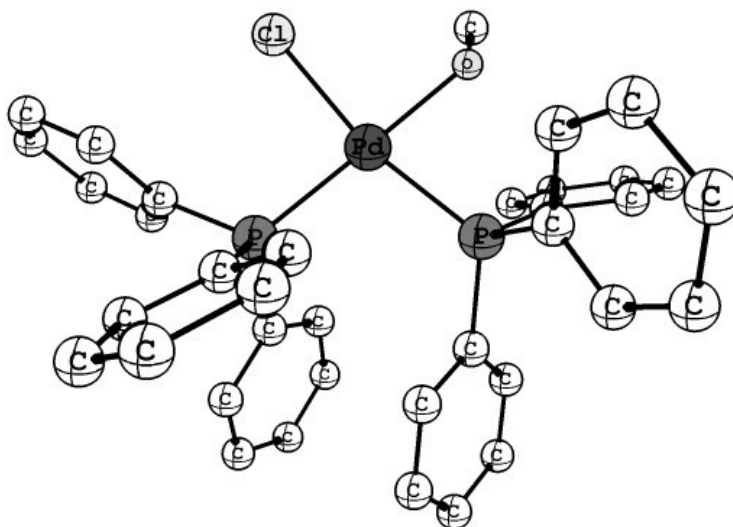
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C	0.630368000	-1.500463000	-1.121500000
H	0.938611000	-2.377222000	-0.530237000
H	-0.372800000	-1.702116000	-1.522135000
H	1.328103000	-1.383806000	-1.961703000
C	-1.810401000	-0.528990000	0.440835000
O	-2.301790000	-1.658081000	0.436823000
N	-2.498704000	0.561492000	-0.011911000
C	-3.835437000	0.385422000	-0.554502000
H	-4.121815000	-0.666470000	-0.455966000
H	-4.557784000	1.016986000	-0.010558000
H	-3.863356000	0.673939000	-1.619633000
C	-1.987395000	1.918840000	-0.075016000
H	-2.727612000	2.615155000	0.352086000
H	-1.058334000	2.029846000	0.491452000
H	-1.800460000	2.226285000	-1.119251000
H	-0.137466000	-1.207811000	1.530991000
H	0.356583000	0.618300000	-0.894984000
H	-0.277537000	0.551978000	1.568145000
C	2.012829000	0.055547000	0.281003000
O	2.337606000	0.053440000	1.447209000
C	4.225962000	0.577543000	-0.352519000
H	4.287594000	1.461739000	0.298688000
H	4.659017000	-0.284113000	0.176209000
H	4.765300000	0.758044000	-1.289403000
O	2.867678000	0.314101000	-0.718174000

Table S1. DFT/B3LYP-D3-PCM/Def2-TZVP computed total electronic energies (E_{tot} , au), zero-point energies (ZPE, kcal/mol) and Gibbs free energies (G_{tot} , 383.15K, au) in methanol for the hydride cycle

Compound	E_{tot} (solv+D3)	ZPE	G_{tot} (solv+D3)
<i>Starting materials</i>			
α,β -Unsaturated Amide	-365.4071898	102.23683	-365.277156
PPh ₃	-1036.670897	170.52590	-1036.441507
CH ₃ OH	-115.7833535	31.79668	-115.755364
CO	-113.3638545	3.09871	-113.378042
<i>Amide coordination and insertion</i>			
1H	-2662.290851	349.23193	-2661.801175
2H	-1990.992956	281.36307	-1990.599278
TSH23-a	-1990.987099	280.92827	-1990.596960
TSH23-b	-1990.98461	279.56357	-1990.593541
3H-a	-1991.019867	283.63598	-1990.626369
3H-b	-1991.025556	283.84569	-1990.631583
<i>CO coordination and insertion</i>			
4H-a	-2104.404766	288.50923	-2104.006738
4H-b	-2104.396434	288.66063	-2103.997987
TSH45-a	-2104.379262	288.57485	-2103.977854
TSH45-b	-2104.377182	288.98354	-2103.972389
5H-a	-2104.421835	290.22099	-2104.020645
5H-b	-2104.420317	290.09619	-2104.019066
<i>Coordination and oxidative addition of methanol</i>			
6H-a	-2220.214878	323.97592	-2219.763532
6H-b	-2220.220087	324.54799	-2219.766202
7H-a	-2220.125194	321.74131	-2219.676082
7H-b	-2220.1337432	321.29208	-2219.686609
<i>Final Products</i>			
Branch alpha ester (AP)	-594.6205144	144.16850	-594.429573
Linear beta ester (BP)	-594.6234938	144.23197	-594.433382

S2. Cartesian coordinates (in Å) of all the B3LYP-D3/ Def2-SVP optimized structures of reactants, intermediates and products in the alkoxy cycle in Methanol phase.

1A

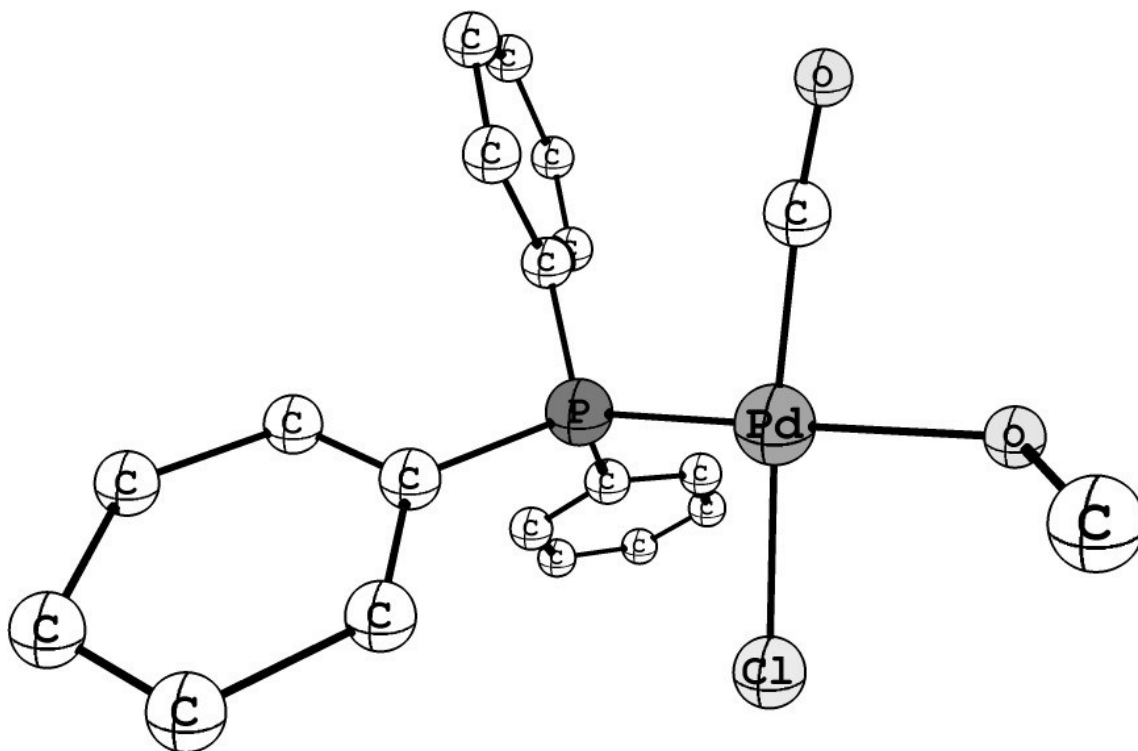


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H	2.011580000	-3.137825000	2.020703000
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C	-4.212561000	-1.484407000	-0.344623000
C	-3.914974000	-0.545435000	1.868358000
C	-5.426168000	-2.043137000	0.057036000
H	-3.857889000	-1.641057000	-1.363949000
C	-5.125800000	-1.116592000	2.271060000
H	-3.334405000	0.042239000	2.581045000
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H	-5.477573000	-0.970152000	3.294894000
H	-6.834754000	-2.303790000	1.679768000
C	-1.719650000	1.473799000	1.083551000
C	-2.443319000	2.639640000	0.794136000
C	-0.928350000	1.423771000	2.239405000
C	-2.367756000	3.740953000	1.647064000
H	-3.055096000	2.703197000	-0.105202000

C	-0.853486000	2.527071000	3.091623000
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C	-1.571726000	3.688142000	2.795579000
H	-2.926462000	4.648620000	1.408090000
H	-0.222862000	2.481568000	3.981940000
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C	-3.304159000	1.110928000	-2.090095000
C	-1.263327000	0.696306000	-3.957751000
H	-0.176256000	-0.229836000	-2.347656000
C	-3.468743000	1.528561000	-3.411961000
H	-4.121303000	1.247901000	-1.380414000
C	-2.446735000	1.328768000	-4.346819000
H	-0.465247000	0.519958000	-4.682181000
H	-4.402543000	2.007703000	-3.714313000
H	-2.579641000	1.656336000	-5.380394000
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C	4.413378000	-0.659193000	0.729418000
C	2.740192000	-0.755816000	2.481376000
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C	2.374136000	2.425430000	1.288823000
C	0.625664000	3.920049000	-0.296699000
H	0.166882000	2.071626000	-1.289025000
C	2.245770000	3.802237000	1.492776000
H	3.060796000	1.854319000	1.912614000
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C	2.366437000	-1.279284000	-2.453578000
C	3.619177000	0.960354000	-3.572506000
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C	2.871849000	-1.333328000	-3.753969000
H	1.902646000	-2.153165000	-1.994059000

