

Supplementary material to:

M.M. Conradie and J. Conradie, *S. Afr. J. Chem.*, 2008, **61**, 102–111.

OPTIMIZED CARTESIAN COORDINATES/Å

1 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/PW91/TZP

Rh	0.763424000	3.248892000	1.062838000
Fe	3.725887000	6.343147000	4.920746000
P	2.559851000	2.001214000	0.392346000
O	1.924315000	3.789085000	2.718471000
O	-0.873861000	4.306178000	1.880082000
C	2.418512000	0.853433000	-1.041809000
C	1.528403000	4.451824000	3.747546000
C	4.072707000	2.972394000	-0.025482000
C	-0.213729000	2.824997000	-0.447981000
C	3.929070000	4.311718000	4.675950000
H	4.368231000	3.811914000	3.819868000
O	-0.862641000	2.607593000	-1.387361000
C	-0.824153000	4.863168000	3.029567000
C	5.137833000	2.392105000	-0.732763000
H	5.081363000	1.348258000	-1.041563000
C	4.148215000	4.323559000	0.343695000
H	3.319386000	4.775322000	0.887551000
C	2.371317000	5.331997000	6.070517000
H	1.448079000	5.732368000	6.475545000
C	2.538069000	4.669660000	4.795420000
C	3.046051000	0.912377000	1.795466000
C	2.112955000	1.390560000	-2.304343000
H	1.972679000	2.465380000	-2.421307000
C	2.453554000	-1.366145000	-2.023670000
H	2.585749000	-2.441436000	-1.907086000
C	6.261858000	3.151302000	-1.059768000
H	7.080087000	2.692616000	-1.614285000
C	2.325172000	-0.644380000	3.513211000
H	1.529071000	-1.210584000	3.995133000
C	2.028955000	0.176778000	2.427045000
H	1.001804000	0.266006000	2.071843000
C	0.220434000	4.967780000	3.936953000
H	0.020273000	5.497902000	4.861134000
C	4.599850000	4.730826000	5.863672000
H	5.659647000	4.616083000	6.069845000
C	2.147680000	-0.826815000	-3.272928000
H	2.035607000	-1.480219000	-4.137964000
C	4.356272000	0.829071000	2.282358000
H	5.150699000	1.407319000	1.811754000
C	3.635077000	-0.723238000	3.995079000
H	3.863191000	-1.351674000	4.855850000
C	3.640393000	5.355066000	6.724814000
H	3.844392000	5.790664000	7.698012000
C	2.591366000	-0.531357000	-0.911173000
H	2.833295000	-0.961743000	0.059582000
C	6.329936000	4.497488000	-0.691788000
H	7.202489000	5.093029000	-0.960829000
C	5.272483000	5.080560000	0.009429000
H	5.314318000	6.134628000	0.282764000
F	-3.155040000	4.558576000	3.477301000
C	4.646359000	0.016039000	3.381039000
H	5.666814000	-0.031972000	3.761163000
C	4.157931000	8.311029000	5.333903000
H	4.242234000	8.741760000	6.327047000
C	2.958468000	8.220021000	4.554124000
H	1.973611000	8.568326000	4.849884000
F	-2.562023000	6.418554000	2.487997000
F	-2.156287000	6.135690000	4.620098000
C	4.679645000	7.254152000	3.336649000
H	5.227683000	6.732070000	2.558682000
C	1.981075000	0.554590000	-3.411129000
H	1.738811000	0.981991000	-4.383306000
C	-2.175924000	5.498529000	3.410808000
C	5.222025000	7.713566000	4.581673000
H	6.253213000	7.611949000	4.905815000
C	3.283610000	7.569758000	3.319892000
H	2.581055000	7.323176000	2.528462000

1 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/BLYP/TZP

Rh	0.746551000	3.244759000	1.041300000
Fe	3.738523000	6.383838000	4.970631000
P	2.578156000	1.972577000	0.364679000
O	1.909597000	3.805788000	2.720381000
O	-0.907783000	4.313093000	1.877078000
C	2.418472000	0.803149000	-1.073400000
C	1.505917000	4.462146000	3.759261000
C	4.102605000	2.948146000	-0.080164000
C	-0.260439000	2.834545000	-0.482350000
C	3.911108000	4.310757000	4.709929000
H	4.355685000	3.811813000	3.857791000
O	-0.919157000	2.644815000	-1.423879000
C	-0.861122000	4.863467000	3.035813000
C	5.169805000	2.362688000	-0.791531000
H	5.115069000	1.319229000	-1.096324000
C	4.186112000	4.306613000	0.282696000
H	3.364889000	4.767775000	0.825899000
C	2.344705000	5.330761000	6.103699000
H	1.421781000	5.731404000	6.506091000
C	2.517373000	4.683254000	4.815341000
C	3.078141000	0.889467000	1.791652000
C	2.113483000	1.334895000	-2.343766000
H	1.982115000	2.408459000	-2.470724000
C	2.433699000	-1.431055000	-2.048523000
H	2.558566000	-2.506146000	-1.925357000
C	6.299892000	3.119613000	-1.125583000
H	7.114893000	2.655055000	-1.679421000
C	2.365761000	-0.634963000	3.558048000
H	1.569090000	-1.177634000	4.064919000
C	2.060156000	0.177303000	2.460698000
H	1.027212000	0.274775000	2.129439000
C	0.185395000	4.964612000	3.949125000
H	-0.021447000	5.484757000	4.875811000
C	4.573550000	4.701169000	5.915778000
H	5.627154000	4.563673000	6.135370000
C	2.129939000	-0.895657000	-3.305832000
H	2.012851000	-1.552180000	-4.167212000
C	4.401593000	0.786488000	2.255710000
H	5.198604000	1.339406000	1.763568000
C	3.688278000	-0.731916000	4.015136000
H	3.923442000	-1.351371000	4.880228000
C	3.608392000	5.325957000	6.777424000
H	3.803854000	5.738282000	7.761549000
C	2.579627000	-0.587718000	-0.937077000
H	2.819566000	-1.018753000	0.032214000
C	6.375562000	4.471457000	-0.760679000
H	7.250092000	5.062609000	-1.031507000
C	5.316917000	5.061844000	-0.057400000
H	5.363460000	6.115021000	0.215853000
F	-3.213732000	4.554088000	3.473606000
C	4.702295000	-0.018646000	3.364223000
H	5.729951000	-0.080038000	3.720452000
C	4.211683000	8.379092000	5.415289000
H	4.295632000	8.791549000	6.415352000
C	3.014740000	8.326598000	4.620807000
H	2.035732000	8.691421000	4.913092000
F	-2.609225000	6.438518000	2.499756000
F	-2.212721000	6.130236000	4.646652000
C	4.734984000	7.355806000	3.393462000
H	5.282260000	6.850198000	2.605429000
C	1.972862000	0.491580000	-3.450727000
H	1.733353000	0.916766000	-4.423987000
C	-2.223511000	5.499738000	3.420308000
C	5.275147000	7.778367000	4.657090000
H	6.302408000	7.657213000	4.984658000
C	3.340666000	7.696718000	3.371559000
H	2.644215000	7.487254000	2.565921000

2 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/BP86/TZP

Rh	0.778217000	3.244382000	1.063763000
Fe	3.719345000	6.387997000	4.956674000
P	2.566362000	1.980859000	0.385860000
O	1.941301000	3.806353000	2.714148000
O	-0.867142000	4.293675000	1.870786000
C	2.405207000	0.836479000	-1.054668000
C	1.535772000	4.470990000	3.741627000
C	4.085483000	2.939988000	-0.050190000
C	-0.223032000	2.822363000	-0.437424000
C	3.935688000	4.355450000	4.687354000
H	4.387264000	3.865887000	3.830261000
O	-0.901085000	2.617966000	-1.359950000
C	-0.823940000	4.855444000	3.019754000
C	5.155329000	2.343855000	-0.741092000
H	5.101527000	1.291693000	-1.025006000
C	4.156008000	4.302945000	0.282152000
H	3.321154000	4.766022000	0.809276000
C	2.354457000	5.351194000	6.077253000
H	1.422890000	5.739883000	6.478133000
C	2.539597000	4.703000000	4.795074000
C	3.054819000	0.882105000	1.786150000
C	2.111638000	1.385693000	-2.316469000
H	1.990643000	2.464887000	-2.427650000
C	2.405424000	-1.380844000	-2.049753000
H	2.519608000	-2.460226000	-1.938216000
C	6.279932000	3.098293000	-1.085490000
H	7.101730000	2.627022000	-1.626766000
C	2.324979000	-0.642488000	3.534777000
H	1.520812000	-1.176266000	4.043131000
C	2.028343000	0.185439000	2.450863000
H	0.994153000	0.311825000	2.123764000
C	0.220124000	4.972678000	3.928366000
H	0.013640000	5.505058000	4.850965000
C	4.591248000	4.762745000	5.889619000
H	5.650142000	4.649252000	6.107529000
C	2.112828000	-0.829164000	-3.299207000
H	1.993596000	-1.476544000	-4.169749000
C	4.376016000	0.751896000	2.237623000
H	5.178840000	1.300134000	1.743144000
C	3.645977000	-0.768203000	3.980499000
H	3.875336000	-1.401499000	4.839258000
C	3.617114000	5.371913000	6.748571000
H	3.806715000	5.795878000	7.731307000
C	2.553436000	-0.553257000	-0.930766000
H	2.785085000	-0.993632000	0.039661000
C	6.343360000	4.456202000	-0.752691000
H	7.215651000	5.048080000	-1.036037000
C	5.280327000	5.055846000	-0.069934000
H	5.318255000	6.118326000	0.174637000
F	-3.159709000	4.534959000	3.449996000
C	4.667686000	-0.068427000	3.332879000
H	5.697379000	-0.152335000	3.684006000
C	4.170586000	8.348338000	5.409846000
H	4.263483000	8.757985000	6.412687000
C	2.965904000	8.285713000	4.632255000
H	1.984904000	8.639970000	4.938810000
F	-2.567690000	6.406730000	2.471840000
F	-2.174368000	6.114818000	4.609942000
C	4.675198000	7.330018000	3.384966000
H	5.216793000	6.823024000	2.591143000
C	1.968992000	0.557647000	-3.430252000
H	1.737154000	0.995596000	-4.401964000
C	-2.183852000	5.482569000	3.395267000
C	5.227416000	7.757232000	4.639095000
H	6.260743000	7.639511000	4.956129000
C	3.280275000	7.659347000	3.381102000
H	2.571986000	7.440089000	2.585357000