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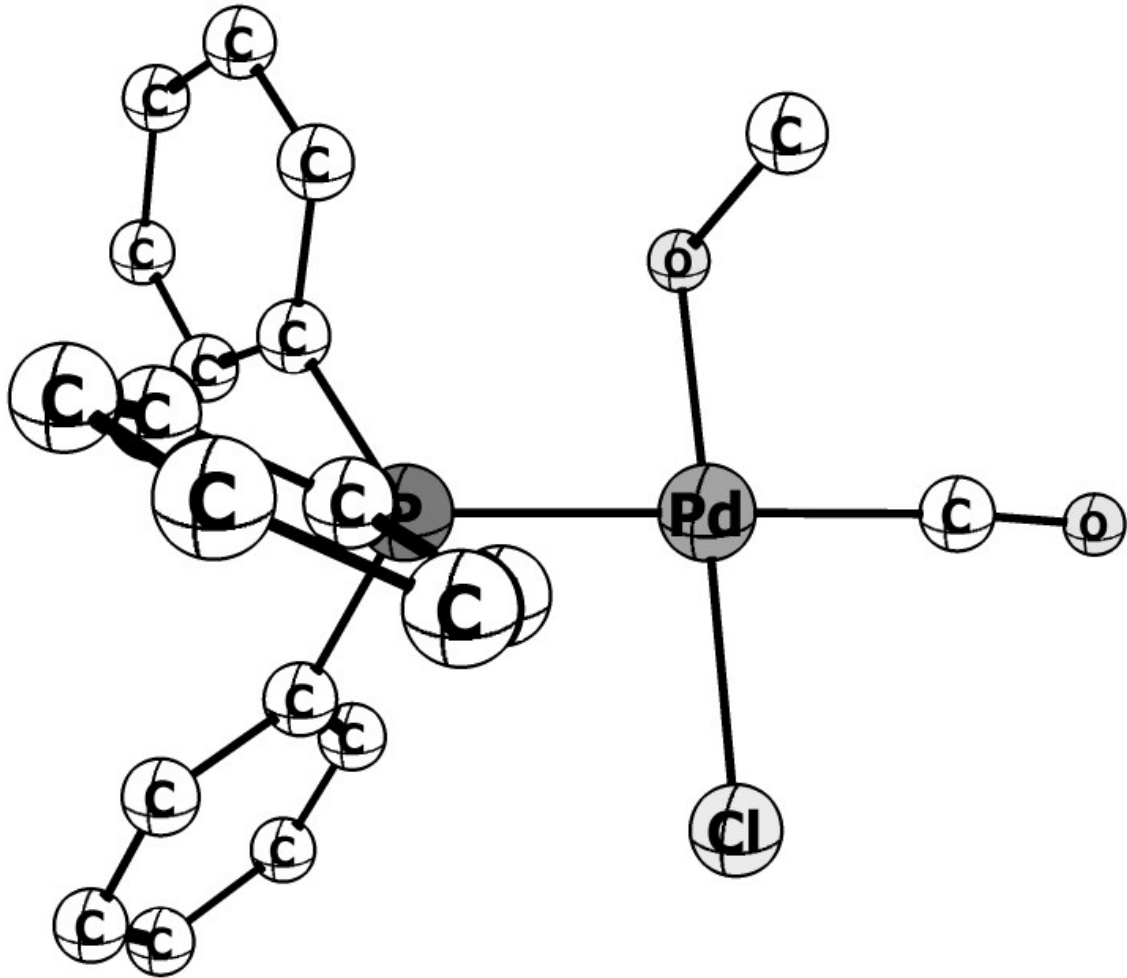
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H	4.489888000	0.773028000	1.429791000
H	4.423569000	-0.980107000	1.074456000
C	1.953505000	2.027947000	-0.239698000
O	2.121829000	3.150041000	-0.276565000
C	-1.039752000	-0.554967000	1.671944000
C	-0.247364000	-1.416779000	2.447354000
C	-2.291271000	-0.134334000	2.154348000
C	-0.706192000	-1.850783000	3.693344000
H	0.715821000	-1.756152000	2.063208000
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H	-2.912937000	0.537058000	1.560104000
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H	-0.085377000	-2.519545000	4.293686000
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H	-2.306063000	-1.771446000	5.146984000
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C	-2.697221000	3.058743000	-1.582861000
H	-2.289863000	1.004420000	-2.106863000
C	-1.682684000	3.861498000	0.463359000
H	-0.474147000	2.444311000	1.546422000
C	-2.483547000	4.087515000	-0.662750000
H	-3.323637000	3.229138000	-2.461199000
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C	-2.293213000	-1.978324000	-0.875035000
C	-1.203272000	-2.050743000	-3.454133000
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H	-2.720252000	-1.953998000	0.128587000
C	-2.304592000	-2.853121000	-3.135000000
H	-0.774961000	-2.079917000	-4.458359000
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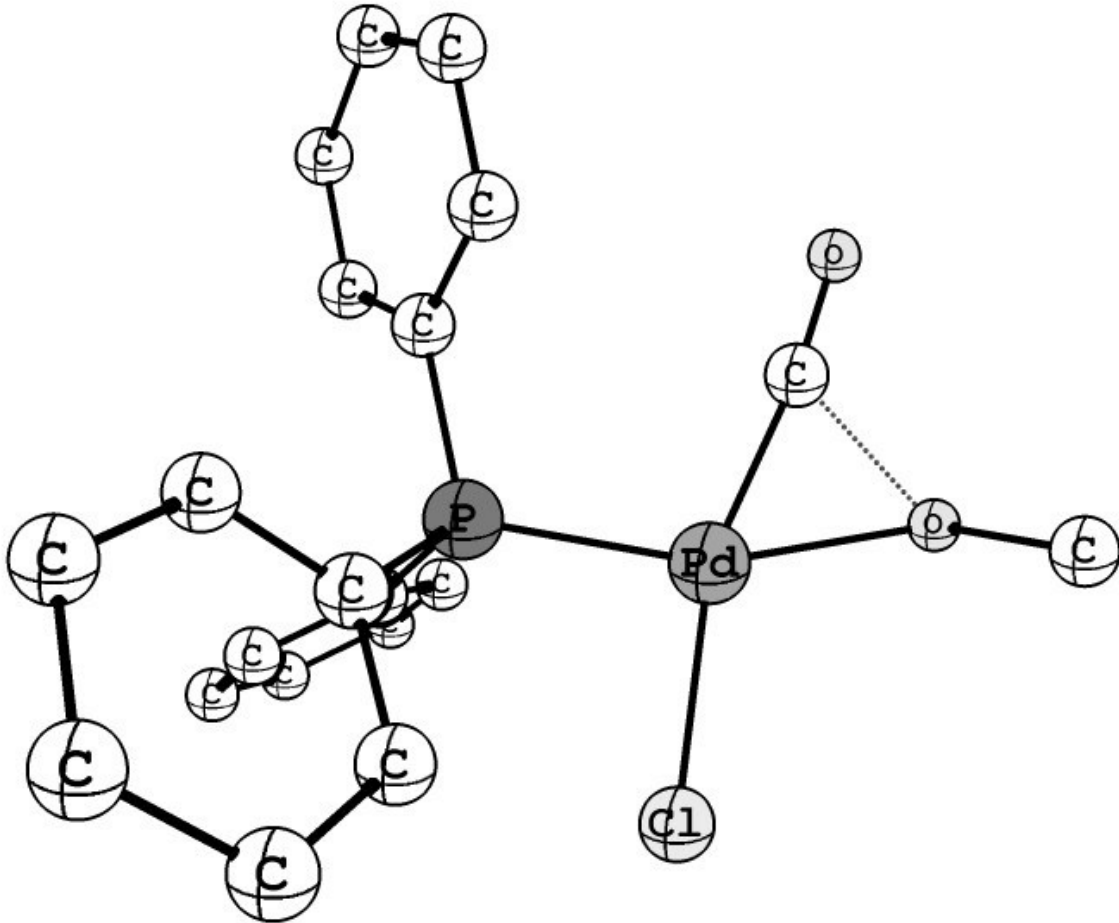
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C	-0.000886000	-0.128908000	-2.731820000
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C	0.331279000	0.042206000	-4.069500000
H	-0.950229000	-0.570468000	-2.462397000
C	2.448584000	0.993406000	-3.427492000
H	2.820714000	1.132013000	-1.323961000
C	1.554270000	0.604038000	-4.419190000
H	-0.367958000	-0.259763000	-4.837961000
H	3.401521000	1.430430000	-3.695130000
H	1.809582000	0.740531000	-5.461861000
C	1.362874000	1.251196000	0.937095000
C	2.163523000	0.923266000	2.031063000
C	1.218852000	2.592966000	0.569285000
C	2.814366000	1.922702000	2.746262000

H	2.288561000	-0.108599000	2.324918000
C	1.876084000	3.585236000	1.280101000
H	0.603032000	2.859558000	-0.276211000
C	2.672237000	3.253143000	2.373124000
H	3.436053000	1.656885000	3.591077000
H	1.763951000	4.619934000	0.983815000
H	3.181419000	4.029934000	2.928548000
C	1.215169000	-1.595311000	0.490555000
C	0.780122000	-2.206774000	1.668783000
C	2.225730000	-2.190793000	-0.262301000
C	1.363403000	-3.389752000	2.097762000
H	-0.021158000	-1.760860000	2.243325000
C	2.800238000	-3.382851000	0.164886000
H	2.562998000	-1.733007000	-1.181418000
C	2.373934000	-3.980805000	1.344787000
H	1.022881000	-3.856013000	3.012787000
H	3.581017000	-3.842613000	-0.426607000
H	2.822907000	-4.908452000	1.674806000
C	-3.833616000	0.043679000	0.520114000
O	-4.950817000	-0.020490000	0.647167000
O	-1.648838000	1.931469000	0.844015000
C	-2.194273000	2.840446000	-0.072832000
H	-3.283949000	2.740055000	-0.188526000
H	-1.992728000	3.854542000	0.295680000
H	-1.750759000	2.761624000	-1.075816000

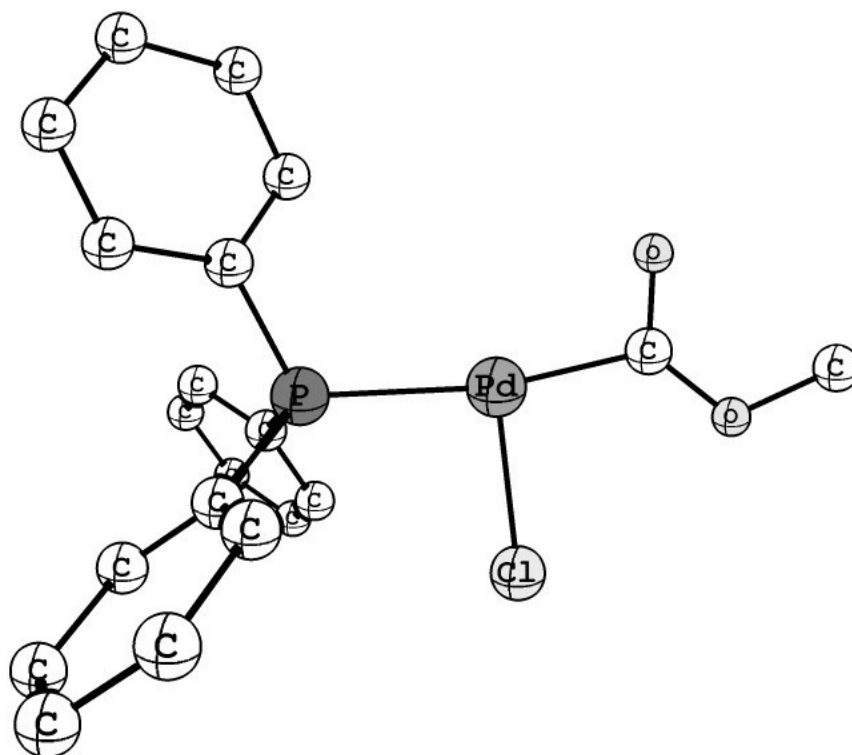
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O	3.874005000	-0.202108000	-0.364769000
C	4.676330000	-0.358783000	0.787232000
H	4.409649000	0.352174000	1.592663000
H	4.595726000	-1.380129000	1.202122000
H	5.733741000	-0.176931000	0.519762000
C	2.628334000	1.228963000	-0.233979000
O	3.022674000	2.308883000	-0.294632000
C	-1.307915000	-0.361776000	1.588489000
C	-0.963560000	-1.531173000	2.286192000
C	-2.334410000	0.465443000	2.075510000
C	-1.644669000	-1.866869000	3.458191000
H	-0.172688000	-2.176563000	1.899666000
C	-3.010385000	0.121335000	3.248162000
H	-2.609886000	1.375673000	1.541343000
C	-2.666508000	-1.043256000	3.941345000

H	-1.373363000	-2.777344000	3.997281000
H	-3.808521000	0.767347000	3.620393000
H	-3.195234000	-1.308446000	4.859784000
C	-0.771674000	1.832191000	-0.214896000
C	-1.573893000	2.322293000	-1.254113000
C	-0.178957000	2.728715000	0.690823000
C	-1.778148000	3.699974000	-1.386303000
H	-2.042497000	1.634536000	-1.959018000
C	-0.391779000	4.099772000	0.558783000
H	0.446773000	2.353534000	1.504328000
C	-1.190183000	4.588207000	-0.482941000
H	-2.402688000	4.076694000	-2.199249000
H	0.069505000	4.790610000	1.267808000
H	-1.352266000	5.663222000	-0.588474000
C	-1.394373000	-0.792676000	-1.308259000
C	-0.811602000	-0.867313000	-2.584461000
C	-2.670070000	-1.330756000	-1.088956000
C	-1.508158000	-1.464759000	-3.635092000
H	0.187367000	-0.457979000	-2.753112000
C	-3.359929000	-1.934388000	-2.144393000
H	-3.125553000	-1.281187000	-0.098685000
C	-2.782656000	-2.000273000	-3.415589000
H	-1.052765000	-1.518451000	-4.626289000
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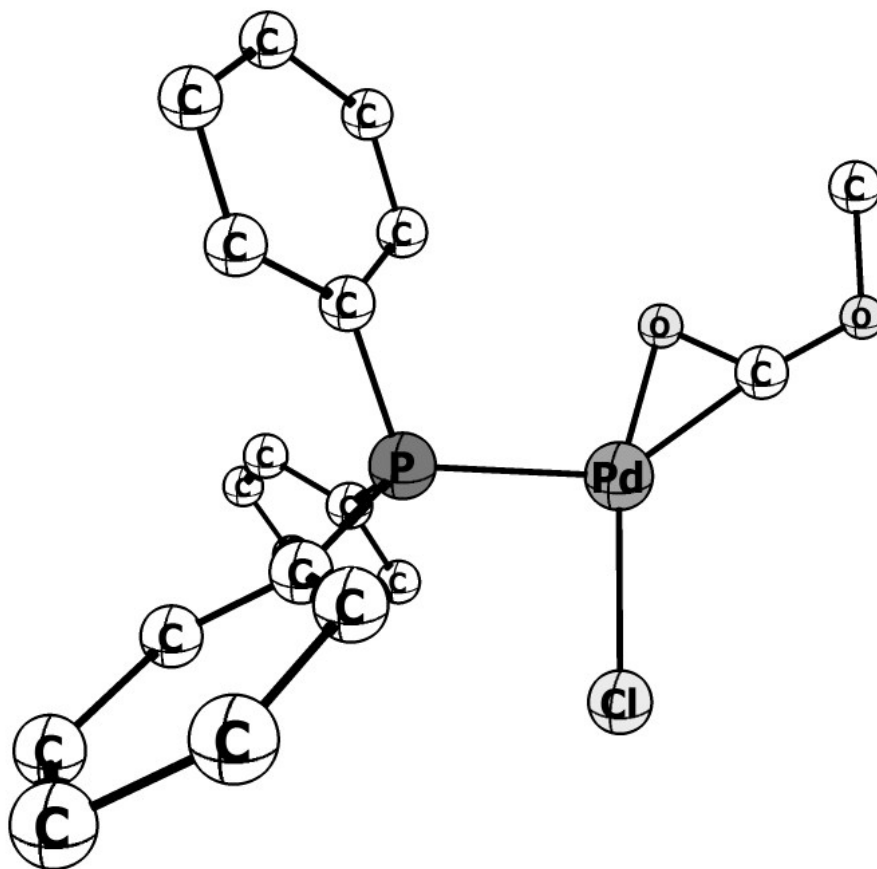
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C	3.634151000	-0.619966000	0.023086000
O	3.699821000	-1.836697000	0.017947000
O	4.663427000	0.202249000	0.032527000
C	5.976666000	-0.399285000	0.039656000
H	6.688761000	0.432958000	0.046385000
H	6.103550000	-1.021449000	0.936843000
H	6.115573000	-1.017304000	-0.858595000
C	-1.486448000	-1.692644000	-0.366305000
C	-0.889703000	-2.841384000	0.180690000
C	-2.637362000	-1.822780000	-1.157720000
C	-1.445122000	-4.101581000	-0.049159000
H	0.013409000	-2.745450000	0.790301000
C	-3.187395000	-3.086509000	-1.391416000
H	-3.104989000	-0.936786000	-1.590874000
C	-2.595007000	-4.225429000	-0.836883000
H	-0.976458000	-4.989189000	0.381866000
H	-4.083472000	-3.180958000	-2.009179000
H	-3.027087000	-5.211582000	-1.022000000
C	-1.401950000	1.065079000	-1.243484000
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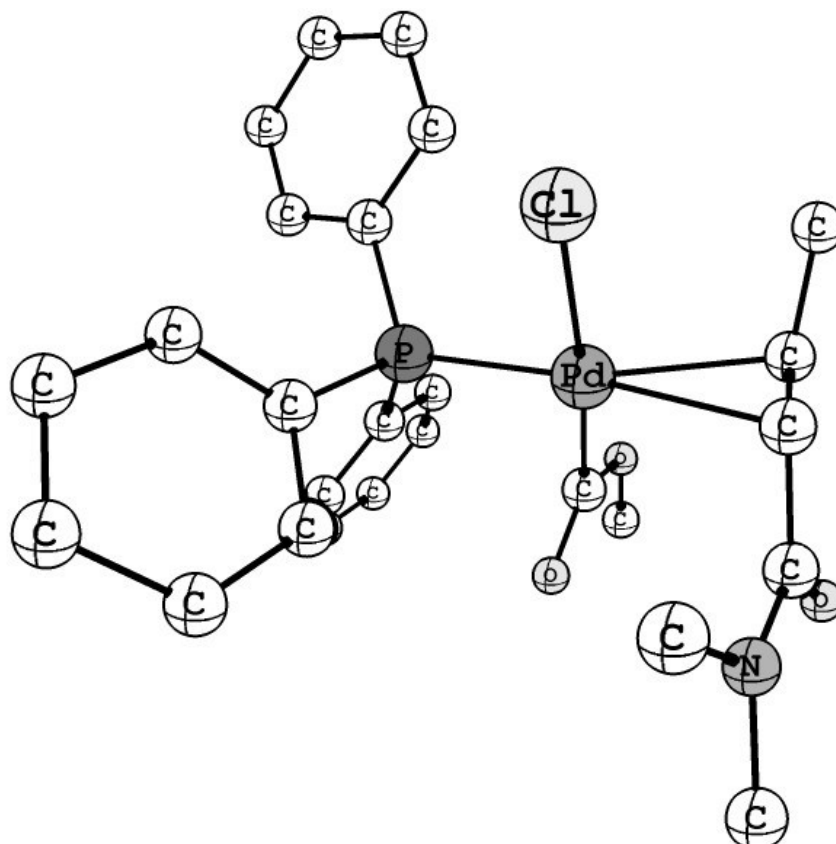
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H	0.154869000	0.565969000	-2.662299000
C	-2.401201000	2.750993000	-3.246765000
H	-3.942656000	3.271395000	-1.820530000
H	-0.741340000	2.050434000	-4.447501000
H	-2.789831000	3.410127000	-4.026557000
C	-1.463839000	0.447865000	1.585397000
C	-0.885638000	1.540139000	2.256349000
C	-2.585469000	-0.189920000	2.135827000
C	-1.434921000	1.992493000	3.457526000
H	-0.007382000	2.031126000	1.829377000
C	-3.126674000	0.263856000	3.342771000
H	-3.039131000	-1.039733000	1.622847000
C	-2.554816000	1.354913000	4.003670000
H	-0.983511000	2.843593000	3.972915000
H	-4.000028000	-0.237667000	3.766284000
H	-2.980065000	1.707428000	4.946308000

3A-G



Pd	-1.545029000	-0.981608000	0.082514000
Cl	-0.525939000	-3.145668000	0.207665000
P	0.530755000	0.099628000	0.004686000
C	-3.458221000	-0.618674000	0.065362000
O	-2.668519000	0.306825000	-0.001310000
O	-4.745098000	-0.531382000	0.062993000
C	-5.330202000	0.811761000	-0.027768000
H	-6.402495000	0.655542000	-0.018045000
H	-5.010285000	1.397518000	0.830272000
H	-5.008879000	1.277908000	-0.955711000
C	0.329114000	1.855936000	-0.423807000
C	-0.543799000	2.623434000	0.354400000
C	0.987835000	2.450678000	-1.499403000
C	-0.740936000	3.966191000	0.067946000
H	-1.067611000	2.170175000	1.185652000
C	0.782137000	3.795623000	-1.788487000
H	1.664089000	1.869095000	-2.109733000
C	-0.079086000	4.555196000	-1.006174000
H	-1.414602000	4.552648000	0.678940000
H	1.299976000	4.248722000	-2.623796000
H	-0.236658000	5.601786000	-1.231709000
C	1.679323000	-0.561172000	-1.237202000
C	3.059568000	-0.583410000	-1.039620000
C	1.148605000	-1.036632000	-2.438402000
C	3.898851000	-1.069427000	-2.035767000
H	3.481402000	-0.225715000	-0.110669000
C	1.989192000	-1.512125000	-3.435016000
H	0.076326000	-1.041851000	-2.585386000
C	3.366346000	-1.530304000	-3.234430000
H	4.968671000	-1.087095000	-1.873792000
H	1.570012000	-1.877456000	-4.363329000
H	4.021340000	-1.908844000	-4.008254000
C	1.458961000	0.127010000	1.569449000
C	1.397890000	-0.985258000	2.412299000
C	2.248212000	1.221406000	1.929927000
C	2.125059000	-1.002628000	3.595591000
H	0.785621000	-1.832277000	2.132857000
C	2.971089000	1.200521000	3.116066000
H	2.297089000	2.089656000	1.287493000
C	2.911496000	0.088956000	3.949845000
H	2.073427000	-1.867552000	4.244055000
H	3.580138000	2.052670000	3.388150000
H	3.473731000	0.074933000	4.874475000

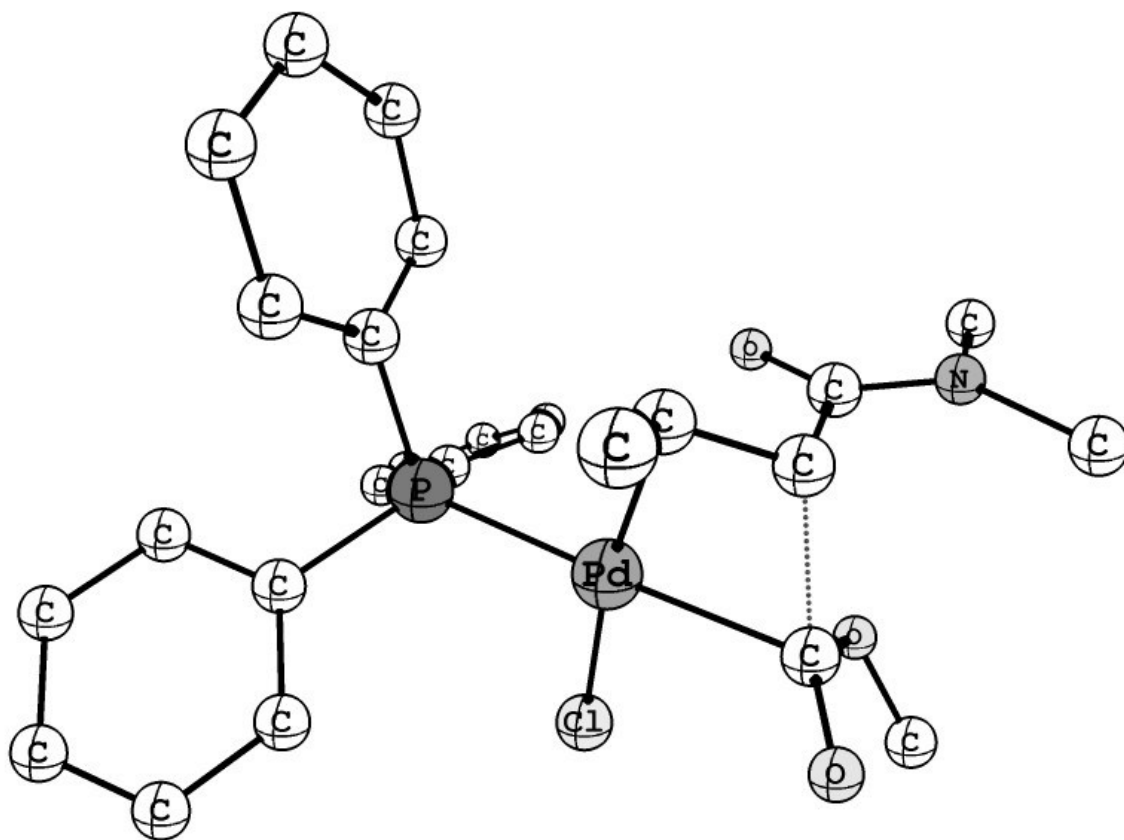
4A



Pd	-0.873532000	-0.356686000	-0.735588000
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O	-1.156367000	2.418886000	-1.201304000
C	-1.441199000	3.786136000	-0.854231000
H	-1.306301000	4.365554000	-1.774601000
H	-2.474747000	3.875767000	-0.491314000
H	-0.744165000	4.133145000	-0.078706000
C	-2.584969000	-0.179180000	-2.400322000
C	-3.076511000	-0.790487000	-1.273149000
H	-2.730735000	0.901723000	-2.481976000
H	-3.077543000	-1.879217000	-1.220039000
C	-3.876542000	-0.000655000	-0.271540000
O	-4.343492000	1.097783000	-0.578955000
N	-4.055643000	-0.556974000	0.958842000
C	-3.410191000	-1.764618000	1.447884000
H	-2.680668000	-2.161847000	0.735628000
H	-2.865113000	-1.538439000	2.379312000
H	-4.158389000	-2.543647000	1.673044000
C	-4.845418000	0.158681000	1.945041000
H	-5.568512000	-0.525809000	2.417072000
H	-4.196306000	0.574051000	2.735730000

H	-5.377469000	0.979546000	1.453847000
C	-2.065542000	-0.891574000	-3.607424000
H	-2.829488000	-0.842530000	-4.404162000
H	-1.164883000	-0.395486000	-4.000799000
H	-1.830808000	-1.942037000	-3.394134000
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P	1.253873000	-0.052800000	0.146317000
C	1.735758000	1.656236000	0.595105000
C	1.863778000	2.089375000	1.920591000
C	1.933880000	2.567005000	-0.456377000
C	2.181351000	3.424499000	2.191449000
H	1.715449000	1.390855000	2.744755000
C	2.252337000	3.896314000	-0.181855000
H	1.832525000	2.235360000	-1.492161000
C	2.373049000	4.329126000	1.144460000
H	2.279461000	3.755773000	3.227707000
H	2.403332000	4.598653000	-1.004608000
H	2.618637000	5.371629000	1.359209000
C	1.286269000	-1.006794000	1.701325000
C	2.293436000	-1.931030000	2.005418000
C	0.213376000	-0.820526000	2.592308000
C	2.234056000	-2.657228000	3.199390000
H	3.119829000	-2.093711000	1.312321000
C	0.165681000	-1.541606000	3.785553000
H	-0.580820000	-0.111610000	2.344355000
C	1.175261000	-2.462711000	4.090223000
H	3.019653000	-3.380084000	3.430658000
H	-0.666746000	-1.390413000	4.476534000
H	1.132355000	-3.032435000	5.021272000
C	2.649353000	-0.601271000	-0.896151000
C	2.426986000	-1.303085000	-2.089360000
C	3.963390000	-0.281646000	-0.509013000
C	3.511531000	-1.690253000	-2.881961000
H	1.409121000	-1.559322000	-2.383164000
C	5.041773000	-0.678079000	-1.300782000
H	4.144031000	0.282957000	0.407976000
C	4.816757000	-1.382255000	-2.489234000
H	3.332892000	-2.234920000	-3.811805000
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H	5.661695000	-1.686506000	-3.111370000