3 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/OLYP/TZP

Rh	0.766993000	3.249504000	1.076553000
Fe	3.743452000	6.369071000	4.976976000
P	2.566248000	1.984660000	0.374066000
O	1.881647000	3.852637000	2.769243000
O	-0.913210000	4.312325000	1.907767000
C	2.405994000	0.823745000	-1.061445000
C	1.469512000	4.512617000	3.786673000
C	4.078583000	2.945428000	-0.105430000
C	-0.213131000	2.832295000	-0.416339000
C	3.861996000	4.337204000	4.743747000
H	4.299193000	3.816653000	3.903655000
O	-0.897051000	2.635869000	-1.336687000
C	-0.891907000	4.877995000	3.048284000
C	5.144529000	2.339945000	-0.794520000
H	5.100374000	1.286483000	-1.055017000
C	4.158924000	4.314613000	0.192431000
H	3.340685000	4.799741000	0.715418000
C	2.331893000	5.422077000	6.109179000
H	1.425858000	5.863193000	6.504576000
C	2.482426000	4.745358000	4.840806000
C	3.080587000	0.900781000	1.781728000
C	2.165005000	1.356997000	-2.340098000
H	2.053354000	2.429709000	-2.475952000
C	2.457889000	-1.399509000	-2.045684000
H	2.577110000	-2.474124000	-1.920653000
C	6.265277000	3.083574000	-1.164254000
H	7.079627000	2.597873000	-1.698841000
C	2.390791000	-0.633033000	3.539299000
H	1.598493000	-1.173269000	4.052938000
C	2.073828000	0.194161000	2.462881000
H	1.036730000	0.299281000	2.154379000
C	0.145291000	5.006138000	3.966420000
H	-0.070545000	5.531876000	4.884314000
C	4.533591000	4.731635000	5.936613000
H	5.583802000	4.573242000	6.155688000
C	2.221762000	-0.860759000	-3.309887000
H	2.152015000	-1.511969000	-4.179590000
C	4.406597000	0.774696000	2.218747000
H	5.202703000	1.321308000	1.724025000
C	3.715191000	-0.753153000	3.966776000
H	3.960782000	-1.387033000	4.816946000
C	3.590751000	5.398200000	6.780502000
H	3.798783000	5.829620000	7.753190000
C	2.551276000	-0.564828000	-0.928336000
H	2.750042000	-1.006245000	0.042672000
C	6.336153000	4.445859000	-0.861953000
H	7.206563000	5.027565000	-1.161182000
C	5.279873000	5.057745000	-0.184918000
H	5.321105000	6.121191000	0.042338000
F	-3.247173000	4.545723000	3.444286000
C	4.719037000	-0.045308000	3.305544000
H	5.752566000	-0.123141000	3.637978000
C	4.257204000	8.313045000	5.392128000
H	4.340798000	8.743307000	6.384130000
C	3.073538000	8.275121000	4.587301000
H	2.101523000	8.671597000	4.858890000
F	-2.653425000	6.418196000	2.465168000
F	-2.307062000	6.145168000	4.612234000
C	4.772174000	7.225785000	3.412123000
H	5.312539000	6.680732000	2.647250000
C	2.076042000	0.521900000	-3.452238000
H	1.891829000	0.954008000	-4.433667000
C	-2.276963000	5.502222000	3.402283000
C	5.307072000	7.663946000	4.666187000
H	6.324379000	7.516673000	5.012132000
C	3.394888000	7.605812000	3.363824000
H	2.702125000	7.392301000	2.557096000

4 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/OPBE/TZP

Rh	0.807611000	3.238210000	1.095132000
Fe	3.719955000	6.388690000	4.998151000
P	2.554190000	1.982933000	0.376876000
O	1.927741000	3.857325000	2.763055000
O	-0.856403000	4.289698000	1.896485000
C	2.383495000	0.839945000	-1.057330000
C	1.512526000	4.526349000	3.765989000
C	4.056168000	2.931291000	-0.107798000
C	-0.170198000	2.800074000	-0.367602000
C	3.896841000	4.399958000	4.741475000
H	4.355342000	3.896361000	3.899576000
O	-0.864400000	2.588915000	-1.275141000
C	-0.837961000	4.873296000	3.023219000
C	5.126335000	2.320350000	-0.777414000
H	5.092217000	1.257933000	-1.009208000
C	4.114379000	4.306250000	0.148049000
H	3.282617000	4.791267000	0.653766000
C	2.329580000	5.443943000	6.092228000
H	1.409118000	5.865980000	6.480800000
C	2.510621000	4.775470000	4.826135000
C	3.059702000	0.887134000	1.763196000
C	2.154712000	1.382590000	-2.330663000
H	2.065728000	2.459896000	-2.461351000
C	2.387857000	-1.374838000	-2.044934000
H	2.484712000	-2.453728000	-1.923460000
C	6.234074000	3.067305000	-1.166478000
H	7.056832000	2.577897000	-1.687591000
C	2.358476000	-0.654945000	3.500326000
H	1.561304000	-1.197919000	4.007108000
C	2.048949000	0.179875000	2.432027000
H	1.012212000	0.291490000	2.118620000
C	0.193459000	5.020161000	3.937996000
H	-0.023521000	5.562443000	4.847089000
C	4.545775000	4.807062000	5.941227000
H	5.599787000	4.676882000	6.169803000
C	2.159434000	-0.828360000	-3.303832000
H	2.071456000	-1.476450000	-4.176163000
C	4.379707000	0.758039000	2.205426000
H	5.177958000	1.312288000	1.717921000
C	3.677702000	-0.780518000	3.932014000
H	3.918255000	-1.423063000	4.779105000
C	3.580015000	5.447872000	6.775817000
H	3.768255000	5.885967000	7.751761000
C	2.500693000	-0.548093000	-0.928117000
H	2.692396000	-0.994298000	0.044711000
C	6.284215000	4.435769000	-0.905704000
H	7.147399000	5.021501000	-1.223179000
C	5.221562000	5.052463000	-0.250091000
H	5.246569000	6.124617000	-0.056561000
F	-3.174137000	4.539564000	3.424084000
C	4.683955000	-0.069092000	3.284640000
H	5.716700000	-0.150594000	3.623531000
C	4.187790000	8.295974000	5.446637000
H	4.258526000	8.717055000	6.445757000
C	3.010322000	8.245287000	4.636574000
H	2.028104000	8.622077000	4.907766000
F	-2.593906000	6.382124000	2.413138000
F	-2.247392000	6.156150000	4.550506000
C	4.728995000	7.232305000	3.463945000
H	5.281670000	6.696809000	2.698408000
C	2.044694000	0.554427000	-3.441958000
H	1.866101000	0.993517000	-4.423063000
C	-2.218151000	5.494978000	3.363257000
C	5.249995000	7.669273000	4.722067000
H	6.268244000	7.530216000	5.074850000
C	3.348131000	7.591615000	3.411395000
H	2.660719000	7.370053000	2.599694000

5 [Rh(fctfa)(CO)(PPh₃)] isomer A ADF/B3LYP/CEP-31G

Rh	-1.007579000	1.637495000	-0.161154000
Fe	3.813836000	-1.632848000	-0.015897000
P	-2.339137000	-0.333767000	0.002589000
O	0.581803000	0.436192000	0.406367000
O	0.301542000	3.248451000	-0.232276000
C	-4.217618000	-0.185767000	0.159084000
C	1.828134000	0.773752000	0.676621000
C	-2.109311000	-1.508141000	-1.465973000
C	-2.418241000	2.715287000	-0.667347000
C	2.262821000	-1.679847000	1.419010000
H	1.254375000	-2.043494000	1.254692000
O	-3.298872000	3.447204000	-1.001832000
C	1.571382000	3.201937000	0.081312000
C	-3.140391000	-2.397470000	-1.884607000
H	-4.103993000	-2.404777000	-1.372640000
C	-0.858309000	-1.496279000	-2.149084000
H	-0.076963000	-0.804685000	-1.830252000
C	4.125143000	-0.235114000	1.522002000
H	4.760771000	0.643101000	1.460333000
C	2.702397000	-0.308246000	1.184442000
C	-1.826061000	-1.356142000	1.508406000
C	-4.946009000	0.435583000	-0.899082000
H	-4.427615000	0.797176000	-1.789263000
C	-6.317117000	-0.488268000	1.413804000
H	-6.838608000	-0.842006000	2.306618000
C	-2.919555000	-3.274222000	-2.983698000
H	-3.715670000	-3.951295000	-3.303915000
C	-1.133761000	-1.397180000	3.874035000
H	-0.890772000	-0.862841000	4.795417000
C	-1.513735000	-0.666637000	2.716146000
H	-1.548819000	0.424448000	2.742033000
C	2.347984000	2.107725000	0.518289000
H	3.391567000	2.289278000	0.756778000
C	3.393189000	-2.435047000	1.907058000
H	3.389605000	-3.489835000	2.167209000
C	-7.043456000	0.128461000	0.358466000
H	-8.126300000	0.253232000	0.437037000
C	-1.748018000	-2.776354000	1.460553000
H	-1.974536000	-3.311497000	0.537196000
C	-1.055810000	-2.817899000	3.828121000
H	-0.757058000	-3.378618000	4.717433000
C	4.542347000	-1.543576000	1.974359000
H	5.544778000	-1.814548000	2.293906000
C	-4.905867000	-0.647234000	1.316136000
H	-4.360301000	-1.122508000	2.132031000
C	-1.671796000	-3.261924000	-3.667362000
H	-1.506147000	-3.929023000	-4.517025000
C	-0.642295000	-2.372429000	-3.247769000
H	0.311027000	-2.348454000	-3.781249000
F	1.674933000	5.554366000	0.768002000
C	-1.362541000	-3.505204000	2.620874000
H	-1.303035000	-4.595770000	2.578934000
C	5.374492000	-2.326541000	-1.263386000
H	6.380292000	-2.570396000	-0.931804000
C	4.916672000	-1.023228000	-1.715786000
H	5.519037000	-0.121694000	-1.786340000
F	2.181857000	5.073614000	-1.378804000
F	3.635790000	4.554330000	0.267592000
C	3.090731000	-2.504521000	-1.798171000
H	2.089304000	-2.904181000	-1.927529000
C	-6.354477000	0.588417000	-0.800061000
H	-6.903434000	1.070158000	-1.612297000
C	2.261679000	4.583298000	-0.062581000
C	4.247174000	-3.241164000	-1.314970000
H	4.262531000	-4.289109000	-1.027635000
C	3.506447000	-1.134456000	-2.046666000
H	2.871564000	-0.324365000	-2.395479000

6 [Rh(fctfa)(CO)(PPh₃)] isomer B ADF/PW91/TZP

C	5.872896000	2.278501000	-2.042192000
C	4.878609000	2.918029000	-2.867092000
C	4.269025000	1.890013000	-3.681904000
C	4.906652000	0.648594000	-3.376456000
C	5.892507000	0.887988000	-2.364624000
Fe	4.027011000	1.447859000	-1.697943000
C	2.703206000	0.031182000	-1.010574000
C	2.007007000	1.245637000	-1.319543000
C	2.558905000	2.288609000	-0.508002000
C	3.596981000	1.724118000	0.299963000
C	3.685624000	0.327037000	-0.009402000
C	4.598601000	4.363830000	-2.853481000
C	3.573212000	4.880305000	-3.697230000
C	3.329727000	6.223817000	-3.914806000
C	2.208094000	6.600972000	-4.901909000
F	1.372943000	7.526995000	-4.375374000
O	5.345674000	5.070855000	-2.091801000
Rh	5.410008000	7.179679000	-1.984639000
P	5.655828000	9.467454000	-1.896761000
O	3.922933000	7.265435000	-3.451459000
C	6.603330000	7.051921000	-0.582752000
O	7.316537000	6.897427000	0.323253000
F	1.437093000	5.537922000	-5.278488000
F	2.729542000	7.130795000	-6.047564000
H	1.209831000	1.357717000	-2.047592000
H	2.266784000	3.334416000	-0.528979000
H	4.218727000	2.263505000	1.007562000
H	4.385785000	-0.379606000	0.425428000
H	2.528542000	-0.939341000	-1.465415000
H	3.480771000	2.029594000	-4.414272000
H	4.668454000	-0.312838000	-3.820560000
H	6.528597000	0.137564000	-1.905579000
H	6.490839000	2.789769000	-1.312859000
H	2.957635000	4.169154000	-4.237037000
C	4.644140000	10.467540000	-3.063262000
C	5.220656000	10.158237000	-0.241234000
C	7.357456000	10.086105000	-2.268409000
C	7.584555000	11.444939000	-2.555022000
C	8.871915000	11.907554000	-2.828930000
C	9.952613000	11.018937000	-2.839825000
C	9.737139000	9.664457000	-2.583878000
C	8.441234000	9.196471000	-2.300600000
H	6.745854000	12.141766000	-2.589389000
H	9.029211000	12.964655000	-3.048591000
H	10.957771000	11.381087000	-3.063435000
H	10.567953000	8.958294000	-2.610096000
H	8.273038000	8.132604000	-2.129726000
C	3.967600000	11.626839000	-2.655877000
C	3.250519000	12.382532000	-3.586796000
C	3.188624000	11.978935000	-4.922371000
C	3.853916000	10.820222000	-5.332388000
C	4.581823000	10.069606000	-4.410424000
H	3.996803000	11.942760000	-1.612257000
H	2.733933000	13.287146000	-3.262202000
H	2.618235000	12.566739000	-5.644236000
H	3.799857000	10.493524000	-6.371977000
H	5.089999000	9.160485000	-4.732242000
C	5.780571000	11.328014000	0.292827000
C	5.364286000	11.805556000	1.539398000
C	4.390428000	11.118655000	2.268198000
C	3.835666000	9.938058000	1.744476000
C	4.249134000	9.465248000	0.499778000
H	6.554961000	11.865391000	-0.255098000
H	5.812721000	12.713996000	1.944777000
H	4.072773000	11.485720000	3.246027000
H	3.086681000	9.385612000	2.313449000
H	3.833839000	8.541267000	0.093285000