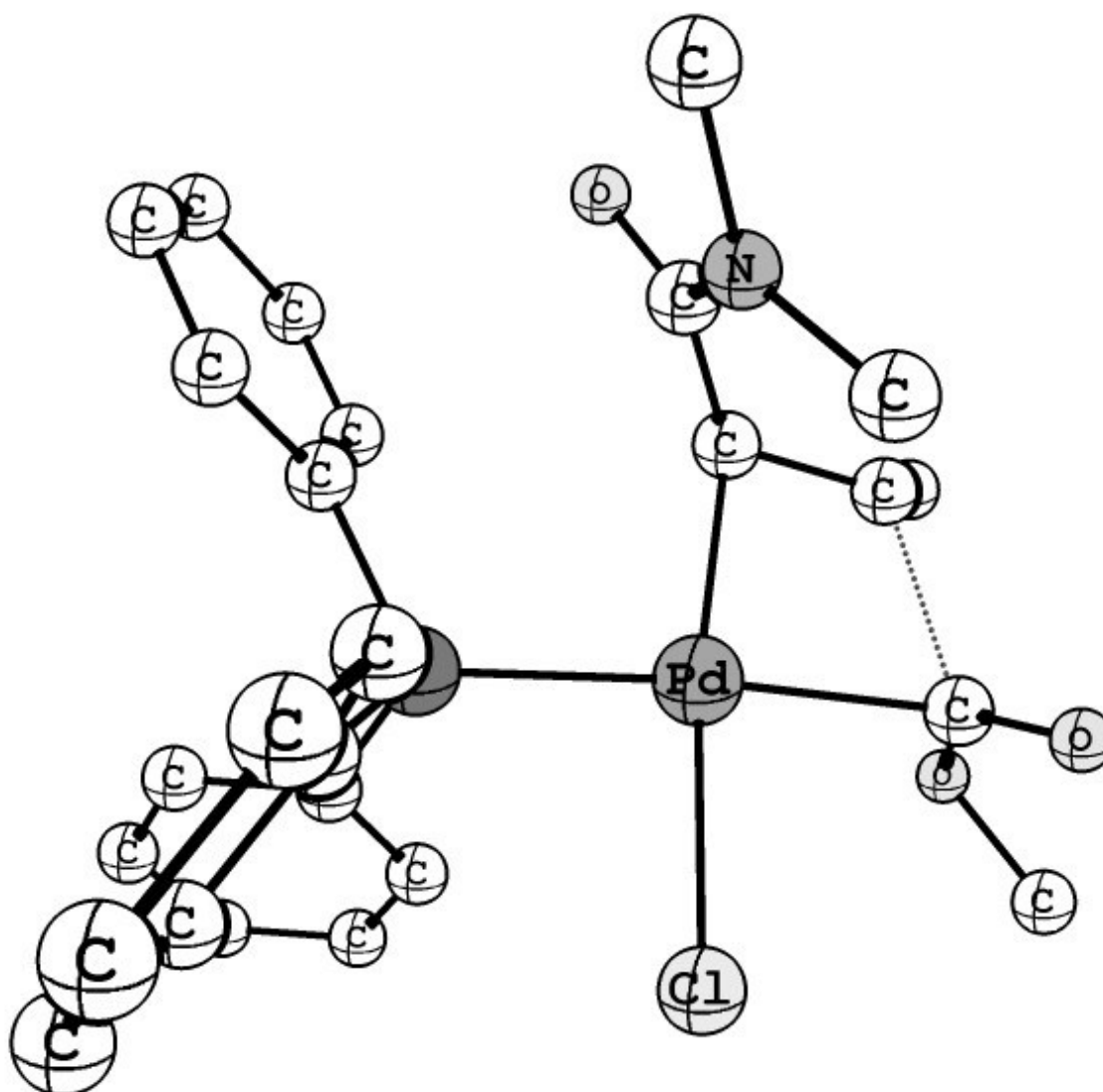
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C	-2.668320000	-1.352240000	-0.963817000
O	-2.695353000	-2.024091000	-1.965103000
O	-3.382919000	-1.559074000	0.138867000
C	-4.070556000	-2.819893000	0.241580000
H	-3.325642000	-3.614557000	0.387618000
H	-4.722479000	-2.736444000	1.117877000
H	-4.658969000	-3.010288000	-0.666130000
C	-2.523336000	0.577966000	-1.135514000
H	-3.208181000	0.474834000	-1.979735000
C	-1.197746000	1.034221000	-1.522509000
H	-0.819254000	1.880912000	-0.943563000
C	-3.086213000	1.198977000	0.131832000
O	-2.313268000	1.625112000	0.992012000
N	-4.435213000	1.299550000	0.255307000
C	-4.981478000	1.900034000	1.463451000
H	-4.184608000	2.423575000	2.000105000
H	-5.781454000	2.608110000	1.197230000

H	-5.410421000	1.124017000	2.121485000
C	-5.431560000	0.693878000	-0.611433000
H	-4.992542000	0.240347000	-1.503352000
H	-5.980577000	-0.092048000	-0.065784000
H	-6.158363000	1.454867000	-0.937873000
C	-0.814854000	0.999298000	-2.979641000
H	-1.257356000	1.860562000	-3.512505000
H	0.274389000	1.064886000	-3.103838000
H	-1.171798000	0.079540000	-3.466711000
C	1.561843000	0.068128000	1.892051000
C	2.719457000	-0.318714000	2.581475000
C	0.414184000	0.444715000	2.612922000
C	2.733391000	-0.320034000	3.979683000
H	3.610312000	-0.628772000	2.033809000
C	0.439519000	0.451817000	4.009143000
H	-0.496719000	0.731835000	2.080227000
C	1.596951000	0.067663000	4.695198000
H	3.637251000	-0.628556000	4.510147000
H	-0.453546000	0.749645000	4.563602000
H	1.610682000	0.064427000	5.787651000
C	2.900382000	-0.847125000	-0.558390000
C	4.197465000	-0.305828000	-0.509749000
C	2.706484000	-2.134648000	-1.081596000
C	5.284143000	-1.046952000	-0.977238000
H	4.359820000	0.698176000	-0.113266000
C	3.798389000	-2.871594000	-1.549296000
H	1.701785000	-2.560461000	-1.098216000
C	5.085928000	-2.330312000	-1.498976000
H	6.288793000	-0.620092000	-0.936056000
H	3.640124000	-3.873089000	-1.955937000
H	5.937462000	-2.906939000	-1.867765000
C	1.817269000	1.825231000	-0.410492000
C	2.328005000	2.102878000	-1.690300000
C	1.467962000	2.891115000	0.432971000
C	2.492039000	3.423309000	-2.113390000
H	2.608654000	1.285414000	-2.357252000
C	1.631954000	4.211437000	0.004789000
H	1.065104000	2.694664000	1.427142000
C	2.143024000	4.481429000	-1.267831000
H	2.894555000	3.625295000	-3.108617000
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TSA45-b

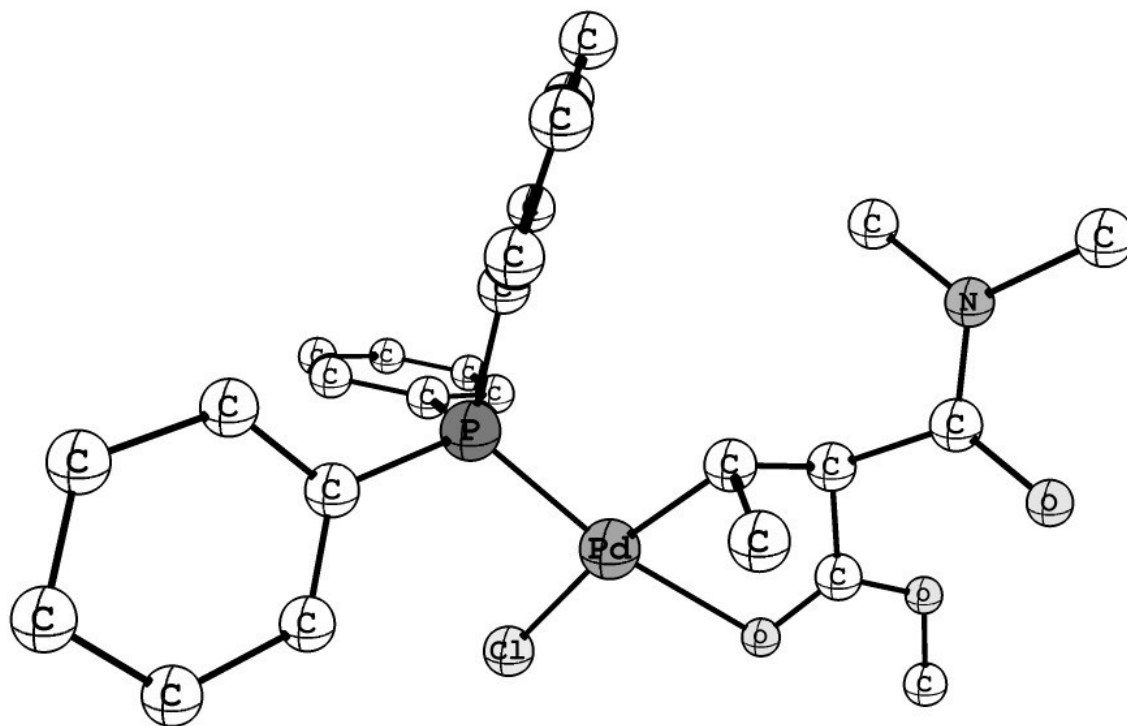


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O	3.984227000	-0.523104000	1.061110000
O	3.594375000	-1.838019000	-0.729435000
C	4.448726000	-2.867892000	-0.197579000
H	3.951983000	-3.330719000	0.666736000
H	4.578945000	-3.597810000	-1.004043000
H	5.416280000	-2.443831000	0.104171000
C	2.967436000	0.782846000	-1.126669000
H	3.616692000	1.391722000	-0.491600000
C	1.578960000	1.217124000	-1.184033000

H	1.110302000	1.063622000	-2.161159000
C	1.118103000	2.567940000	-0.680114000
N	1.343209000	2.974418000	0.610009000
C	0.930635000	4.317865000	0.988360000
H	1.800629000	4.994062000	1.066749000
H	0.242744000	4.707804000	0.231976000
H	0.428896000	4.289973000	1.968618000
C	2.191393000	2.305147000	1.579363000
H	2.226135000	1.223979000	1.414094000
H	3.222670000	2.700287000	1.565520000
H	1.782975000	2.465667000	2.588389000
C	3.598270000	0.365921000	-2.438750000
H	4.601302000	-0.058038000	-2.306440000
H	2.970639000	-0.365753000	-2.965383000
H	3.681000000	1.266654000	-3.069190000
O	0.521871000	3.284566000	-1.482283000
C	-1.969155000	-1.728327000	-0.692847000
C	-1.265790000	-2.884058000	-1.059170000
C	-3.361121000	-1.670711000	-0.884552000
C	-1.949825000	-3.974984000	-1.604408000
H	-0.188558000	-2.930178000	-0.899810000
C	-4.040102000	-2.765225000	-1.420884000
H	-3.913362000	-0.766856000	-0.619050000
C	-3.334519000	-3.918920000	-1.782837000
H	-1.395712000	-4.871800000	-1.890735000
H	-5.122073000	-2.715963000	-1.562626000
H	-3.866698000	-4.772902000	-2.208408000
C	-1.651015000	-0.067052000	1.715870000
C	-1.110878000	1.003748000	2.449111000
C	-2.532830000	-0.958617000	2.340129000
C	-1.467092000	1.191532000	3.784535000
H	-0.411470000	1.688626000	1.967953000
C	-2.879921000	-0.771832000	3.682192000
H	-2.944948000	-1.802938000	1.786267000
C	-2.352457000	0.301731000	4.404453000
H	-1.046655000	2.029799000	4.344556000
H	-3.565116000	-1.472800000	4.164310000
H	-2.626022000	0.443550000	5.452462000
C	-1.860059000	1.098438000	-0.949525000
C	-1.742158000	1.060153000	-2.349213000
C	-2.542623000	2.160464000	-0.344232000
C	-2.307386000	2.065604000	-3.130408000
H	-1.212674000	0.233503000	-2.829775000
C	-3.104006000	3.171208000	-1.131983000
H	-2.649899000	2.201109000	0.739781000
C	-2.990332000	3.125502000	-2.522608000

H	-2.21366000	2.024585000	-4.218005000
H	-3.637372000	3.994587000	-0.651289000
H	-3.432323000	3.914882000	-3.134977000

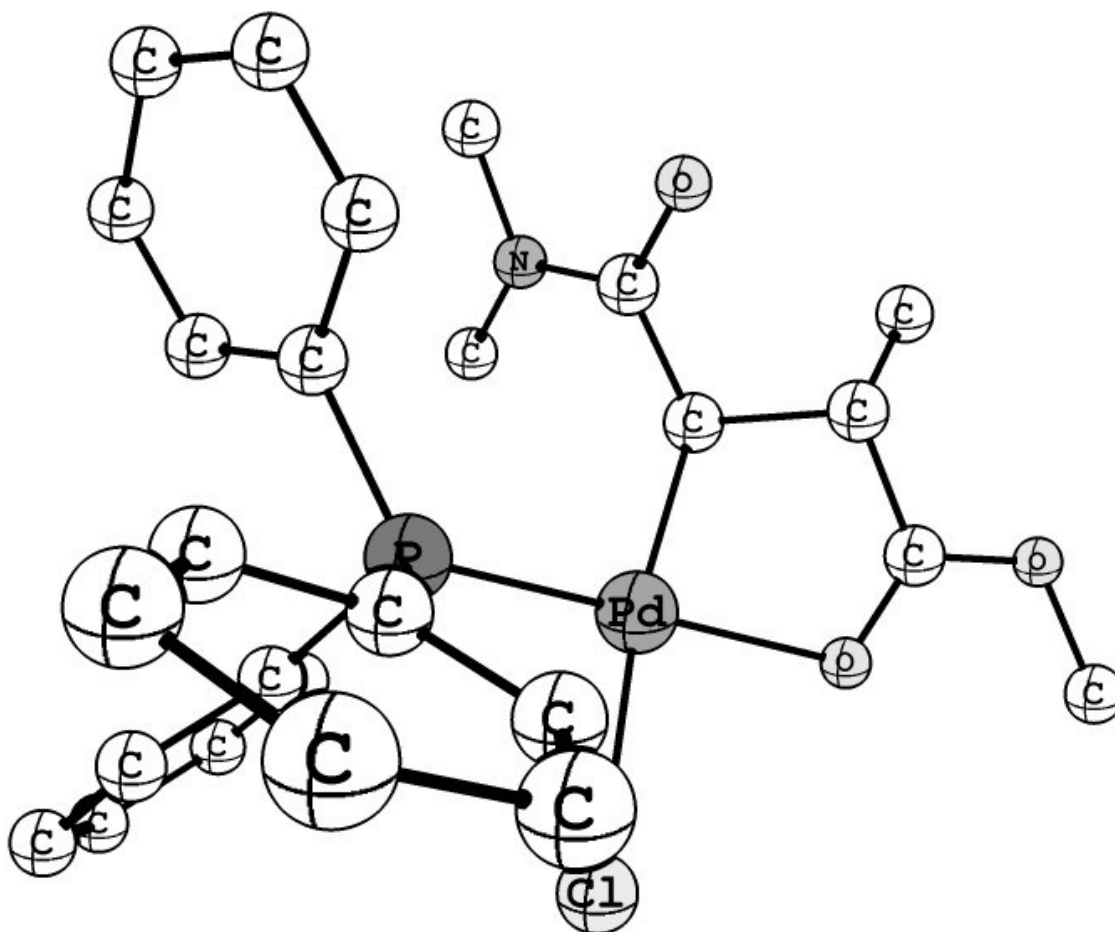
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Pd	-0.243305000	-1.275867000	-0.228468000
C	-1.621370000	0.196654000	-0.582796000
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H	-1.304626000	1.170009000	-0.199510000
C	-4.093024000	0.598994000	-0.204854000
O	-4.873806000	0.179704000	-1.055091000
N	-4.192447000	1.845109000	0.339854000
C	-3.251230000	2.453616000	1.266716000
H	-2.588104000	1.716199000	1.727591000
H	-2.624246000	3.205868000	0.758519000
H	-3.804906000	2.958995000	2.073699000
C	-5.234419000	2.740693000	-0.138542000
H	-5.845197000	3.101150000	0.705331000
H	-4.788976000	3.617345000	-0.639641000
H	-5.869913000	2.202235000	-0.848492000
C	-1.828800000	0.272311000	-2.091916000
H	-2.592678000	1.021930000	-2.366153000
H	-0.893044000	0.558173000	-2.594400000
H	-2.152629000	-0.692572000	-2.512956000

H	-2.674220000	-0.127590000	1.282275000
C	-3.085268000	-1.728224000	0.041860000
O	-2.150820000	-2.459355000	-0.295562000
O	-4.262906000	-2.198551000	0.367659000
C	-4.460671000	-3.622630000	0.294863000
H	-5.496265000	-3.794845000	0.605769000
H	-4.302672000	-3.972821000	-0.734153000
H	-3.762118000	-4.136806000	0.969017000
Cl	1.168218000	-3.252583000	0.055852000
P	1.447475000	0.183937000	-0.003768000
C	2.652404000	0.163897000	-1.382331000
C	2.795634000	-1.006641000	-2.144977000
C	3.459151000	1.279272000	-1.667104000
C	3.730910000	-1.055413000	-3.181865000
H	2.188280000	-1.881294000	-1.903305000
C	4.390896000	1.224329000	-2.706202000
H	3.360192000	2.194605000	-1.081770000
C	4.526433000	0.058552000	-3.466800000
H	3.836421000	-1.969188000	-3.771234000
H	5.012235000	2.096495000	-2.921784000
H	5.252970000	0.019194000	-4.281796000
C	0.980099000	1.950369000	0.166364000
C	0.846542000	2.540098000	1.432053000
C	0.619633000	2.687595000	-0.975091000
C	0.364022000	3.846715000	1.553468000
H	1.117062000	1.981061000	2.328798000
C	0.140430000	3.992363000	-0.850305000
H	0.710527000	2.242189000	-1.967389000
C	0.009498000	4.575237000	0.414948000
H	0.266585000	4.295406000	2.544567000
H	-0.134558000	4.554753000	-1.745366000
H	-0.368282000	5.595480000	0.511804000
C	2.409224000	-0.168146000	1.514373000
C	3.790312000	0.061694000	1.588775000
C	1.724434000	-0.649618000	2.641687000
C	4.476770000	-0.183537000	2.781436000
H	4.335740000	0.426289000	0.717011000
C	2.411569000	-0.883230000	3.834242000
H	0.651001000	-0.842396000	2.577795000
C	3.789712000	-0.652699000	3.905043000
H	5.553877000	-0.008184000	2.830598000
H	1.871302000	-1.254874000	4.707826000
H	4.329254000	-0.844127000	4.835490000

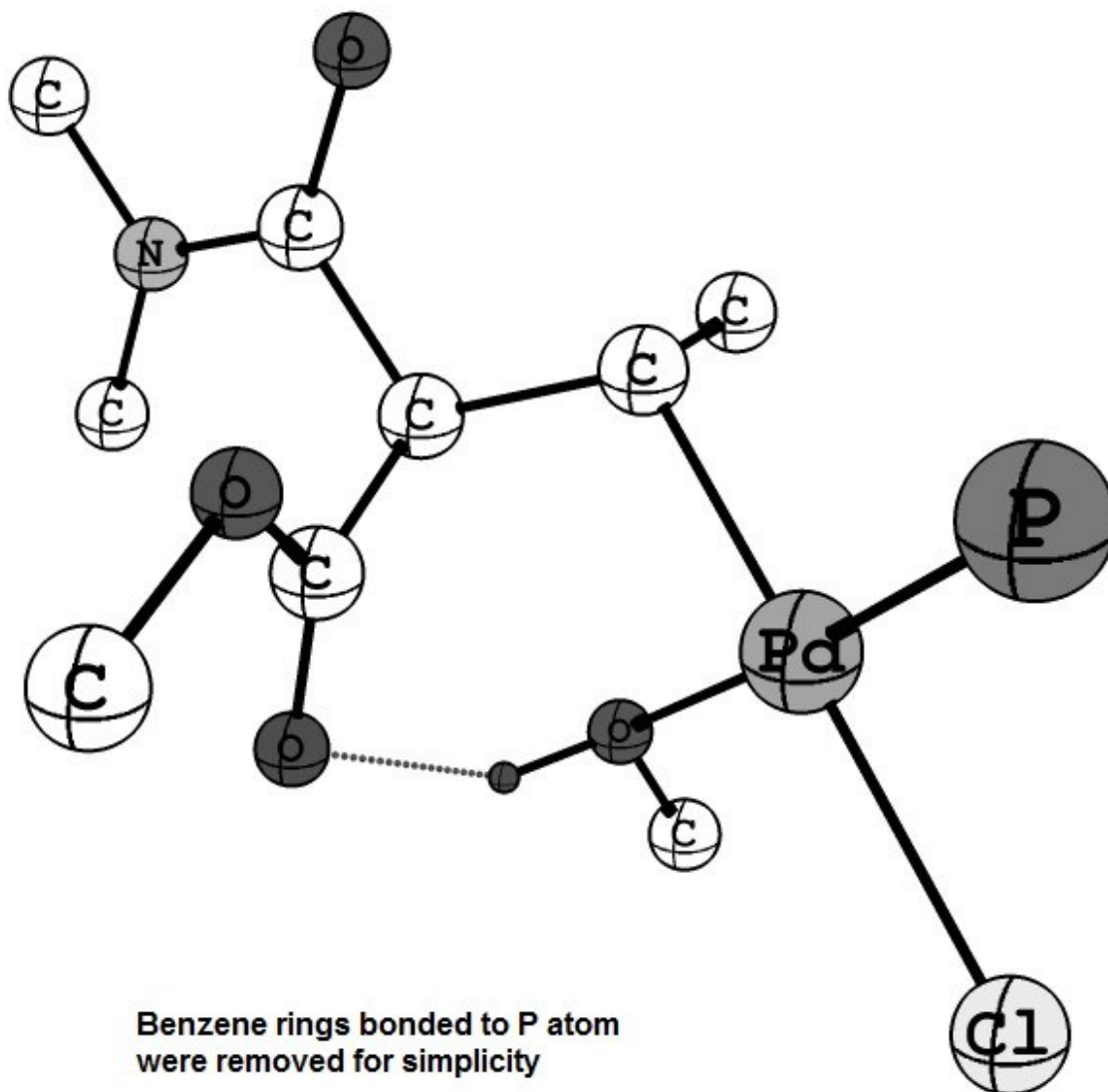
5A-b



Pd	1.132558000	-0.803853000	-0.284664000
C	3.967903000	-0.531135000	0.150137000
O	3.247862000	-1.421771000	-0.313137000
O	5.255170000	-0.709188000	0.333298000
C	5.813790000	-1.992960000	-0.003410000
H	6.882791000	-1.919882000	0.221635000
H	5.343084000	-2.779493000	0.601901000
H	5.655619000	-2.205297000	-1.069336000
C	3.412982000	0.809401000	0.545134000
C	2.115845000	1.035699000	-0.255273000
H	3.146740000	0.713492000	1.613051000
H	2.373585000	1.098490000	-1.322792000
C	1.418321000	2.272181000	0.214860000
O	1.457708000	2.608994000	1.405341000
N	0.784229000	3.038203000	-0.724195000
C	0.658195000	2.673685000	-2.122260000
H	0.612553000	1.586187000	-2.243744000
H	-0.282113000	3.088205000	-2.514027000

H	1.489275000	3.064855000	-2.736916000
C	0.320793000	4.367542000	-0.372359000
H	0.931692000	5.136486000	-0.879451000
H	-0.727567000	4.502547000	-0.673837000
H	0.403464000	4.493698000	0.710975000
C	4.431214000	1.948334000	0.404022000
H	3.987361000	2.881799000	0.773055000
H	5.339539000	1.740446000	0.986927000
H	4.720094000	2.086214000	-0.649749000
P	-1.045541000	-0.288279000	0.042063000
Cl	0.435057000	-3.113040000	-0.582550000
C	-2.012698000	-0.944050000	-1.374467000
C	-3.239627000	-1.601088000	-1.214204000
C	-1.500416000	-0.749063000	-2.667124000
C	-3.948716000	-2.046899000	-2.333732000
H	-3.643979000	-1.779993000	-0.218109000
C	-2.215688000	-1.184197000	-3.783893000
H	-0.529943000	-0.266919000	-2.799548000
C	-3.443043000	-1.835044000	-3.619208000
H	-4.900929000	-2.564593000	-2.197096000
H	-1.808120000	-1.023590000	-4.784514000
H	-4.000144000	-2.183342000	-4.491958000
C	-1.693631000	-1.093002000	1.565566000
C	-2.983063000	-0.774059000	2.030827000
C	-0.909141000	-1.999082000	2.294011000
C	-3.482740000	-1.368529000	3.190469000
H	-3.598013000	-0.049995000	1.494522000
C	-1.409122000	-2.583161000	3.461602000
H	0.087041000	-2.258212000	1.937513000
C	-2.695526000	-2.273783000	3.910076000
H	-4.487647000	-1.116692000	3.536784000
H	-0.786032000	-3.283418000	4.022644000
H	-3.084014000	-2.732348000	4.822431000
C	-1.730862000	1.402180000	0.259744000
C	-2.537400000	2.004254000	-0.716881000
C	-1.535419000	2.051173000	1.490221000
C	-3.168472000	3.223520000	-0.452252000
H	-2.697297000	1.512674000	-1.676859000
C	-2.169080000	3.265634000	1.750484000
H	-0.898619000	1.597816000	2.249876000
C	-2.996475000	3.849158000	0.785373000
H	-3.805491000	3.677683000	-1.214516000
H	-2.017568000	3.758215000	2.713509000
H	-3.498954000	4.796130000	0.995181000

6A-a

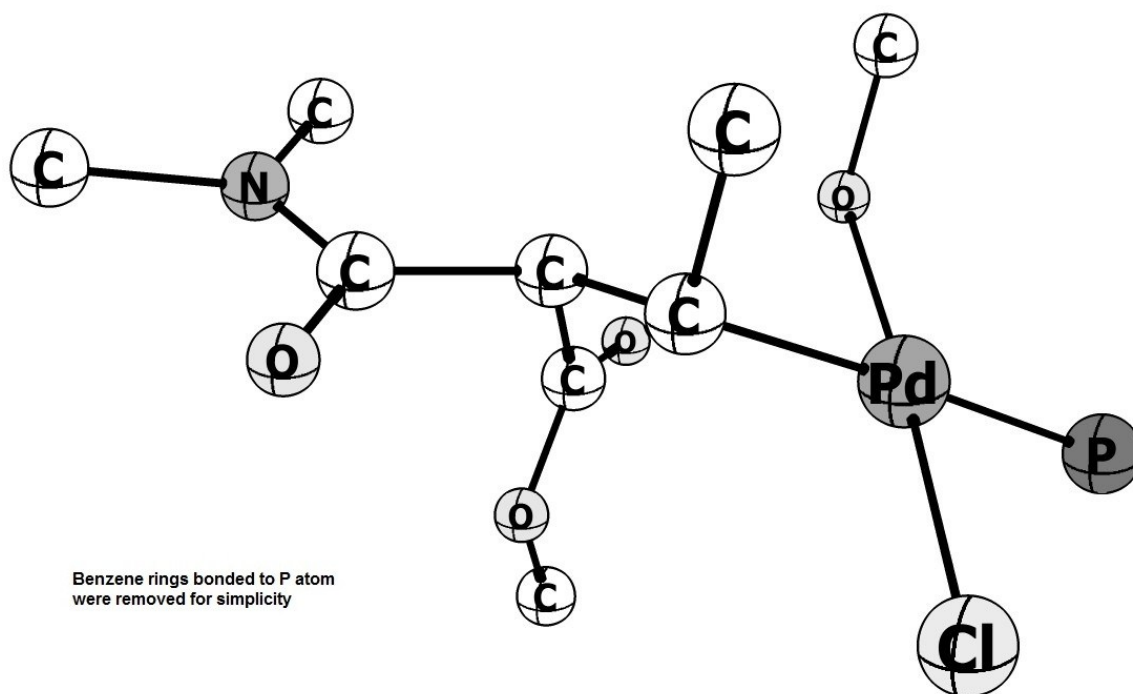


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P	1.389393000	0.325376000	-0.051050000
Cl	1.599902000	-3.104515000	0.284149000
C	-2.468923000	-0.523156000	1.019321000
O	-2.530912000	-1.600088000	1.592407000
O	-2.120656000	0.603155000	1.633391000
C	-1.754992000	0.514447000	3.020490000
H	-0.925852000	-0.192463000	3.147869000
H	-1.439051000	1.521703000	3.311376000
H	-2.617384000	0.189588000	3.618604000
C	-2.765721000	-0.323701000	-0.456510000
H	-3.247258000	-1.248421000	-0.791064000
C	-1.455409000	-0.142800000	-1.245327000