7 [Rh(fctfa)(CO)₂] A ADF/PW91/TZP

Rh	5.506503000	7.179254000	-2.192387000
Fe	4.069142000	1.686465000	-1.512855000
O	7.828987000	7.052728000	-0.245611000
O	5.553170000	10.208234000	-2.021870000
O	5.505046000	5.109742000	-2.286995000
O	3.919768000	7.259570000	-3.522860000
C	2.585434000	2.706204000	-0.494196000
C	3.675952000	2.396187000	0.380885000
C	3.832246000	0.972133000	0.400668000
C	2.841389000	0.405116000	-0.466385000
C	2.071259000	1.479209000	-1.019811000
C	4.940870000	2.934063000	-2.894710000
C	4.219563000	1.860866000	-3.545535000
C	4.798003000	0.625589000	-3.123335000
C	5.854679000	0.914841000	-2.201130000
C	5.941457000	2.330518000	-2.048678000
C	6.945240000	7.112732000	-0.986805000
C	5.534857000	9.056317000	-2.087042000
C	4.703099000	4.377450000	-2.979562000
C	3.659932000	4.869906000	-3.811216000
C	3.368561000	6.205456000	-4.011288000
H	2.234041000	3.702681000	-0.746023000
H	4.284039000	3.115351000	0.919998000
H	4.582639000	0.420507000	0.958547000
H	2.710576000	-0.651420000	-0.679403000
H	1.253069000	1.380220000	-1.726285000
H	3.397234000	1.964546000	-4.245594000
H	4.474001000	-0.363364000	-3.432343000
H	6.468036000	0.181479000	-1.687533000
H	6.632067000	2.878345000	-1.417681000
H	3.055366000	4.144136000	-4.343546000
C	2.224199000	6.574262000	-4.973440000
F	1.550337000	5.486305000	-5.447448000
F	2.700011000	7.250792000	-6.051411000
F	1.313190000	7.373329000	-4.361352000

8 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl I ADF/PW91/TZP

C	4.432402000	2.917061000	-1.696409000
C	4.304029000	3.387458000	-3.010056000
C	3.625297000	2.602243000	-3.957698000
C	3.078849000	1.373145000	-3.591028000
C	3.205454000	0.910146000	-2.278824000
C	3.883227000	1.683482000	-1.335935000
P	4.985663000	5.036451000	-3.501607000
C	3.490072000	6.106279000	-3.575617000
C	2.274517000	5.692194000	-3.013704000
C	1.151015000	6.519624000	-3.078458000
C	1.230846000	7.765152000	-3.701123000
C	2.443548000	8.188090000	-4.252949000
C	3.570149000	7.370207000	-4.186529000
Rh	6.760380000	5.863196000	-2.165235000
I	7.537582000	7.391806000	-4.286816000
O	6.162215000	4.983750000	-0.273904000
C	6.804238000	5.133349000	0.829857000
C	7.982241000	5.902511000	1.023673000
C	8.632729000	6.668047000	0.069425000
O	8.387411000	6.843829000	-1.167798000
C	6.236134000	4.448766000	2.005278000
C	5.103584000	3.554782000	1.988847000
C	4.904485000	3.060147000	3.312883000
C	5.906193000	3.632220000	4.159887000
C	6.734951000	4.477672000	3.363879000
Fe	6.791398000	2.569807000	2.625740000
C	8.239549000	1.859240000	1.326672000
C	8.760341000	1.958727000	2.657286000
C	7.964996000	1.125373000	3.509323000
C	6.949040000	0.516196000	2.701829000
C	7.118557000	0.971354000	1.352570000
C	9.858932000	7.495370000	0.520337000
F	9.608252000	8.823743000	0.409434000
F	10.943275000	7.217096000	-0.245877000
F	10.218223000	7.264621000	1.818372000
C	5.584367000	7.489221000	-1.515619000
C	8.047499000	4.353133000	-2.533750000
C	5.404622000	4.730513000	-5.277271000
C	4.554070000	5.131406000	-6.318233000
C	4.890713000	4.860117000	-7.648630000
C	6.067702000	4.177013000	-7.954450000
C	6.903462000	3.750313000	-6.917717000
C	6.575414000	4.025496000	-5.592050000
H	9.607522000	2.567512000	2.965137000
H	8.611016000	2.391468000	0.454765000
H	6.501989000	0.699805000	0.500920000
H	6.176553000	-0.162279000	3.056802000
H	8.099593000	0.990965000	4.580594000
H	7.581727000	5.047456000	3.730009000
H	6.031856000	3.440165000	5.220930000
H	4.135160000	2.359747000	3.621990000
H	4.500616000	3.319843000	1.120460000
H	8.399881000	5.919385000	2.022844000
H	3.630786000	5.667637000	-6.099892000
H	4.225539000	5.194056000	-8.446486000
H	6.335557000	3.978046000	-8.993497000
H	7.826125000	3.213785000	-7.142258000
H	7.249955000	3.699565000	-4.803362000
H	2.196735000	4.718124000	-2.532998000
H	0.211395000	6.182697000	-2.641944000
H	0.352150000	8.407879000	-3.753788000
H	2.515746000	9.162743000	-4.734352000
H	4.516306000	7.708369000	-4.611810000
H	3.528707000	2.947592000	-4.986062000
H	2.558406000	0.773155000	-4.337082000
H	2.781645000	-0.053649000	-1.996929000
H	3.990644000	1.325621000	-0.311612000
H	4.969394000	3.517112000	-0.965537000
O	8.874234000	3.553268000	-2.577206000
H	4.720751000	7.066930000	-0.989250000
H	6.237134000	8.039281000	-0.830098000
H	5.271291000	8.133577000	-2.338596000

9 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl II ADF/PW91/TZP

C	6.802778000	4.533759000	-5.596782000
C	7.225904000	5.868178000	-5.561572000
C	7.829145000	6.424310000	-6.703069000
C	7.999138000	5.658668000	-7.854526000
C	7.575872000	4.327770000	-7.882300000
C	6.979256000	3.769114000	-6.752513000
P	6.963396000	6.953284000	-4.083961000
C	5.574248000	8.038677000	-4.613952000
C	4.703752000	7.619059000	-5.629538000
C	3.638525000	8.429461000	-6.025894000
C	3.427865000	9.664018000	-5.410603000
C	4.282592000	10.083369000	-4.388258000
C	5.345273000	9.275258000	-3.985373000
Rh	6.726480000	5.860168000	-2.008410000
I	4.336015000	4.797630000	-2.806236000
O	6.280090000	4.956919000	-0.106480000
C	6.958009000	5.120249000	0.962759000
C	8.164925000	5.873303000	1.077340000
C	8.764377000	6.604836000	0.070496000
O	8.439886000	6.798574000	-1.156630000
C	6.409615000	4.480433000	2.167367000
C	5.242058000	3.623520000	2.176670000
C	5.048479000	3.147662000	3.508691000
C	6.091912000	3.678359000	4.336245000
C	6.947739000	4.482836000	3.522569000
Fe	6.894743000	2.579365000	2.793651000
C	8.234140000	1.734446000	1.451566000
C	8.822232000	1.836990000	2.753729000
C	8.008681000	1.089389000	3.668876000
C	6.911967000	0.529852000	2.931651000
C	7.046321000	0.932407000	1.561915000
C	10.067738000	7.353946000	0.411408000
F	9.932705000	8.690256000	0.224922000
F	11.086155000	6.933019000	-0.391971000
F	10.486198000	7.170240000	1.695831000
C	5.637985000	7.510165000	-1.269607000
C	7.765653000	4.192097000	-2.471739000
C	8.453786000	8.037515000	-4.157163000
C	8.433810000	9.320302000	-4.727866000
C	9.609057000	10.071760000	-4.821305000
C	10.815698000	9.549977000	-4.350978000
C	10.843855000	8.266752000	-3.795350000
C	9.674616000	7.515172000	-3.698546000
H	9.723036000	2.391975000	3.006361000
H	8.594543000	2.215401000	0.544306000
H	6.364472000	0.690703000	0.750287000
H	6.108208000	-0.076733000	3.344124000
H	8.182784000	0.979154000	4.737141000
H	7.825155000	5.021937000	3.870867000
H	6.226331000	3.483281000	5.397847000
H	4.259408000	2.473791000	3.834997000
H	4.633684000	3.403010000	1.304431000
H	8.645589000	5.892549000	2.048513000
H	7.503449000	9.735020000	-5.114264000
H	9.574952000	11.066863000	-5.267652000
H	11.732033000	10.139332000	-4.416517000
H	11.781675000	7.851963000	-3.422706000
H	9.710655000	6.523572000	-3.254091000
H	4.855527000	6.656152000	-6.114023000
H	2.972917000	8.089117000	-6.818058000
H	2.597398000	10.296978000	-5.723468000
H	4.120481000	11.042357000	-3.897642000
H	5.999758000	9.612586000	-3.184793000
H	8.169657000	7.458371000	-6.693243000
H	8.468183000	6.105590000	-8.731158000
H	7.712863000	3.728929000	-8.783224000
H	6.641757000	2.733320000	-6.764547000
H	6.300827000	4.095971000	-4.734627000
O	8.341051000	3.200211000	-2.566627000
H	5.242056000	7.166922000	-0.308656000
H	6.355931000	8.326553000	-1.128647000
H	4.819007000	7.796496000	-1.931841000