H	-1.168718000	0.905112000	-1.166202000
C	-3.733378000	0.863258000	-0.673332000
O	-3.333561000	1.923305000	-1.143916000
C	-6.003316000	1.725729000	-0.553785000
H	-5.479078000	2.608708000	-0.932653000
H	-6.753726000	1.401849000	-1.295628000
H	-6.530944000	1.981699000	0.379604000
C	-5.599887000	-0.584892000	0.166684000
H	-4.844702000	-1.241023000	0.608519000
H	-6.343665000	-0.366983000	0.948202000
H	-6.111440000	-1.131056000	-0.645870000
N	-5.034477000	0.667800000	-0.311965000
C	-1.608602000	-0.518053000	-2.710720000
H	-0.686322000	-0.296932000	-3.270516000
H	-1.842618000	-1.587014000	-2.836515000
H	-2.426831000	0.062087000	-3.177700000
H	-2.036632000	-2.879780000	0.260496000
C	-1.356852000	-4.338791000	-0.931092000
H	-0.590458000	-4.782171000	-0.278808000
H	-2.296404000	-4.909506000	-0.859388000
H	-0.999433000	-4.371576000	-1.969182000
O	-1.593677000	-2.971574000	-0.607968000
C	1.008271000	1.996826000	-0.702839000
C	1.775108000	2.578579000	-1.723741000
C	-0.110234000	2.690143000	-0.205173000
C	1.433270000	3.836129000	-2.231289000
H	2.643833000	2.055896000	-2.124857000
C	-0.445418000	3.945113000	-0.712317000
H	-0.733772000	2.241280000	0.568288000
C	0.325842000	4.522508000	-1.726428000
H	2.039340000	4.279641000	-3.024605000
H	-1.323286000	4.464577000	-0.322906000
H	0.060549000	5.504176000	-2.125804000
C	3.064895000	-0.005488000	-0.706952000
C	4.214053000	0.454914000	-0.049451000
C	3.186969000	-0.682055000	-1.930275000
C	5.475019000	0.239793000	-0.613071000
H	4.126661000	0.981455000	0.902697000
C	4.447154000	-0.886997000	-2.495091000
H	2.290377000	-1.047873000	-2.435572000
C	5.593067000	-0.428408000	-1.835713000
H	6.367930000	0.596665000	-0.094639000
H	4.536005000	-1.412196000	-3.448784000
H	6.579638000	-0.595020000	-2.274483000
C	1.623987000	0.594863000	1.753700000
C	1.702055000	-0.527268000	2.596760000

C	1.747939000	1.879428000	2.306422000
C	1.888057000	-0.361263000	3.970424000
H	1.621696000	-1.527797000	2.165825000
C	1.924476000	2.039150000	3.684146000
H	1.706186000	2.761752000	1.668151000
C	1.991070000	0.921232000	4.519670000
H	1.945402000	-1.240389000	4.616550000
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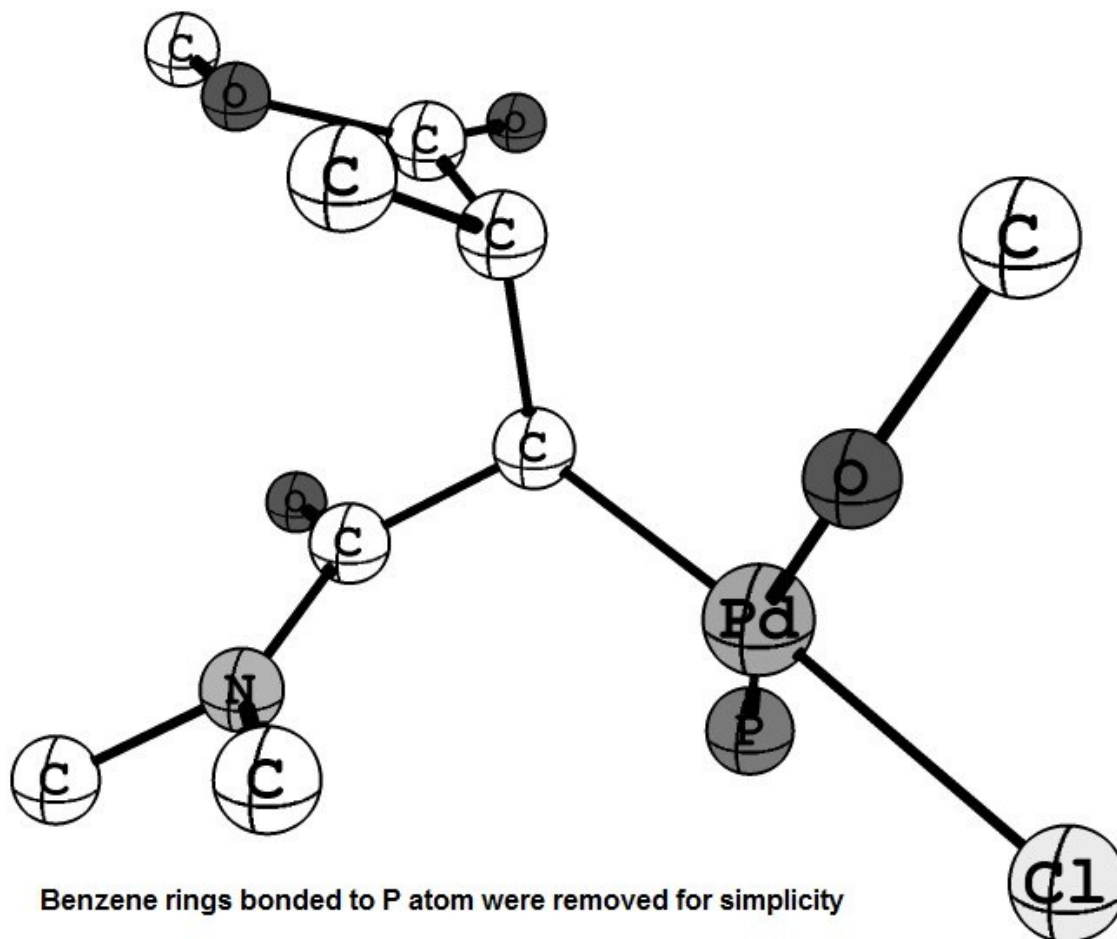
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Pd	0.475246000	-0.436592000	-0.667889000
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O	2.381969000	1.524048000	1.256755000
O	3.055378000	-0.528391000	1.863109000
C	2.524011000	-0.315272000	3.188403000
H	1.470168000	-0.055558000	3.131237000
H	2.663231000	-1.257902000	3.706530000
H	3.075005000	0.481189000	3.684650000
C	3.416305000	0.096760000	-0.390955000
H	3.409362000	1.022988000	-0.958065000
C	2.474474000	-0.896994000	-1.074500000
H	2.631996000	-1.886270000	-0.661403000
C	4.858202000	-0.462773000	-0.309555000
O	5.067481000	-1.670161000	-0.383184000

C	7.242512000	-0.020544000	-0.141701000
H	7.264114000	-1.102081000	-0.205923000
H	7.786822000	0.405457000	-0.987899000
H	7.729586000	0.300878000	0.780669000
C	5.702387000	1.883071000	-0.103780000
H	4.691035000	2.175746000	0.151295000
H	6.367243000	2.277756000	0.664767000
H	5.974089000	2.340154000	-1.058900000
N	5.859454000	0.435833000	-0.156837000
C	2.647996000	-0.880038000	-2.581696000
H	2.006910000	-1.625675000	-3.049742000
H	2.406546000	0.096424000	-3.007219000
H	3.683326000	-1.110400000	-2.865755000
H	1.405503000	2.183116000	-0.110194000
C	0.928627000	2.587211000	-2.069084000
H	0.282570000	3.465328000	-1.984473000
H	1.939780000	2.901972000	-2.328713000
H	0.542748000	1.931428000	-2.844765000
O	0.885745000	1.841901000	-0.858435000
Cl	0.170901000	-2.752887000	-0.391253000
P	-1.856407000	0.069123000	-0.097186000
C	-3.006451000	-1.278038000	-0.576142000
C	-3.021802000	-1.668465000	-1.916556000
C	-3.838449000	-1.935627000	0.328752000
C	-3.863087000	-2.684423000	-2.345180000
H	-2.365553000	-1.181230000	-2.625049000
C	-4.674653000	-2.961601000	-0.099238000
H	-3.840542000	-1.653877000	1.369345000
C	-4.692053000	-3.334794000	-1.435472000
H	-3.861903000	-2.977964000	-3.386084000
H	-5.318001000	-3.461955000	0.612677000
H	-5.345187000	-4.131106000	-1.766853000

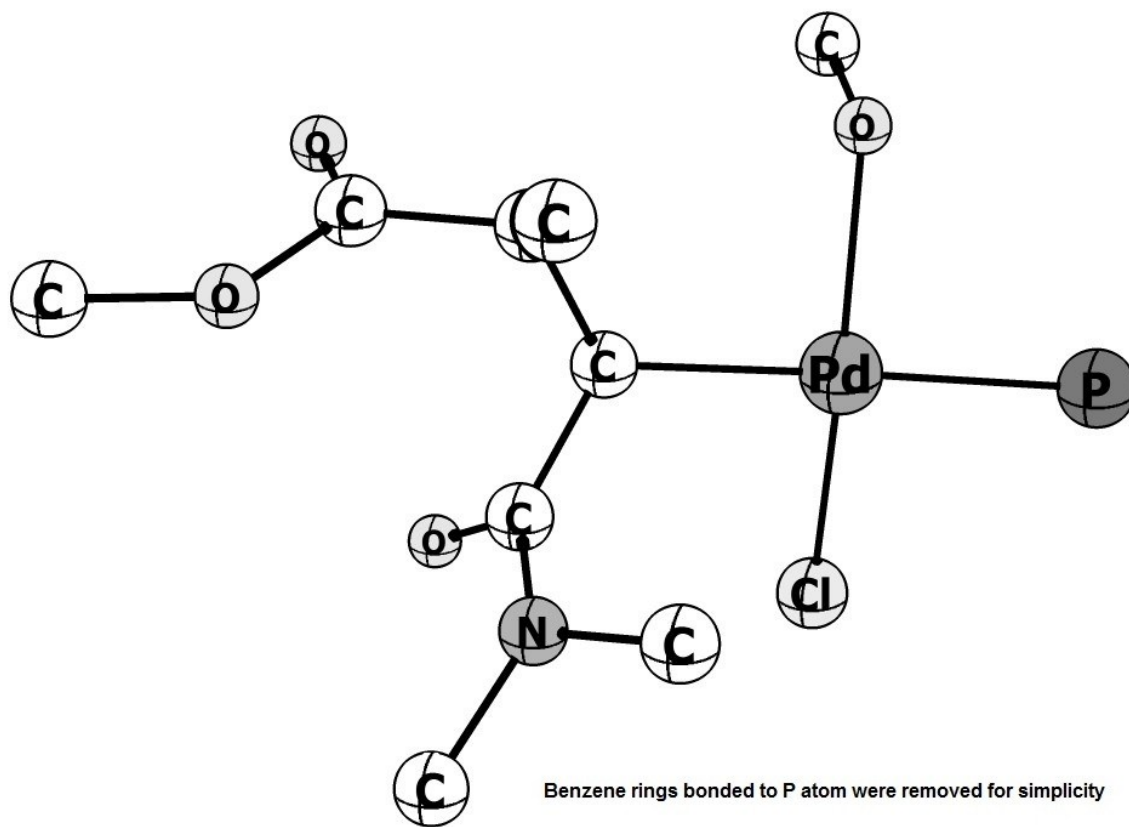
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Pd	0.04134000	-1.42848800	-0.21501000
P	-1.30360900	0.37515800	-0.09866700
Cl	-1.87468700	-2.98676100	-0.00850400
C	3.82723100	0.27444300	-1.38557200
O	3.54947600	0.94385900	-2.35751700
O	4.89368900	0.51463500	-0.61422700
C	5.64252800	1.69558800	-0.90959900
H	5.00794200	2.58433400	-0.77829300
H	6.47625600	1.71616700	-0.19815800
H	6.02085400	1.67266200	-1.94154900
C	2.97592600	-0.88864100	-0.88128600
H	2.63077600	-1.38367700	-1.80104900
C	1.72310200	-0.22903100	-0.23403200
H	1.46420500	0.59256100	-0.90496700
C	2.07212900	0.49067900	1.06585300
N	1.94162400	-0.12661600	2.28331900
C	2.28087700	0.61958900	3.48408000

H	3.267894000	0.316302000	3.876782000
H	2.305304000	1.688343000	3.249457000
H	1.528635000	0.425644000	4.265585000
C	1.681159000	-1.535834000	2.507263000
H	1.529914000	-2.067521000	1.565118000
H	2.534663000	-2.002203000	3.027884000
H	0.781771000	-1.673398000	3.130181000
C	3.763548000	-1.876715000	-0.021611000
H	4.647085000	-2.240204000	-0.567248000
H	4.119631000	-1.403544000	0.903776000
H	3.144687000	-2.741399000	0.243005000
O	2.480856000	1.651317000	0.991958000
H	0.136705000	-3.850634000	-0.158315000
C	1.356314000	-3.954387000	-1.699422000
H	1.508185000	-5.044431000	-1.663124000
H	0.577973000	-3.714302000	-2.441179000
H	2.298171000	-3.479469000	-1.998437000
O	1.005966000	-3.463293000	-0.403082000
H	-1.005925000	2.636085000	1.879698000
H	-0.031194000	1.788362000	-2.245917000
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H	1.055746000	4.004382000	-2.443681000
H	1.107412000	5.551470000	-0.483901000
H	-0.436599000	0.282521000	2.635137000
H	-4.226776000	0.235439000	0.566953000
H	-1.619604000	0.123507000	4.812592000
H	-5.406185000	0.055031000	2.738594000
H	-4.114161000	0.004347000	4.869895000
H	-1.958237000	-1.464926000	-2.318888000
H	-3.276097000	2.384230000	-0.869664000
H	-3.578930000	-1.305419000	-4.200465000
H	-4.917797000	2.523219000	-2.720792000
H	-5.071576000	0.682000000	-4.397662000