10 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl III ADF/PW91/TZP

Rh	5.503681000	5.218327000	7.746911000
I	4.979841000	7.869955000	7.431739000
Fe	8.632128000	5.085324000	2.843835000
P	3.143274000	4.578291000	7.394907000
F	8.184172000	1.424299000	8.528754000
F	7.910852000	0.509864000	6.559788000
F	6.281014000	0.472817000	8.019643000
O	5.930469000	5.099586000	5.575423000
O	6.096203000	3.190558000	7.962769000
O	8.331404000	6.231135000	8.366934000
C	6.593386000	4.154297000	5.045958000
C	7.036878000	2.966423000	5.723346000
C	6.750100000	2.597976000	7.019770000
C	7.285630000	1.244959000	7.521001000
C	7.274360000	5.852790000	8.112099000
C	5.165489000	5.277608000	9.833580000
C	6.895361000	4.295149000	3.612688000
C	6.619223000	5.484625000	2.845571000
C	7.072559000	5.266397000	1.509866000
C	7.641869000	3.953136000	1.438116000
C	7.547852000	3.353764000	2.730887000
C	9.595363000	6.801091000	3.481613000
C	10.077996000	6.394463000	2.193355000
C	10.619811000	5.073020000	2.319553000
C	10.467157000	4.661408000	3.683953000
C	9.837412000	5.731576000	4.399018000
C	2.882783000	3.931459000	5.697896000
C	2.507247000	2.600647000	5.471783000
C	2.359854000	2.123246000	4.158230000
C	2.586495000	2.983156000	3.070521000
C	2.967675000	4.308497000	3.301176000
C	3.127955000	4.779134000	4.603497000
C	1.889300000	5.917127000	7.587892000
C	1.822496000	6.588606000	8.825735000
C	0.888207000	7.602092000	9.027287000
C	0.018426000	7.972431000	7.995095000
C	0.080743000	7.311043000	6.768432000
C	1.009978000	6.279406000	6.564286000
C	2.478014000	3.256451000	8.495734000
C	3.337820000	2.370955000	9.167855000
C	2.810139000	1.355322000	9.970865000
C	1.427938000	1.209323000	10.108771000
C	0.565609000	2.084555000	9.440346000
C	1.082694000	3.104345000	8.641564000
H	7.619838000	2.259967000	5.142723000
H	5.316830000	6.290289000	10.216855000
H	4.155238000	4.933045000	10.066313000
H	5.891497000	4.582859000	10.270317000
H	6.156988000	6.380730000	3.244531000
H	7.021927000	5.982111000	0.695085000
H	8.089719000	3.499053000	0.559746000
H	7.891127000	2.357578000	2.988907000
H	9.109008000	7.742665000	3.716121000
H	10.027819000	6.978896000	1.278741000
H	11.053693000	4.481819000	1.518471000
H	10.767269000	3.705511000	4.102052000
H	9.560563000	5.722496000	5.449418000
H	2.326849000	1.930428000	6.310637000
H	2.072012000	1.084576000	3.989735000
H	2.475231000	2.613290000	2.049772000
H	3.160391000	4.975560000	2.461242000
H	3.454624000	5.804318000	4.773662000
H	2.510521000	6.325510000	9.629190000
H	0.849747000	8.115853000	9.988811000
H	-0.702046000	8.778147000	8.147356000
H	-0.591618000	7.592396000	5.956836000
H	1.041166000	5.768223000	5.603284000
H	4.415375000	2.471509000	9.057780000
H	3.488441000	0.676732000	10.490990000
H	1.020977000	0.416712000	10.739485000
H	-0.514931000	1.977734000	9.544899000
H	0.404824000	3.789952000	8.131092000

11 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl IV ADF/PW91/TZP

Rh	5.557137000	5.441649000	7.516390000
I	5.178737000	6.017412000	10.153542000
Fe	8.658514000	4.941535000	2.758287000
P	3.191259000	4.759233000	7.215678000
F	8.214467000	1.505787000	8.526188000
F	7.822898000	0.510805000	6.616828000
F	6.259749000	0.597118000	8.147066000
O	5.957547000	5.133669000	5.460775000
O	6.131007000	3.322061000	7.931552000
O	8.389133000	6.502283000	7.992251000
C	6.608701000	4.127845000	4.992867000
C	7.024656000	2.973821000	5.707184000
C	6.746863000	2.663881000	7.034252000
C	7.264889000	1.309885000	7.572348000
C	7.332768000	6.075768000	7.822321000
C	5.071869000	7.430264000	7.001022000
C	6.908664000	4.211658000	3.553198000
C	6.653770000	5.368252000	2.728237000
C	7.109863000	5.082140000	1.406015000
C	7.660042000	3.758625000	1.399704000
C	7.549752000	3.221936000	2.718708000
C	9.659590000	6.668339000	3.298331000
C	10.157404000	6.161098000	2.052179000
C	10.655594000	4.836984000	2.281278000
C	10.460574000	4.525057000	3.667717000
C	9.848958000	5.659484000	4.294151000
C	2.955352000	3.956380000	5.578490000
C	2.598327000	2.603992000	5.479636000
C	2.479729000	1.993343000	4.218850000
C	2.716593000	2.738919000	3.050839000
C	3.082649000	4.084666000	3.152386000
C	3.216348000	4.685499000	4.404057000
C	1.951297000	6.126202000	7.268485000
C	1.754210000	6.774921000	8.503985000
C	0.861582000	7.842147000	8.603333000
C	0.158809000	8.279659000	7.475223000
C	0.346226000	7.631734000	6.252004000
C	1.233953000	6.557967000	6.147144000
C	2.502401000	3.551379000	8.418647000
C	3.339445000	2.794171000	9.256020000
C	2.783650000	1.858758000	10.134201000
C	1.400878000	1.668463000	10.182561000
C	0.562815000	2.415346000	9.347730000
C	1.107168000	3.353894000	8.470941000
H	7.578533000	2.230419000	5.144357000
H	5.229753000	7.473731000	5.917732000
H	4.032850000	7.635541000	7.265526000
H	5.721422000	8.144418000	7.515334000
H	6.199868000	6.290112000	3.075460000
H	7.072825000	5.758648000	0.558706000
H	8.106031000	3.257258000	0.547011000
H	7.878535000	2.235050000	3.024658000
H	9.200663000	7.640520000	3.454559000
H	10.145461000	6.682271000	1.099657000
H	11.087454000	4.179337000	1.533382000
H	10.720944000	3.591064000	4.157074000
H	9.551500000	5.729783000	5.335011000
H	2.413569000	2.019202000	6.377738000
H	2.208245000	0.938994000	4.153481000
H	2.628217000	2.265769000	2.072517000
H	3.287404000	4.663591000	2.253137000
H	3.541340000	5.721629000	4.467878000
H	2.310754000	6.448636000	9.384072000
H	0.718868000	8.334171000	9.565637000
H	-0.533593000	9.118766000	7.550630000
H	-0.204322000	7.959987000	5.369411000
H	1.353586000	6.057194000	5.189175000
H	4.417378000	2.934232000	9.221743000
H	3.440871000	1.282945000	10.786931000
H	0.972824000	0.940886000	10.875548000
H	-0.517923000	2.272493000	9.382260000
H	0.449160000	3.939722000	7.827417000

12 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl V ADF/PW91/TZP

C	5.415291000	2.167325000	-1.845421000
C	4.611441000	2.801559000	-2.802012000
C	3.769019000	2.031437000	-3.619788000
C	3.739310000	0.643316000	-3.488593000
C	4.558310000	0.011797000	-2.550435000
C	5.389724000	0.776220000	-1.731305000
P	4.626279000	4.634481000	-3.026884000
C	3.064944000	5.175569000	-2.211425000
C	2.428417000	4.353368000	-1.271348000
C	1.287760000	4.801587000	-0.601312000
C	0.770035000	6.069810000	-0.864775000
C	1.398431000	6.894873000	-1.801129000
C	2.541245000	6.454678000	-2.466038000
Rh	6.457117000	5.808762000	-2.123946000
C	5.418001000	7.264489000	-1.484872000
O	6.246617000	4.722978000	-0.185819000
C	6.946910000	4.998904000	0.845688000
C	8.078953000	5.869275000	0.882780000
C	8.576856000	6.646280000	-0.149509000
O	8.177361000	6.826893000	-1.353750000
C	6.499897000	4.389666000	2.112395000
C	5.318242000	3.573181000	2.243353000
C	5.185775000	3.197108000	3.614243000
C	6.285421000	3.758712000	4.341057000
C	7.103608000	4.484357000	3.422642000
Fe	6.972787000	2.523680000	2.845583000
C	8.158240000	1.533798000	1.469661000
C	8.887189000	1.766165000	2.681105000
C	8.174166000	1.128904000	3.754765000
C	7.010992000	0.501140000	3.201106000
C	7.001218000	0.754480000	1.790869000
C	9.849306000	7.479723000	0.129557000
F	9.681306000	8.772514000	-0.247680000
F	10.907531000	6.988769000	-0.567648000
F	10.212212000	7.496486000	1.445001000
I	8.244897000	3.961171000	-3.112528000
C	6.749111000	6.998288000	-3.853040000
C	4.300015000	4.829839000	-4.827716000
C	3.004867000	5.076906000	-5.334077000
C	2.791190000	5.155012000	-6.712129000
C	3.855952000	4.983172000	-7.600228000
C	5.136873000	4.721023000	-7.105906000
C	5.360735000	4.643073000	-5.727597000
H	9.804252000	2.339487000	2.773011000
H	8.420490000	1.915702000	0.486146000
H	6.229406000	0.434228000	1.098793000
H	6.259213000	-0.051940000	3.756376000
H	8.459643000	1.133429000	4.803768000
H	8.013441000	5.016549000	3.677601000
H	6.478144000	3.634890000	5.402102000
H	4.401298000	2.573006000	4.030820000
H	4.652966000	3.313375000	1.427259000
H	8.593374000	5.957253000	1.833171000
H	2.163195000	5.201603000	-4.652603000
H	1.785269000	5.348368000	-7.088677000
H	3.687339000	5.049363000	-8.676801000
H	5.970932000	4.576949000	-7.794084000
H	6.361172000	4.423307000	-5.350433000
H	2.822957000	3.359552000	-1.064096000
H	0.805005000	4.153160000	0.128974000
H	-0.119556000	6.417982000	-0.339565000
H	1.002218000	7.887541000	-2.010053000
H	3.025099000	7.111484000	-3.188820000
H	3.145931000	2.511021000	-4.373157000
H	3.088408000	0.055908000	-4.135354000
H	4.555903000	-1.074861000	-2.466311000
H	6.048847000	0.286222000	-1.016655000
H	6.065858000	2.757425000	-1.205336000
H	7.391104000	7.812093000	-3.501276000
H	7.272080000	6.393673000	-4.594579000
H	5.808959000	7.381432000	-4.259911000
O	4.908665000	8.231271000	-1.118400000