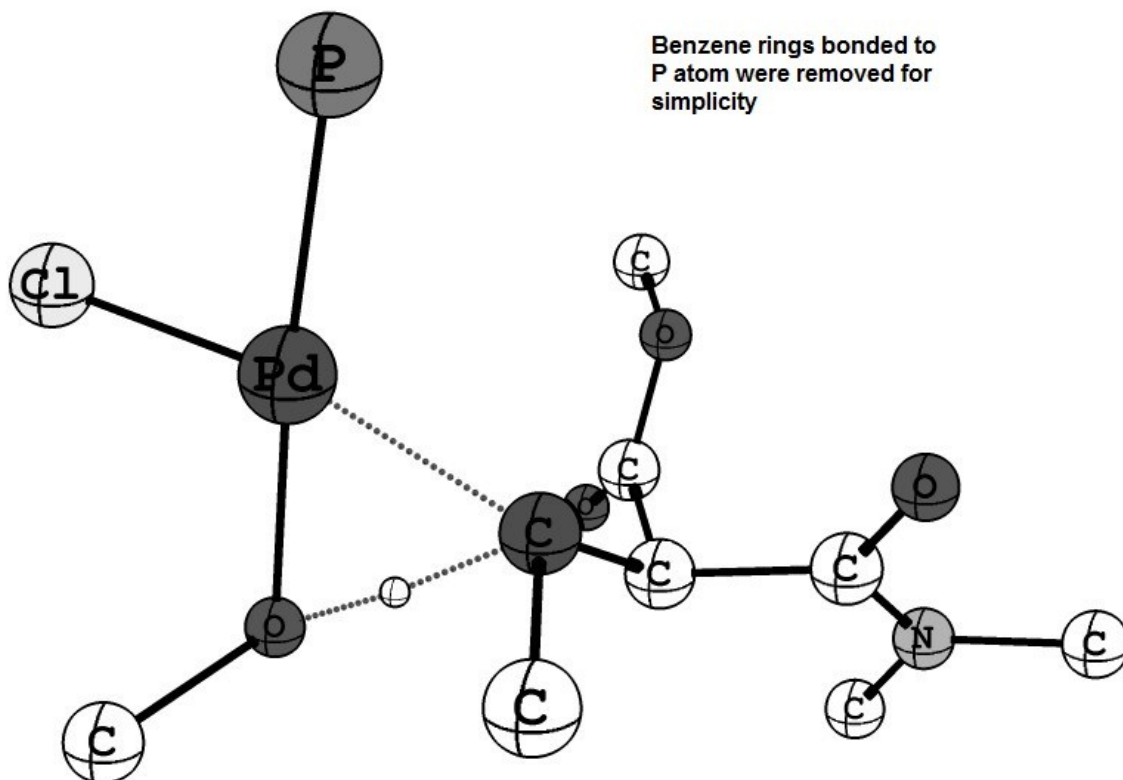
6A-b-t



Pd	-0.455301000	-0.165723000	0.308853000
C	-4.663318000	-1.504011000	0.144240000
O	-4.953124000	-2.290874000	1.019670000
O	-5.559448000	-0.694026000	-0.433643000
C	-6.900163000	-0.744881000	0.082191000
H	-6.905267000	-0.489939000	1.140595000
H	-7.460690000	-0.010880000	-0.488674000
H	-7.323215000	-1.738677000	-0.055463000
C	-3.253388000	-1.298989000	-0.384855000
H	-2.769660000	-2.256735000	-0.216407000
C	-2.554620000	-0.276846000	0.551594000
H	-2.595693000	-0.693232000	1.558433000
C	-3.302729000	1.032331000	0.675124000
N	-3.294130000	1.952556000	-0.325093000
C	-4.097323000	3.152212000	-0.159769000
H	-4.344396000	3.548101000	-1.144631000
H	-5.010289000	2.914957000	0.377308000
H	-3.554749000	3.922679000	0.398527000
C	-2.314945000	2.031363000	-1.390390000
H	-1.717375000	1.128713000	-1.427006000
H	-2.813453000	2.166915000	-2.352242000
H	-1.642375000	2.876430000	-1.219687000

C	-3.221753000	-1.011287000	-1.883500000
H	-3.704773000	-1.822776000	-2.430553000
H	-3.737314000	-0.087888000	-2.132853000
H	-2.190475000	-0.942065000	-2.225289000
O	-3.997229000	1.220480000	1.684023000
H	0.335148000	-2.305582000	-1.087577000
C	-0.411709000	-3.250437000	0.482187000
H	-0.434099000	-4.217714000	-0.018037000
H	0.470252000	-3.171612000	1.116182000
H	-1.302962000	-3.129627000	1.089865000
O	-0.432970000	-2.198683000	-0.506603000
Cl	-0.451006000	1.845136000	1.503517000
P	1.908919000	0.021921000	0.009477000
C	2.404091000	1.656183000	-0.620377000
C	3.569122000	2.306362000	-0.216045000
C	1.560842000	2.279341000	-1.544665000
C	3.891433000	3.554416000	-0.738035000
H	4.223219000	1.850563000	0.512998000
C	1.889462000	3.519230000	-2.073089000
H	0.640976000	1.794403000	-1.840216000
C	3.056702000	4.160553000	-1.669510000
H	4.795541000	4.052500000	-0.412981000
H	1.229227000	3.990114000	-2.789615000
H	3.309401000	5.132011000	-2.073843000

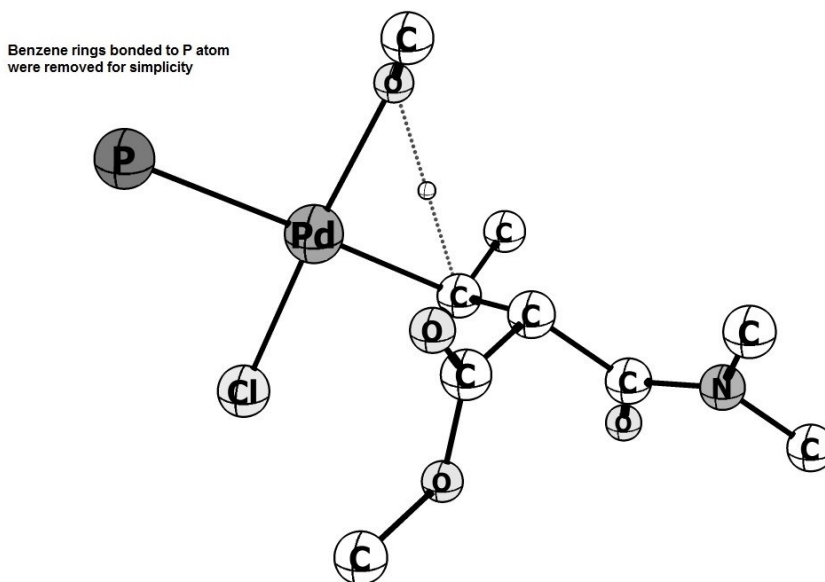
TSA61-a



Pd	0.174059000	-1.557199000	0.037203000
P	1.456022000	0.336383000	-0.083748000
Cl	1.917694000	-2.655100000	1.191775000
C	-2.681127000	-0.452721000	1.281133000
O	-2.972152000	-1.200096000	2.187564000
O	-2.005865000	0.689625000	1.461101000
C	-1.601867000	0.995426000	2.802973000
H	-0.978528000	0.186128000	3.203285000
H	-1.020774000	1.921025000	2.740299000
H	-2.484867000	1.131286000	3.443162000
C	-3.038024000	-0.673698000	-0.181867000
H	-3.628319000	-1.597876000	-0.207181000
C	-1.775929000	-0.867938000	-1.044589000
H	-1.253851000	0.088240000	-1.086023000
C	-3.900346000	0.511182000	-0.681961000
O	-3.408653000	1.379669000	-1.395382000
C	-6.066449000	1.608225000	-0.758660000
H	-6.501684000	2.162197000	0.089259000
H	-5.480004000	2.292200000	-1.379898000
H	-6.893394000	1.188532000	-1.356472000
C	-5.869297000	-0.478450000	0.517747000
H	-5.163820000	-1.085758000	1.091365000

H	-6.542375000	0.011860000	1.237643000
H	-6.479809000	-1.141261000	-0.120665000
N	-5.200070000	0.543583000	-0.274954000
C	-2.072823000	-1.304005000	-2.482205000
H	-1.136250000	-1.399696000	-3.051618000
H	-2.593208000	-2.274730000	-2.521039000
H	-2.703598000	-0.556032000	-2.987946000
H	-1.478321000	-2.085423000	-0.576098000
C	-0.725276000	-4.218578000	-0.861759000
H	0.199522000	-4.691761000	-0.488522000
H	-1.511380000	-4.992324000	-0.936802000
H	-0.524237000	-3.842798000	-1.882620000
O	-1.157738000	-3.195244000	0.010701000
C	0.882103000	1.594443000	-1.283748000
C	1.622656000	1.893008000	-2.439141000
C	-0.342197000	2.248563000	-1.060099000
C	1.146316000	2.837366000	-3.352080000
H	2.573483000	1.394134000	-2.627261000
C	-0.812691000	3.189196000	-1.976657000
H	-0.941569000	2.018236000	-0.179112000
C	-0.070232000	3.487131000	-3.123028000
H	1.731111000	3.064777000	-4.246237000
H	-1.775827000	3.669399000	-1.798241000
H	-0.441665000	4.221927000	-3.841121000
C	3.157073000	-0.051084000	-0.622212000
C	4.261765000	0.642630000	-0.110748000
C	3.343431000	-1.033116000	-1.607951000
C	5.545515000	0.353740000	-0.583443000
H	4.122964000	1.405809000	0.657000000
C	4.625277000	-1.311613000	-2.083318000
H	2.481933000	-1.579530000	-1.998107000
C	5.728492000	-0.620168000	-1.569220000
H	6.404884000	0.893023000	-0.178691000
H	4.765336000	-2.075254000	-2.851592000
H	6.732683000	-0.843979000	-1.936527000
C	1.624800000	1.235272000	1.501612000
C	1.801911000	0.498185000	2.684693000
C	1.599992000	2.638223000	1.557041000
C	1.941852000	1.159096000	3.905862000
H	1.826892000	-0.592011000	2.641228000
C	1.733044000	3.293152000	2.784531000
H	1.473514000	3.223938000	0.646549000
C	1.900114000	2.556144000	3.960464000
H	2.074551000	0.578350000	4.821405000
H	1.706520000	4.384520000	2.818892000
H	1.999525000	3.070602000	4.918994000

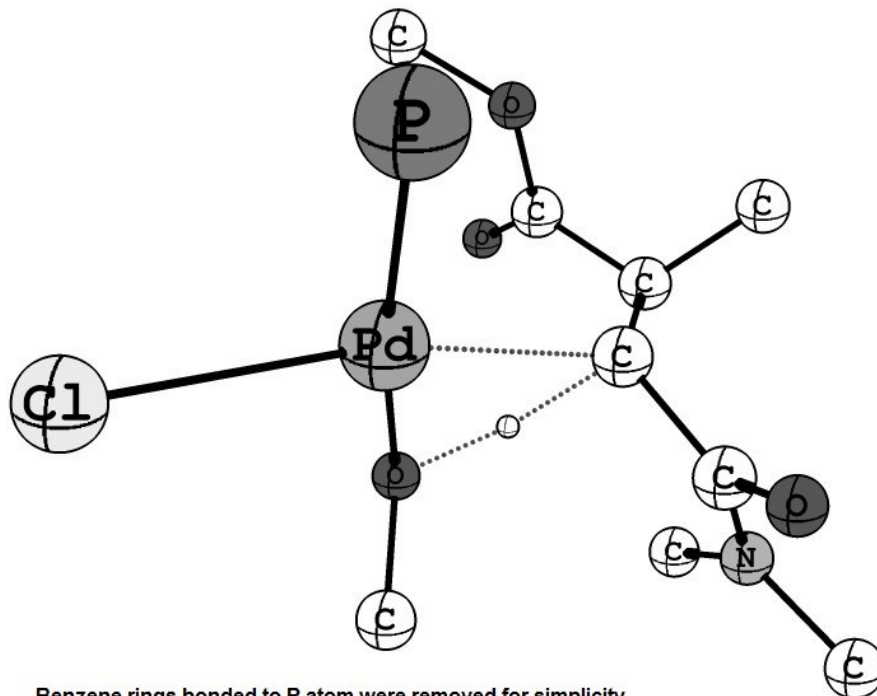
TSA61-a-t



Pd	0.399667000	0.053868000	-0.880410000
C	2.890044000	-0.450296000	0.875483000
O	2.363170000	0.019408000	1.865156000
O	3.162419000	-1.745545000	0.732168000
C	2.680608000	-2.632514000	1.748233000
H	1.582677000	-2.660650000	1.724656000
H	3.088009000	-3.620381000	1.505846000
H	3.021575000	-2.307728000	2.741090000
C	3.314723000	0.347658000	-0.349464000
H	3.217039000	1.405906000	-0.076364000
C	2.379556000	0.029703000	-1.524580000
H	2.564532000	-1.001451000	-1.841150000
C	4.795178000	0.054253000	-0.696112000
O	5.097887000	-0.622349000	-1.674848000
C	7.138840000	0.309446000	-0.250864000
H	7.352302000	-0.771001000	-0.239345000
H	7.353059000	0.680703000	-1.265124000
H	7.802716000	0.813043000	0.462438000
C	5.528144000	1.391116000	1.301563000
H	4.470196000	1.425260000	1.574713000
H	6.076051000	0.971289000	2.160246000
H	5.881626000	2.424232000	1.141645000
N	5.752814000	0.573110000	0.119382000
C	2.551007000	0.970652000	-2.706613000
H	1.833251000	0.736327000	-3.508150000
H	2.424039000	2.037539000	-2.447137000
H	3.567556000	0.878522000	-3.127848000