13 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl VI ADF/PW91/TZP

C	6.155298000	4.222019000	-5.795795000
C	6.618726000	5.543806000	-5.835768000
C	7.163304000	6.044142000	-7.029307000
C	7.240617000	5.233172000	-8.161181000
C	6.776693000	3.917374000	-8.115500000
C	6.233392000	3.416129000	-6.932103000
P	6.461490000	6.676808000	-4.385585000
C	4.910202000	7.601520000	-4.768142000
C	3.933771000	7.039732000	-5.603881000
C	2.721420000	7.699209000	-5.815792000
C	2.473900000	8.928389000	-5.205081000
C	3.445746000	9.499392000	-4.378241000
C	4.652884000	8.839195000	-4.155295000
Rh	6.392441000	5.812053000	-2.188700000
C	5.230692000	7.172784000	-1.557428000
O	6.171590000	4.939537000	-0.226193000
C	6.928421000	5.155041000	0.790075000
C	8.097340000	5.963596000	0.812381000
C	8.593731000	6.728804000	-0.235276000
O	8.166299000	6.913038000	-1.421134000
C	6.483516000	4.519972000	2.044795000
C	5.319656000	3.666460000	2.169705000
C	5.195416000	3.270139000	3.536558000
C	6.283601000	3.844810000	4.272209000
C	7.091011000	4.597507000	3.362969000
Fe	6.991234000	2.647631000	2.758855000
C	8.261684000	1.744414000	1.385006000
C	8.909489000	1.883301000	2.654497000
C	8.132966000	1.177162000	3.633056000
C	6.996793000	0.605578000	2.968498000
C	7.070353000	0.961152000	1.581212000
C	9.877620000	7.551048000	0.019839000
F	9.619642000	8.882251000	-0.066822000
F	10.821874000	7.262418000	-0.912016000
F	10.459538000	7.345058000	1.234264000
I	8.115517000	3.753169000	-2.783149000
C	4.685421000	4.654135000	-2.664913000
C	7.812645000	7.892126000	-4.644985000
C	7.614471000	9.080421000	-5.369545000
C	8.681950000	9.951881000	-5.595048000
C	9.952527000	9.645023000	-5.100986000
C	10.153851000	8.457717000	-4.390853000
C	9.093742000	7.580789000	-4.162810000
H	9.825851000	2.437464000	2.845465000
H	8.575464000	2.196874000	0.445202000
H	6.350638000	0.698926000	0.808810000
H	6.209133000	0.020589000	3.437970000
H	8.357337000	1.099612000	4.694683000
H	7.988580000	5.149915000	3.629221000
H	6.477931000	3.712504000	5.334044000
H	4.422796000	2.621816000	3.943441000
H	4.664725000	3.394798000	1.347834000
H	8.644980000	6.006876000	1.747433000
H	6.628795000	9.325939000	-5.764868000
H	8.515724000	10.871965000	-6.157538000
H	10.784896000	10.331647000	-5.267976000
H	11.142459000	8.213795000	-3.999723000
H	9.258841000	6.662494000	-3.602504000
H	4.121061000	6.085932000	-6.095495000
H	1.971111000	7.246652000	-6.463607000
H	1.526856000	9.441506000	-5.370806000
H	3.261710000	10.460279000	-3.899111000
H	5.399081000	9.295228000	-3.505290000
H	7.539667000	7.064514000	-7.076415000
H	7.674676000	5.632419000	-9.077425000
H	6.849243000	3.281461000	-8.997681000
H	5.882783000	2.386305000	-6.883347000
H	5.754743000	3.812807000	-4.873431000
H	4.049375000	5.115234000	-3.425490000
H	5.034312000	3.667221000	-2.975394000
H	4.149500000	4.573080000	-1.714301000
O	4.545251000	7.945083000	-1.045222000

14 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl VII ADF/PW91/TZP

Rh	5.521733000	5.252993000	7.681802000
I	4.986302000	7.871089000	7.172712000
Fe	8.674868000	5.012008000	2.893325000
P	3.049421000	4.565335000	7.359982000
F	8.341613000	1.558584000	8.633241000
F	8.031213000	0.541679000	6.720384000
F	6.443728000	0.548002000	8.226819000
O	5.937069000	5.043427000	5.627806000
O	6.200103000	3.262774000	8.021502000
O	5.174474000	5.838854000	10.618061000
C	6.628555000	4.102880000	5.104123000
C	7.097688000	2.939936000	5.789541000
C	6.845923000	2.626179000	7.108118000
C	7.419490000	1.310640000	7.663353000
C	5.277251000	5.615266000	9.489355000
C	7.553295000	5.847185000	7.898122000
C	6.926920000	4.246243000	3.674015000
C	6.660779000	5.430548000	2.895332000
C	7.110192000	5.193905000	1.561876000
C	7.668446000	3.875638000	1.502443000
C	7.574048000	3.291168000	2.801268000
C	9.687220000	6.754825000	3.371168000
C	10.187905000	6.196789000	2.149604000
C	10.675588000	4.878940000	2.431765000
C	10.472840000	4.621491000	3.826463000
C	9.866622000	5.784359000	4.404588000
C	2.696475000	4.102484000	5.619946000
C	2.240254000	2.826699000	5.262711000
C	2.049046000	2.500130000	3.918548000
C	2.307604000	3.442640000	2.922938000
C	2.768310000	4.715096000	3.273725000
C	2.973502000	5.043270000	4.612345000
C	1.803600000	5.868510000	7.758164000
C	1.803659000	6.397944000	9.058866000
C	0.887594000	7.382592000	9.422367000
C	-0.036440000	7.859672000	8.488383000
C	-0.044000000	7.336708000	7.195543000
C	0.868418000	6.343242000	6.830713000
C	2.432582000	3.154461000	8.378001000
C	3.341953000	2.298284000	9.015197000
C	2.879508000	1.254262000	9.820774000
C	1.510098000	1.058212000	9.998071000
C	0.598197000	1.906809000	9.363106000
C	1.054185000	2.950222000	8.559839000
H	7.685829000	2.229986000	5.219524000
H	7.863383000	6.135467000	6.891221000
H	7.661206000	6.690439000	8.583141000
H	8.087100000	4.963158000	8.263089000
H	6.204532000	6.334865000	3.283629000
H	7.066217000	5.901653000	0.739982000
H	8.111631000	3.409472000	0.628193000
H	7.908416000	2.294470000	3.067779000
H	9.230319000	7.732433000	3.487347000
H	10.183563000	6.679795000	1.176997000
H	11.107144000	4.190199000	1.711498000
H	10.727854000	3.707776000	4.354385000
H	9.566037000	5.897779000	5.441449000
H	2.036100000	2.085357000	6.034516000
H	1.698637000	1.503308000	3.652957000
H	2.159585000	3.185042000	1.874396000
H	2.981733000	5.451884000	2.500008000
H	3.356970000	6.028314000	4.880130000
H	2.519584000	6.039654000	9.798170000
H	0.902768000	7.785562000	10.434137000
H	-0.745242000	8.638645000	8.768529000
H	-0.762172000	7.701222000	6.461674000
H	0.848961000	5.941225000	5.819370000
H	4.411902000	2.447607000	8.885584000
H	3.597091000	0.599900000	10.315535000
H	1.150857000	0.250466000	10.635623000
H	-0.473112000	1.762469000	9.502648000
H	0.338428000	3.618676000	8.082656000

15 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl VIII ADF/PW91/TZP

Rh	5.561492000	5.423699000	7.576042000
I	5.260391000	5.780401000	10.262340000
Fe	8.691523000	4.936910000	2.712959000
P	3.124141000	4.653391000	7.231005000
F	8.310149000	1.660281000	8.527237000
F	7.904756000	0.627880000	6.639151000
F	6.360670000	0.722057000	8.189073000
O	6.004507000	5.222237000	5.511566000
O	6.199563000	3.438890000	7.928737000
O	4.951453000	8.357343000	7.260933000
C	6.642877000	4.230292000	5.006218000
C	7.067070000	3.061963000	5.700429000
C	6.815203000	2.767171000	7.027375000
C	7.350436000	1.434737000	7.589515000
C	5.148377000	7.228839000	7.397812000
C	7.590453000	6.013815000	7.824850000
C	6.919207000	4.330926000	3.566234000
C	6.720131000	5.514742000	2.767149000
C	7.104814000	5.215240000	1.425793000
C	7.553406000	3.855491000	1.380949000
C	7.455660000	3.308430000	2.695996000
C	9.852007000	6.594078000	3.150481000
C	10.267468000	5.997702000	1.914874000
C	10.658709000	4.646104000	2.185496000
C	10.482227000	4.406406000	3.587038000
C	9.987673000	5.612723000	4.181169000
C	2.851138000	3.905899000	5.572601000
C	2.418690000	2.580374000	5.422156000
C	2.292442000	2.019524000	4.149809000
C	2.591143000	2.773618000	3.014671000
C	3.026634000	4.094177000	3.155479000
C	3.166915000	4.654069000	4.424303000
C	1.907960000	6.041007000	7.323443000
C	1.839137000	6.762300000	8.528646000
C	0.979967000	7.852736000	8.648543000
C	0.183942000	8.244960000	7.569023000
C	0.241872000	7.528526000	6.373519000
C	1.094697000	6.428467000	6.250299000
C	2.435883000	3.415043000	8.404605000
C	3.303782000	2.587832000	9.131309000
C	2.786507000	1.625559000	10.000649000
C	1.406683000	1.486286000	10.154584000
C	0.538242000	2.312939000	9.436139000
C	1.048637000	3.275107000	8.565845000
H	7.620686000	2.324578000	5.130768000
H	7.954979000	6.292950000	6.830804000
H	7.690366000	6.838104000	8.533719000
H	8.086148000	5.117830000	8.209204000
H	6.348158000	6.461910000	3.141824000
H	7.087813000	5.906614000	0.588957000
H	7.927166000	3.335139000	0.504657000
H	7.713485000	2.293065000	2.976553000
H	9.480390000	7.606089000	3.277409000
H	10.269240000	6.479134000	0.941258000
H	11.009817000	3.924623000	1.453537000
H	10.680709000	3.475144000	4.108298000
H	9.729795000	5.747969000	5.227555000
H	2.181741000	1.983206000	6.301573000
H	1.960070000	0.986346000	4.050219000
H	2.494215000	2.332317000	2.022663000
H	3.273080000	4.686038000	2.274500000
H	3.534348000	5.674222000	4.523289000
H	2.467293000	6.473937000	9.373015000
H	0.939964000	8.401912000	9.588659000
H	-0.478448000	9.105845000	7.660174000
H	-0.379155000	7.823246000	5.527933000
H	1.122694000	5.874146000	5.313726000
H	4.380728000	2.701314000	9.025817000
H	3.468960000	0.992021000	10.566241000
H	1.005810000	0.739567000	10.840250000
H	-0.539979000	2.212859000	9.557187000
H	0.368305000	3.923461000	8.014336000

16 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl IX ADF/PW91/TZP

C	4.628340000	2.793035000	-1.793521000
C	4.343111000	3.348388000	-3.046511000
C	3.529840000	2.645474000	-3.950791000
C	2.996434000	1.408008000	-3.594059000
C	3.266679000	0.863684000	-2.335508000
C	4.081620000	1.557491000	-1.439813000
P	4.984128000	5.007425000	-3.522861000
C	3.483830000	6.075516000	-3.509161000
C	2.310980000	5.680627000	-2.851941000
C	1.191792000	6.516980000	-2.845088000
C	1.232941000	7.753277000	-3.489682000
C	2.403349000	8.159197000	-4.137467000
C	3.523071000	7.330934000	-4.141932000
Rh	6.773193000	5.920326000	-2.228693000
I	8.483218000	3.632532000	-2.542182000
O	6.108639000	5.117365000	-0.376963000
C	6.746930000	5.222481000	0.737267000
C	7.927980000	5.983501000	0.954683000
C	8.613551000	6.723429000	0.009797000
O	8.401144000	6.884491000	-1.239869000
C	6.176770000	4.501228000	1.885116000
C	5.084819000	3.558153000	1.824821000
C	4.884471000	3.021472000	3.132129000
C	5.844507000	3.613636000	4.012816000
C	6.651879000	4.513300000	3.254104000
Fe	6.803975000	2.632690000	2.472931000
C	8.363971000	2.030113000	1.236199000
C	8.792831000	2.078502000	2.600073000
C	7.968183000	1.182816000	3.356839000
C	7.025490000	0.584279000	2.456782000
C	7.271758000	1.111510000	1.146465000
C	9.831990000	7.546584000	0.479862000
F	9.555230000	8.880554000	0.421064000
F	10.913932000	7.323882000	-0.300849000
F	10.199236000	7.276009000	1.766616000
C	5.648829000	7.636905000	-1.675671000
C	7.399169000	6.763913000	-3.770622000
C	5.350631000	4.828006000	-5.326927000
C	4.407395000	5.180337000	-6.306562000
C	4.692599000	4.989826000	-7.659568000
C	5.913746000	4.439353000	-8.050894000
C	6.846760000	4.070629000	-7.080441000
C	6.570833000	4.260746000	-5.727165000
H	9.595607000	2.694677000	2.993561000
H	8.760406000	2.615970000	0.409698000
H	6.730667000	0.867533000	0.237532000
H	6.256864000	-0.133925000	2.726556000
H	8.037528000	0.997324000	4.424478000
H	7.465326000	5.110102000	3.651714000
H	5.958937000	3.398923000	5.071464000
H	4.143424000	2.278813000	3.408464000
H	4.508924000	3.319416000	0.939334000
H	8.331948000	5.989276000	1.960001000
H	3.448400000	5.607895000	-6.020764000
H	3.954768000	5.277199000	-8.407574000
H	6.136935000	4.298654000	-9.108252000
H	7.801033000	3.633339000	-7.372219000
H	7.308384000	3.961704000	-4.978992000
H	2.263371000	4.712609000	-2.355594000
H	0.283693000	6.193411000	-2.337785000
H	0.356927000	8.401533000	-3.487662000
H	2.444879000	9.124493000	-4.640081000
H	4.426842000	7.655414000	-4.657182000
H	3.320892000	3.057191000	-4.937095000
H	2.375027000	0.865127000	-4.305378000
H	2.850594000	-0.105585000	-2.060597000
H	4.304011000	1.134011000	-0.460532000
H	5.280036000	3.326791000	-1.107248000
O	7.831349000	7.364547000	-4.654411000
H	4.747589000	7.260657000	-1.183227000
H	6.304263000	8.162183000	-0.975299000
H	5.392342000	8.278284000	-2.521663000