H	1.464291730	1.148867630	-1.008750230
C	0.720183000	2.726203000	0.811533000
H	1.588428000	2.292618000	1.326310000
H	0.789796000	3.822982000	0.774119000
H	-0.191256000	2.444601000	1.348576000
O	0.599727000	2.206038000	-0.521494000
P	-1.906621000	0.030745000	-0.062982000
Cl	0.337061000	-2.275633000	-1.222574000
C	-2.516769000	1.656570000	0.528213000
C	-2.534774000	2.716195000	-0.396062000
C	-2.895922000	1.897635000	1.856311000
C	-2.929567000	3.992813000	0.002442000
H	-2.231541000	2.539244000	-1.430628000
C	-3.283375000	3.181650000	2.255292000
H	-2.885595000	1.084263000	2.583380000
C	-3.299893000	4.230075000	1.332045000
H	-2.941384000	4.808997000	-0.723712000
H	-3.574990000	3.360087000	3.292963000
H	-3.601078000	5.232225000	1.645825000
C	-3.264492000	-0.528693000	-1.166885000
C	-4.570026000	-0.023291000	-1.045967000
C	-2.988830000	-1.495735000	-2.148236000
C	-5.584019000	-0.481497000	-1.891094000
H	-4.796821000	0.730976000	-0.290566000
C	-4.007259000	-1.952067000	-2.989367000
H	-1.976572000	-1.895275000	-2.237939000
C	-5.305022000	-1.446181000	-2.864459000
H	-6.595919000	-0.082421000	-1.788102000
H	-3.783801000	-2.704876000	-3.749188000
H	-6.098575000	-1.801582000	-3.526118000
C	-2.019284000	-1.049922000	1.412868000
C	-0.904797000	-1.094445000	2.268292000
C	-3.152244000	-1.819019000	1.713740000
C	-0.932511000	-1.889731000	3.415732000
H	-0.006519000	-0.518836000	2.032710000
C	-3.172681000	-2.620498000	2.859597000
H	-4.020088000	-1.795315000	1.052168000
C	-2.065388000	-2.655935000	3.712568000
H	-0.060690000	-1.918920000	4.073638000
H	-4.057623000	-3.220318000	3.085075000
H	-2.082863000	-3.284528000	4.606058000

TSA61-b

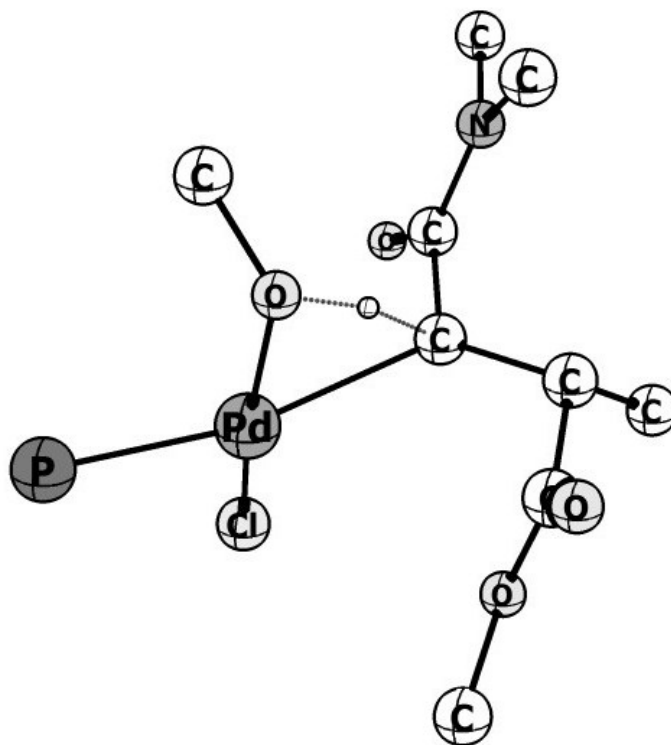


Benzene rings bonded to P atom were removed for simplicity

Pd	-0.364750000	0.185548000	-1.254899000
P	1.374226000	0.252840000	0.202377000
Cl	1.064558000	0.976022000	-2.942753000
C	-2.085236000	-2.709584000	-0.514248000
O	-2.552047000	-3.239655000	-1.497547000
O	-0.815052000	-2.893273000	-0.119863000
C	-2.825877000	-1.730194000	0.377156000
H	-3.853532000	-1.751891000	0.000915000
C	-2.198268000	-0.327376000	0.179778000
H	-1.261977000	-0.349544000	0.752008000
C	-2.878285000	0.898352000	0.739376000
N	-4.208894000	1.102767000	0.500606000
O	-2.217666000	1.718099000	1.389648000
H	-2.330761000	-0.109089000	-1.178329000
C	-2.626488000	1.396031000	-2.797979000
H	-3.621895000	1.314535000	-3.270772000
H	-2.714431000	2.084431000	-1.936241000
H	-1.929797000	1.850916000	-3.521722000
O	-2.175068000	0.113513000	-2.408370000
C	-5.015031000	0.400020000	-0.484154000
H	-4.395082000	-0.165374000	-1.185455000
H	-5.741482000	-0.282069000	-0.009974000
H	-5.580573000	1.138430000	-1.074743000
C	-4.875390000	2.219496000	1.151264000

H	-5.042554000	3.050665000	0.442967000
H	-5.854962000	1.894330000	1.536361000
H	-4.254141000	2.581008000	1.976874000
C	0.017169000	-3.678027000	-0.977969000
H	1.001035000	-3.720665000	-0.498070000
H	-0.393526000	-4.689836000	-1.101698000
H	0.103239000	-3.197922000	-1.963532000
C	-2.823554000	-2.148228000	1.852263000
H	-1.800776000	-2.171765000	2.252210000
H	-3.407769000	-1.426280000	2.443004000
H	-3.275892000	-3.143379000	1.986837000
C	0.942358000	-0.372532000	1.872755000
C	0.376625000	0.460121000	2.850218000
C	1.112049000	-1.741039000	2.145480000
C	-0.004069000	-0.069628000	4.085255000
H	0.216640000	1.517654000	2.650920000
C	0.732079000	-2.263821000	3.381563000
H	1.546091000	-2.401720000	1.395710000
C	0.172640000	-1.429482000	4.354705000
H	-0.442480000	0.587435000	4.839473000
H	0.870496000	-3.328261000	3.582599000
H	-0.127295000	-1.840374000	5.321314000
C	1.853751000	2.001881000	0.398640000
C	0.823081000	2.936000000	0.615575000
C	3.180230000	2.439073000	0.281717000
C	1.132211000	4.291124000	0.744589000
H	-0.217252000	2.604170000	0.684437000
C	3.478232000	3.799586000	0.404165000
H	3.982617000	1.727439000	0.086072000
C	2.458473000	4.725338000	0.640070000
H	0.330845000	5.012525000	0.919646000
H	4.513574000	4.134838000	0.310438000
H	2.695540000	5.787505000	0.734728000
C	2.851631000	-0.723394000	-0.229977000
C	2.915883000	-1.440980000	-1.432240000
C	3.913049000	-0.808310000	0.690012000
C	4.035942000	-2.227698000	-1.716428000
H	2.094799000	-1.376890000	-2.145131000
C	5.032122000	-1.587284000	0.396280000
H	3.860538000	-0.275775000	1.641682000
C	5.094388000	-2.298958000	-0.807509000
H	4.077723000	-2.787820000	-2.653045000
H	5.854705000	-1.645064000	1.112355000
H	5.968567000	-2.914101000	-1.032694000

TSA61-b-t



Benzene rings bonded to P atom
were removed for simplicity

Pd	-0.455301000	-0.165723000	0.308853000
C	-4.663318000	-1.504011000	0.144240000
O	-4.953124000	-2.290874000	1.019670000
O	-5.559448000	-0.694026000	-0.433643000
C	-6.900163000	-0.744881000	0.082191000
H	-6.905267000	-0.489939000	1.140595000
H	-7.460690000	-0.010880000	-0.488674000
H	-7.323215000	-1.738677000	-0.055463000
C	-3.253388000	-1.298989000	-0.384855000
H	-2.769660000	-2.256735000	-0.216407000
C	-2.554620000	-0.276846000	0.551594000
H	-2.595693000	-0.693232000	1.558433000
C	-3.302729000	1.032331000	0.675124000
N	-3.294130000	1.952556000	-0.325093000
C	-4.097323000	3.152212000	-0.159769000
H	-4.344396000	3.548101000	-1.144631000
H	-5.010289000	2.914957000	0.377308000
H	-3.554749000	3.922679000	0.398527000
C	-2.314945000	2.031363000	-1.390390000
H	-1.717375000	1.128713000	-1.427006000
H	-2.813453000	2.166915000	-2.352242000

H	-1.642375000	2.876430000	-1.219687000
C	-3.221753000	-1.011287000	-1.883500000
H	-3.704773000	-1.822776000	-2.430553000
H	-3.737314000	-0.087888000	-2.132853000
H	-2.190475000	-0.942065000	-2.225289000
O	-3.997229000	1.220480000	1.684023000
H	-1.475724400	-1.254133240	0.013482580
C	-0.411709000	-3.250437000	0.482187000
H	-0.434099000	-4.217714000	-0.018037000
H	0.470252000	-3.171612000	1.116182000
H	-1.302962000	-3.129627000	1.089865000
O	-0.432970000	-2.198683000	-0.506603000
Cl	-0.451006000	1.845136000	1.503517000
P	1.908919000	0.021921000	0.009477000
C	2.404091000	1.656183000	-0.620377000
C	3.569122000	2.306362000	-0.216045000
C	1.560842000	2.279341000	-1.544665000
C	3.891433000	3.554416000	-0.738035000
H	4.223219000	1.850563000	0.512998000
C	1.889462000	3.519230000	-2.073089000
H	0.640976000	1.794403000	-1.840216000
C	3.056702000	4.160553000	-1.669510000
H	4.795541000	4.052500000	-0.412981000
H	1.229227000	3.990114000	-2.789615000
H	3.309401000	5.132011000	-2.073843000
C	2.944053000	-0.314177000	1.463915000
C	4.297318000	-0.648735000	1.352237000
C	2.360231000	-0.235835000	2.729233000
C	5.052970000	-0.893023000	2.490180000
H	4.758394000	-0.728311000	0.377109000
C	3.120491000	-0.479349000	3.867370000
H	1.313103000	0.019057000	2.816355000
C	4.465904000	-0.807484000	3.749569000
H	6.099079000	-1.153079000	2.394922000
H	2.659072000	-0.417363000	4.844226000
H	5.056675000	-1.001242000	4.635384000
C	2.516545000	-1.159207000	-1.248612000
C	2.656651000	-0.797303000	-2.590114000
C	2.722939000	-2.496862000	-0.886286000
C	2.997705000	-1.748100000	-3.544625000
H	2.508499000	0.229239000	-2.893513000
C	3.059628000	-3.445407000	-1.843932000
H	2.638589000	-2.798911000	0.148963000
C	3.196920000	-3.073825000	-3.177015000
H	3.109281000	-1.448436000	-4.578440000
H	3.219382000	-4.472842000	-1.544632000

H	3.460833000	-3.812092000	-3.922450000
H	5.788323740	-0.258418060	-3.735242320
H	3.036116040	-3.559901920	-3.289635440
H	5.351466950	-2.713826860	-3.675728160
Cl	1.381164800	0.246638520	0.200338570

Table S2. DFT/B3LYP-D3-PCM/Def2-TZVP computed total electronic energies (E_{tot} , au), zero-point energies (ZPE, kcal/mol) and Gibbs free energies (G_{tot} , 383.15K, au) in methanol for the alkoxy cycle

Compound	E_{tot} (solv+D3)	ZPE	G_{tot} (solv+D3)
1A	-2776.8763486	370.62906	-2776.354210
2A	-1853.5375541	203.46793	-1853.267876
2A-t	-1853.5355261	204.17552	-1853.271251
TSA23	-1853.52885023	203.28141	-1853.258824
3A	-1853.53351992	204.54622	-1853.263963
3A-G	-1853.4674365	200.19211	-1853.209557
4A	-2218.98384753	309.15048	-2218.554959
TSA45-a	-2218.95445949	308.38407	-2218.526430
TSA45-b	-2218.95550859	308.83705	-2218.525748
5A-a	-2219.0002333	310.6055	-2218.568967
5A-b	-2219.0054911	311.25264	-2218.571065
6A-a	-2334.7962143	344.64670	-2334.313922
6A-a-t	-2334.7700657	343.88858	-2334.295846
6A-b	-2334.7902529	344.59919	-2334.308641
6A-b-t	-2334.776824	345.85206	-2334.298934
TSA61-a	-2334.741365	342.01752	-2334.273642
TSA61-a-t	-2334.6917645	339.87993	-2334.216854
TSA61-b	-2334.74258926	342.02708	-2334.264149
TSA61-b-t	-2334.68705305	339.88452	-2334.208456