17 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl X ADF/PW91/TZP

C	5.794840000	2.208663000	-2.003695000
C	4.797230000	2.887941000	-2.794320000
C	3.946117000	1.873903000	-3.380171000
C	4.440963000	0.597329000	-2.973992000
C	5.575730000	0.804121000	-2.124303000
Fe	3.912654000	1.737363000	-1.342330000
C	2.443404000	0.695689000	-0.351227000
C	1.965007000	1.999427000	-0.709009000
C	2.813074000	2.969471000	-0.084646000
C	3.818648000	2.269884000	0.653213000
C	3.591387000	0.863716000	0.491338000
C	4.685928000	4.347353000	-2.907061000
C	3.601359000	4.906887000	-3.641799000
C	3.426173000	6.243489000	-3.936631000
C	2.215140000	6.629551000	-4.809660000
F	1.421067000	7.533506000	-4.175806000
O	5.628125000	5.011902000	-2.351039000
Rh	5.791476000	7.141559000	-2.345126000
C	7.341955000	6.915061000	-1.338425000
O	8.314376000	6.678493000	-0.761348000
O	4.120123000	7.278745000	-3.624125000
P	6.127114000	9.490738000	-2.329480000
F	1.421253000	5.568736000	-5.137115000
F	2.618523000	7.195624000	-5.978611000
H	1.114955000	2.213980000	-1.349229000
H	2.744598000	4.050360000	-0.186376000
H	4.623063000	2.729686000	1.218739000
H	4.191024000	0.065404000	0.918833000
H	2.020851000	-0.251644000	-0.672731000
H	3.095366000	2.040896000	-4.032168000
H	4.014708000	-0.363088000	-3.246065000
H	6.154930000	0.026363000	-1.636529000
H	6.566162000	2.702035000	-1.423795000
H	2.863016000	4.216727000	-4.035397000
C	4.785364000	10.476845000	-3.100794000
C	6.409269000	10.292551000	-0.688686000
C	7.646424000	9.961007000	-3.259497000
C	5.073442000	11.633660000	-3.844872000
C	4.038844000	12.404329000	-4.373281000
C	2.710433000	12.027060000	-4.169329000
C	2.419678000	10.885772000	-3.419260000
H	6.105359000	11.937084000	-4.013228000
H	4.276100000	13.300221000	-4.945946000
H	1.902994000	12.623235000	-4.594919000
H	1.385235000	10.586446000	-3.256034000
H	3.212987000	9.227267000	-2.291574000
C	8.844214000	10.213630000	-2.573909000
C	10.019252000	10.478761000	-3.279912000
C	3.447906000	10.112579000	-2.880171000
C	10.011344000	10.498370000	-4.675163000
C	8.822956000	10.244371000	-5.365294000
C	7.649431000	9.968321000	-4.665135000
H	8.860354000	10.212336000	-1.484509000
H	10.940430000	10.675629000	-2.732862000
H	10.928417000	10.709950000	-5.224715000
H	8.809250000	10.254786000	-6.454662000
H	6.731765000	9.762312000	-5.213985000
C	6.398810000	11.696771000	-0.628137000
C	6.670770000	12.352267000	0.570913000
C	6.958349000	11.616344000	1.723375000
C	6.961554000	10.223376000	1.672021000
C	6.681988000	9.561621000	0.473831000
H	6.168650000	12.282891000	-1.516250000
H	6.650843000	13.440916000	0.604451000
H	7.165952000	12.129707000	2.662305000
H	7.163334000	9.639879000	2.569190000
H	6.634413000	8.475816000	0.468127000
C	6.936894000	6.866506000	-4.117014000
I	3.981138000	7.149841000	-0.116757000
H	7.917613000	7.344555000	-4.074873000
H	7.026737000	5.780854000	-4.216702000
H	6.319605000	7.289813000	-4.914734000

18 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl XI ADF/PW91/TZP

Rh	5.595391000	5.266584000	7.585484000
I	8.196643000	6.194026000	7.950230000
Fe	8.805311000	4.837542000	2.711341000
P	3.297629000	4.658128000	7.314041000
F	8.264119000	1.487157000	8.568535000
F	8.051565000	0.504629000	6.624710000
F	6.372653000	0.525553000	8.031832000
O	6.069892000	5.041455000	5.433257000
O	6.241708000	3.270982000	7.873039000
O	4.997055000	8.216769000	7.395830000
C	6.722484000	4.068139000	4.935025000
C	7.148894000	2.900798000	5.649800000
C	6.882429000	2.610851000	6.969160000
C	7.403232000	1.279118000	7.539584000
C	5.218980000	7.086756000	7.473896000
C	5.360350000	5.333873000	9.692317000
C	7.030631000	4.152804000	3.498119000
C	6.810610000	5.324664000	2.688286000
C	7.257588000	5.041819000	1.362227000
C	7.767127000	3.703644000	1.337488000
C	7.644738000	3.154204000	2.650210000
C	9.995234000	6.529007000	2.701220000
C	10.590474000	5.498812000	1.903939000
C	10.819544000	4.364657000	2.747544000
C	10.362248000	4.693251000	4.061999000
C	9.850683000	6.033073000	4.034190000
C	2.914834000	4.099293000	5.612555000
C	2.363999000	2.833191000	5.363659000
C	2.106280000	2.427805000	4.052294000
C	2.393792000	3.278703000	2.984467000
C	2.950351000	4.537529000	3.227088000
C	3.220811000	4.943950000	4.531615000
C	2.147021000	6.067851000	7.621633000
C	2.160836000	6.671767000	8.891121000
C	1.320102000	7.746770000	9.169357000
C	0.460645000	8.240658000	8.184400000
C	0.439083000	7.644164000	6.924353000
C	1.273161000	6.558906000	6.642826000
C	2.634102000	3.346117000	8.420482000
C	3.489184000	2.393457000	8.993065000
C	2.966110000	1.390928000	9.812219000
C	1.594636000	1.330140000	10.063015000
C	0.739973000	2.276822000	9.491970000
C	1.254813000	3.283780000	8.676956000
H	7.720678000	2.164245000	5.096569000
H	5.396984000	6.355263000	10.078229000
H	4.436221000	4.833446000	9.994411000
H	6.228861000	4.769367000	10.040023000
H	6.395260000	6.257398000	3.052418000
H	7.245983000	5.731460000	0.523836000
H	8.199213000	3.200644000	0.477887000
H	7.946571000	2.154713000	2.944536000
H	9.681012000	7.505658000	2.346530000
H	10.811570000	5.560326000	0.842084000
H	11.242989000	3.414589000	2.435260000
H	10.369990000	4.039560000	4.928886000
H	9.402614000	6.552325000	4.877596000
H	2.136749000	2.164203000	6.192164000
H	1.682917000	1.440762000	3.869635000
H	2.196141000	2.957806000	1.961750000
H	3.193050000	5.198454000	2.395880000
H	3.683675000	5.913049000	4.708558000
H	2.831292000	6.302467000	9.665788000
H	1.340626000	8.203365000	10.158143000
H	-0.189075000	9.088470000	8.400362000
H	-0.229778000	8.020042000	6.151089000
H	1.238758000	6.096600000	5.657998000
H	4.559630000	2.440704000	8.804164000
H	3.639873000	0.659484000	10.257224000
H	1.190289000	0.549253000	10.707181000
H	-0.331253000	2.236394000	9.685338000
H	0.583559000	4.024160000	8.243209000

19 [Rh(fctfa)(CH₃)(CO)(PPh₃)(I)]-alkyl XII ADF/PW91/TZP

Rh	5.612315000	5.293868000	7.509080000
I	8.251926000	6.031969000	7.980419000
Fe	8.744790000	4.921150000	2.733241000
P	3.303538000	4.699546000	7.247063000
F	8.276227000	1.378473000	8.533937000
F	8.047818000	0.428835000	6.574825000
F	6.377457000	0.433213000	7.993407000
O	6.047315000	4.991549000	5.461882000
O	6.256736000	3.192648000	7.864401000
O	5.241257000	6.073202000	10.399068000
C	6.716258000	4.017106000	4.955586000
C	7.150070000	2.851576000	5.643909000
C	6.885059000	2.538197000	6.967589000
C	7.406484000	1.189758000	7.508803000
C	5.382739000	5.768640000	9.293102000
C	5.190512000	7.288169000	6.949583000
C	7.012821000	4.136211000	3.519773000
C	6.729564000	5.297843000	2.710717000
C	7.189522000	5.040588000	1.383876000
C	7.772320000	3.733051000	1.357331000
C	7.679149000	3.175582000	2.668134000
C	9.830129000	6.682884000	2.763738000
C	10.477536000	5.717421000	1.927641000
C	10.784686000	4.572892000	2.730796000
C	10.324802000	4.830799000	4.060590000
C	9.734023000	6.136948000	4.081381000
C	2.927151000	4.050171000	5.577988000
C	2.434473000	2.750925000	5.394361000
C	2.184231000	2.273077000	4.106868000
C	2.422824000	3.084676000	2.997295000
C	2.925729000	4.376600000	3.174453000
C	3.189086000	4.855406000	4.455982000
C	2.118101000	6.090651000	7.505473000
C	2.055516000	6.670290000	8.784675000
C	1.194476000	7.735682000	9.036120000
C	0.384924000	8.241077000	8.014590000
C	0.435821000	7.665927000	6.745612000
C	1.296006000	6.594606000	6.489857000
C	2.666005000	3.444191000	8.431764000
C	3.538707000	2.609988000	9.144757000
C	3.025709000	1.665209000	10.037133000
C	1.649101000	1.545933000	10.223832000
C	0.775819000	2.373207000	9.511666000
C	1.278596000	3.319804000	8.621263000
H	7.716642000	2.124667000	5.073244000
H	5.252958000	7.242039000	5.857174000
H	4.203906000	7.616505000	7.284530000
H	5.974360000	7.936816000	7.346958000
H	6.262010000	6.206805000	3.072310000
H	7.138412000	5.729550000	0.546447000
H	8.232778000	3.256631000	0.497191000
H	8.039483000	2.195097000	2.960411000
H	9.453146000	7.649613000	2.443954000
H	10.679190000	5.824231000	0.865554000
H	11.259972000	3.659948000	2.384120000
H	10.381681000	4.152249000	4.906767000
H	9.267039000	6.601700000	4.945488000
H	2.247019000	2.111491000	6.255679000
H	1.804934000	1.260449000	3.975235000
H	2.229580000	2.707747000	1.993380000
H	3.131450000	5.007442000	2.310282000
H	3.610134000	5.850517000	4.584684000
H	2.674738000	6.285001000	9.593765000
H	1.157259000	8.173231000	10.032885000
H	-0.284455000	9.078067000	8.210656000
H	-0.197692000	8.046870000	5.945202000
H	1.315013000	6.148499000	5.497360000
H	4.613839000	2.685795000	8.993298000
H	3.712824000	1.023773000	10.587769000
H	1.253671000	0.811933000	10.926043000
H	-0.300691000	2.286839000	9.653778000
H	0.592208000	3.967807000	8.078018000

20 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl I ADF/PW91/TZP

C	-0.606864000	1.836523000	2.825126000
C	-1.735734000	2.053753000	2.021270000
C	-2.893143000	2.605966000	2.593158000
C	-2.920203000	2.927702000	3.949000000
C	-1.798174000	2.693127000	4.748635000
C	-0.643307000	2.150541000	4.184805000
P	-1.672654000	1.622498000	0.231433000
C	-1.388159000	3.233318000	-0.611643000
C	-1.146112000	4.392168000	0.140969000
C	-0.944955000	5.617032000	-0.496764000
C	-0.984758000	5.700847000	-1.888459000
C	-1.210914000	4.548213000	-2.644528000
C	-1.401483000	3.319331000	-2.014761000
Rh	-0.057228000	-0.024764000	0.007385000
I	-0.123771000	-0.096596000	-2.670984000
O	1.572456000	1.473775000	0.307999000
C	2.805914000	1.209927000	0.138121000
C	3.362629000	-0.074707000	-0.086665000
C	2.676096000	-1.280075000	-0.060976000
O	1.426649000	-1.530297000	0.002387000
C	3.560860000	-2.552298000	-0.036953000
F	2.830890000	-3.676996000	0.071319000
F	4.421728000	-2.516801000	1.024205000
F	4.335108000	-2.674688000	-1.152387000
C	-1.305064000	-1.506535000	0.347556000
O	-1.338747000	-1.607659000	1.562741000
C	-3.423098000	1.167142000	-0.135704000
C	-4.158215000	1.743060000	-1.179965000
C	-5.468050000	1.328402000	-1.433319000
C	-6.059245000	0.339888000	-0.647073000
C	-5.337798000	-0.229329000	0.405177000
C	-4.030188000	0.178508000	0.661255000
H	4.442755000	-0.118288000	-0.181853000
H	-3.718790000	2.526931000	-1.793005000
H	-6.026322000	1.786908000	-2.248692000
H	-7.080473000	0.016408000	-0.848614000
H	-5.793532000	-0.994568000	1.032571000
H	-3.483784000	-0.267616000	1.490882000
H	-1.111696000	4.343038000	1.227550000
H	-0.753039000	6.506364000	0.102365000
H	-0.829141000	6.659408000	-2.384156000
H	-1.227982000	4.600239000	-3.732937000
H	-1.534136000	2.421153000	-2.615684000
H	-3.773371000	2.783743000	1.976749000
H	-3.822325000	3.358581000	4.382136000
H	-1.826559000	2.933636000	5.811584000
H	0.233916000	1.966266000	4.803242000
H	0.307124000	1.438909000	2.385110000
C	-1.940490000	-2.447227000	-0.624688000
H	-2.548071000	-1.879810000	-1.339473000
H	-1.134773000	-2.917097000	-1.204555000
H	-2.535563000	-3.204334000	-0.100701000
C	4.174836000	3.151775000	-0.921336000
C	3.724250000	2.392468000	0.210222000
C	4.128629000	3.107744000	1.400712000
C	4.798387000	4.303666000	0.990459000
C	4.825266000	4.331109000	-0.440243000
Fe	5.784894000	2.661065000	0.258856000
C	7.027759000	1.400779000	-0.802285000
C	7.631831000	2.691711000	-0.640803000
C	7.757137000	2.950095000	0.764506000
C	7.231630000	1.819057000	1.471847000
C	6.785328000	0.862313000	0.504801000
H	6.787740000	0.919945000	-1.748148000
H	6.350379000	-0.108323000	0.732148000
H	7.173065000	1.709689000	2.552502000
H	8.162226000	3.854372000	1.214335000
H	5.282686000	5.101544000	-1.056281000
H	5.237362000	5.047023000	1.652173000
H	3.943258000	2.788893000	2.424211000
H	7.924483000	3.365890000	-1.443010000
H	4.020007000	2.878209000	-1.962855000

21 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl II ADF/PW91/TZP

C	-1.919737000	-1.208800000	2.947184000
C	-2.158463000	-2.101817000	1.890897000
C	-2.743228000	-3.349572000	2.165648000
C	-3.089952000	-3.690263000	3.472070000
C	-2.848999000	-2.797524000	4.519936000
C	-2.263623000	-1.559013000	4.254499000
P	-1.731453000	-1.639428000	0.155428000
C	-3.346668000	-1.131027000	-0.576189000
C	-4.495351000	-1.004468000	0.219362000
C	-5.709056000	-0.612331000	-0.350460000
C	-5.792150000	-0.344581000	-1.716555000
C	-4.651359000	-0.463928000	-2.514747000
C	-3.435429000	-0.849024000	-1.951627000
Rh	0.003022000	-0.085317000	0.158567000
I	0.206296000	-0.105357000	-2.516750000
O	1.553260000	1.357796000	0.273989000
C	2.781027000	1.185223000	-0.050747000
C	3.412400000	-0.055152000	-0.297527000
C	2.839185000	-1.294784000	-0.019464000
O	1.670679000	-1.578926000	0.388918000
C	3.717133000	-2.557169000	-0.191744000
F	3.060866000	-3.480880000	-0.920766000
F	3.996362000	-3.140880000	1.010654000
F	4.906142000	-2.345581000	-0.823659000
C	-1.218473000	1.434812000	0.398057000
O	-1.272210000	1.619375000	1.604568000
C	-1.361212000	-3.271034000	-0.604202000
C	-2.182908000	-3.868934000	-1.569777000
C	-1.861680000	-5.128247000	-2.080026000
C	-0.725263000	-5.801456000	-1.629341000
C	0.092971000	-5.210895000	-0.663468000
C	-0.217162000	-3.952397000	-0.153139000
H	4.450011000	-0.026393000	-0.616170000
H	-3.076996000	-3.360157000	-1.924111000
H	-2.504879000	-5.581239000	-2.833775000
H	-0.474395000	-6.782300000	-2.032640000
H	0.986466000	-5.725006000	-0.311014000
H	0.441611000	-3.489209000	0.577903000
H	-4.447682000	-1.217021000	1.286261000
H	-6.591638000	-0.520523000	0.281056000
H	-6.741185000	-0.042397000	-2.159407000
H	-4.704420000	-0.254112000	-3.582712000
H	-2.546863000	-0.921065000	-2.578493000
H	-2.925726000	-4.055476000	1.356266000
H	-3.545409000	-4.659801000	3.671159000
H	-3.113349000	-3.069906000	5.541972000
H	-2.069283000	-0.858709000	5.065757000
H	-1.478242000	-0.233973000	2.751157000
C	-1.831286000	2.327671000	-0.632611000
H	-1.021045000	2.729276000	-1.255100000
H	-2.475222000	1.735389000	-1.294415000
H	-2.395754000	3.135253000	-0.152399000
C	4.743702000	4.225776000	-1.082244000
C	4.274305000	2.894239000	-1.332965000
C	3.560995000	2.446832000	-0.161353000
C	3.613172000	3.507540000	0.808649000
C	4.347812000	4.596422000	0.244288000
Fe	5.521514000	2.907108000	0.276554000
C	7.549516000	2.929990000	-0.053587000
C	7.254819000	3.433709000	1.256783000
C	6.571063000	2.403307000	1.984609000
C	6.445304000	1.264080000	1.125685000
C	7.046466000	1.588408000	-0.136198000
H	8.046390000	3.476934000	-0.852310000
H	7.101929000	0.937829000	-1.006441000
H	5.953984000	0.326661000	1.377295000
H	6.203554000	2.477499000	3.005511000
H	4.580955000	5.534699000	0.743885000
H	3.174264000	3.470451000	1.802868000
H	7.493954000	4.428688000	1.626991000
H	5.317851000	4.838027000	-1.773399000
H	4.395359000	2.328198000	-2.253700000

22 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl III ADF/PW91/TZP

C	0.181789000	2.805959000	-2.557378000
C	0.178994000	1.650115000	-3.345668000
C	0.233537000	1.773554000	-4.745225000
C	0.312383000	3.032166000	-5.337402000
C	0.314801000	4.183413000	-4.543452000
C	0.244484000	4.067101000	-3.156211000
P	0.032507000	-0.033104000	-2.599508000
C	1.502523000	-0.977353000	-3.166090000
C	2.561713000	-0.373512000	-3.860227000
C	3.677803000	-1.128344000	-4.227459000
C	3.747525000	-2.484579000	-3.905769000
C	2.704027000	-3.085640000	-3.197379000
C	1.593540000	-2.337061000	-2.814123000
Rh	0.127981000	-0.142624000	-0.342508000
I	-1.566858000	-2.234913000	-0.254881000
O	1.490937000	1.453433000	-0.202286000
C	2.749372000	1.382484000	0.069740000
C	3.475420000	0.214400000	0.398779000
C	2.957025000	-1.076934000	0.490303000
O	1.784422000	-1.507926000	0.273158000
C	3.922053000	-2.191560000	0.968373000
F	3.815463000	-3.305382000	0.203733000
F	3.633307000	-2.553000000	2.250775000
F	5.239686000	-1.821038000	0.951224000
C	-1.363508000	1.006725000	0.273961000
O	-1.110124000	1.207044000	1.446313000
C	-1.374112000	-0.691315000	-3.609393000
C	-1.284594000	-1.882836000	-4.340524000
C	-2.354318000	-2.305476000	-5.131974000
C	-3.524702000	-1.550494000	-5.199949000
C	-3.618908000	-0.358239000	-4.477956000
C	-2.550557000	0.070092000	-3.693651000
H	4.531412000	0.336708000	0.611111000
H	-0.376582000	-2.480842000	-4.309196000
H	-2.265264000	-3.230659000	-5.700299000
H	-4.358009000	-1.883671000	-5.818288000
H	-4.524102000	0.245674000	-4.531485000
H	-2.629979000	1.014701000	-3.159840000
H	2.523844000	0.685987000	-4.107684000
H	4.498107000	-0.647288000	-4.759053000
H	4.622272000	-3.069474000	-4.189748000
H	2.763135000	-4.137287000	-2.919130000
H	0.806612000	-2.800401000	-2.217140000
H	0.210004000	0.882473000	-5.371486000
H	0.364477000	3.114387000	-6.422526000
H	0.371724000	5.167705000	-5.008941000
H	0.247337000	4.960123000	-2.532176000
H	0.164520000	2.714022000	-1.474911000
C	-2.606464000	1.492457000	-0.413762000
H	-2.332564000	2.162760000	-1.238173000
H	-3.127917000	0.624453000	-0.835803000
H	-3.250763000	2.017380000	0.301196000
C	5.119667000	4.305958000	-0.065547000
C	4.884152000	2.910373000	0.128530000
C	3.464224000	2.670500000	-0.006061000
C	2.838869000	3.946863000	-0.249403000
C	3.858977000	4.945754000	-0.294269000
Fe	3.854684000	3.992620000	1.526822000
C	4.793276000	4.759191000	3.189117000
C	3.576926000	5.471754000	2.927860000
C	2.494420000	4.533748000	2.981697000
C	3.040799000	3.245310000	3.276190000
C	4.460914000	3.381176000	3.402821000
H	5.791579000	5.186291000	3.205434000
H	5.161414000	2.578927000	3.612087000
H	2.477549000	2.319855000	3.350740000
H	1.445423000	4.754893000	2.812329000
H	3.704204000	6.008771000	-0.450105000
H	1.773899000	4.105183000	-0.367386000
H	3.493485000	6.532517000	2.711038000
H	6.086436000	4.797730000	-0.024143000
H	5.647555000	2.163912000	0.319150000

23 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl IV ADF/PW91/TZP

C	0.250738000	2.928463000	-2.321513000
C	-0.105553000	1.840880000	-3.128775000
C	-0.355960000	2.046003000	-4.496898000
C	-0.240293000	3.321401000	-5.046006000
C	0.116103000	4.404579000	-4.236888000
C	0.360280000	4.204784000	-2.878371000
P	-0.241491000	0.136317000	-2.437354000
C	1.116630000	-0.809546000	-3.237704000
C	2.097707000	-0.175470000	-4.011226000
C	3.127342000	-0.920982000	-4.590147000
C	3.187821000	-2.301998000	-4.402629000
C	2.222250000	-2.938756000	-3.617320000
C	1.202616000	-2.197192000	-3.026711000
Rh	-0.022015000	-0.018603000	-0.181274000
I	-2.114326000	1.605355000	0.353582000
O	1.342951000	1.661405000	0.288296000
C	2.611019000	1.584427000	0.404731000
C	3.359640000	0.373349000	0.311131000
C	2.843129000	-0.887187000	0.060341000
O	1.650663000	-1.290122000	-0.189866000
C	3.854741000	-2.055407000	0.147967000
F	3.405211000	-3.180679000	-0.446292000
F	4.112990000	-2.366631000	1.455413000
F	5.057775000	-1.744948000	-0.420384000
C	-1.162084000	-1.564536000	0.302457000
O	-0.867853000	-1.713387000	1.473686000
C	-1.769827000	-0.477037000	-3.287183000
C	-1.740330000	-1.510073000	-4.235594000
C	-2.912029000	-1.903972000	-4.886554000
C	-4.121267000	-1.269398000	-4.604647000
C	-4.154489000	-0.231036000	-3.670224000
C	-2.990470000	0.163964000	-3.015201000
H	4.433818000	0.433518000	0.456412000
H	-0.802570000	-2.002957000	-4.484041000
H	-2.871103000	-2.705823000	-5.622966000
H	-5.033988000	-1.577391000	-5.115339000
H	-5.092105000	0.278111000	-3.449487000
H	-3.029660000	0.970005000	-2.281868000
H	2.061135000	0.901778000	-4.163913000
H	3.884721000	-0.414039000	-5.186936000
H	3.992345000	-2.881730000	-4.854953000
H	2.275439000	-4.013417000	-3.447476000
H	0.478682000	-2.698868000	-2.386640000
H	-0.644646000	1.209546000	-5.132997000
H	-0.435424000	3.470482000	-6.107241000
H	0.197729000	5.403124000	-4.667144000
H	0.633976000	5.043681000	-2.239603000
H	0.441561000	2.778024000	-1.261105000
C	-2.172346000	-2.383717000	-0.437773000
H	-3.005511000	-1.726811000	-0.722200000
H	-1.746651000	-2.775847000	-1.369058000
H	-2.532526000	-3.200719000	0.197469000
C	4.941262000	4.494997000	0.944948000
C	4.742517000	3.092063000	0.762357000
C	3.322317000	2.855437000	0.623527000
C	2.660583000	4.130412000	0.753946000
C	3.658099000	5.133775000	0.941738000
Fe	3.753212000	3.723422000	2.439946000
C	4.724079000	4.068427000	4.220849000
C	3.456006000	4.736586000	4.206067000
C	2.434964000	3.745856000	4.029399000
C	3.072358000	2.468303000	3.937794000
C	4.485953000	2.664943000	4.053350000
H	5.694652000	4.543910000	4.326200000
H	5.242763000	1.887795000	4.009893000
H	2.571128000	1.519669000	3.770339000
H	1.367762000	3.930221000	3.956035000
H	3.476036000	6.194701000	1.083496000
H	1.585743000	4.272230000	0.722056000
H	3.298113000	5.807048000	4.297531000
H	5.898584000	4.987371000	1.083311000
H	5.527675000	2.344746000	0.720701000

24 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl V ADF/PW91/TZP

C	-1.451977000	-0.789975000	2.849521000
C	-1.618763000	-1.946383000	2.068540000
C	-1.754315000	-3.189534000	2.704179000
C	-1.710817000	-3.274343000	4.096711000
C	-1.534557000	-2.122797000	4.866833000
C	-1.411739000	-0.880548000	4.241367000
P	-1.636233000	-1.767550000	0.236110000
C	-3.404142000	-1.458464000	-0.183690000
C	-4.401692000	-1.630965000	0.785428000
C	-5.743047000	-1.419032000	0.460160000
C	-6.100310000	-1.040833000	-0.833417000
C	-5.109724000	-0.870063000	-1.803528000
C	-3.767206000	-1.068803000	-1.483077000
Rh	0.016496000	-0.188062000	-0.218971000
I	-1.756826000	1.841261000	-0.257528000
O	1.507886000	1.335176000	-0.144834000
C	2.700682000	1.179742000	0.285134000
C	3.336463000	-0.076815000	0.515248000
C	2.738445000	-1.313824000	0.365541000
O	1.526870000	-1.637994000	0.087789000
C	3.628202000	-2.563781000	0.518826000
F	3.076367000	-3.468173000	1.373885000
F	4.878882000	-2.287671000	0.987664000
F	3.784700000	-3.192388000	-0.679701000
C	-0.073425000	-0.355698000	-2.204162000
O	-0.797181000	-1.135080000	-2.770709000
C	-1.318928000	-3.465598000	-0.398668000
C	-2.193376000	-4.081298000	-1.305764000
C	-1.910400000	-5.354473000	-1.803387000
C	-0.753565000	-6.024878000	-1.404364000
C	0.121550000	-5.417562000	-0.500083000
C	-0.154787000	-4.146633000	0.000407000
H	4.386128000	-0.058385000	0.789429000
H	-3.100888000	-3.571226000	-1.623771000
H	-2.600726000	-5.820550000	-2.505824000
H	-0.533068000	-7.017635000	-1.796975000
H	1.029701000	-5.930953000	-0.184380000
H	0.538790000	-3.678938000	0.692955000
H	-4.135741000	-1.921230000	1.800628000
H	-6.506974000	-1.546887000	1.225917000
H	-7.147736000	-0.872458000	-1.083936000
H	-5.380760000	-0.567099000	-2.814431000
H	-2.999793000	-0.920459000	-2.239040000
H	-1.890570000	-4.092472000	2.110998000
H	-1.812554000	-4.246024000	4.578782000
H	-1.491956000	-2.193829000	5.953691000
H	-1.278744000	0.023170000	4.834829000
H	-1.366204000	0.185706000	2.367032000
C	0.859357000	0.594224000	-2.929161000
H	0.572418000	1.623492000	-2.682171000
H	1.891751000	0.448998000	-2.593440000
H	0.772538000	0.410745000	-4.006064000
C	3.448081000	2.419377000	0.551902000
C	4.585911000	2.593087000	1.428308000
C	4.939279000	3.978267000	1.415420000
C	4.053744000	4.659337000	0.518312000
C	3.134439000	3.705598000	-0.011638000
Fe	5.077118000	3.159900000	-0.464596000
C	5.615345000	1.825791000	-1.949288000
C	5.269749000	3.091874000	-2.521055000
C	6.145948000	4.080172000	-1.964530000
C	7.031056000	3.423367000	-1.048571000
C	6.701366000	2.028557000	-1.037552000
H	5.119765000	0.878999000	-2.144435000
H	7.182819000	1.262879000	-0.436765000
H	7.805291000	3.901339000	-0.456282000
H	6.133027000	5.142725000	-2.187159000
H	2.330912000	3.894044000	-0.715388000
H	4.087916000	5.715665000	0.270678000
H	5.752797000	4.430800000	1.973664000
H	5.059043000	1.819430000	2.024284000
H	4.477207000	3.273552000	-3.239972000

25 [Rh(fctfa)(COCH₃)(PPh₃)(I)]-acyl VI ADF/PW91/TZP

I	-1.723302000	-2.212374000	0.306515000
Rh	-0.032231000	-0.178388000	-0.224787000
O	1.357196000	1.416596000	-0.107193000
C	2.572208000	1.288839000	0.296781000
C	3.254296000	0.068974000	0.552400000
C	2.706216000	-1.201822000	0.477885000
O	1.509804000	-1.572462000	0.231459000
C	3.651661000	-2.407242000	0.668777000
F	3.141062000	-3.318293000	1.525760000
F	4.888298000	-2.058857000	1.134419000
F	3.849944000	-3.039794000	-0.527974000
C	0.067586000	-0.528865000	-2.184894000
O	-0.465252000	0.182858000	-3.002864000
H	4.308309000	0.143950000	0.798762000
C	0.882504000	-1.746777000	-2.571623000
H	1.941906000	-1.556713000	-2.360632000
H	0.579534000	-2.614667000	-1.977718000
H	0.741751000	-1.923838000	-3.644011000
C	3.306722000	2.545993000	0.523626000
C	4.410772000	2.740041000	1.440231000
C	4.802352000	4.112680000	1.369350000
C	3.973773000	4.764592000	0.398914000
C	3.051135000	3.807323000	-0.120434000
Fe	5.000056000	3.190509000	-0.454291000
C	5.544140000	1.776997000	-1.862774000
C	5.293423000	3.036191000	-2.494968000
C	6.189930000	3.999564000	-1.927876000
C	6.992406000	3.333731000	-0.944623000
C	6.590740000	1.958092000	-0.904040000
H	5.008126000	0.851007000	-2.049419000
H	7.002710000	1.191006000	-0.255078000
H	7.759131000	3.793463000	-0.328412000
H	6.243012000	5.053212000	-2.185873000
H	2.289172000	3.979632000	-0.873960000
H	4.049370000	5.803818000	0.095390000
H	5.604097000	4.572568000	1.938503000
H	4.835449000	1.986991000	2.096050000
H	4.545668000	3.228774000	-3.257408000
C	-3.596863000	-0.083488000	-1.951515000
C	-3.363376000	1.073770000	-1.199845000
C	-4.356802000	2.066642000	-1.141352000
C	-5.572904000	1.885275000	-1.797698000
C	-5.804311000	0.720839000	-2.535208000
C	-4.812846000	-0.256304000	-2.615863000
P	-1.779974000	1.361852000	-0.298648000
C	-2.246395000	1.619387000	1.459765000
C	-3.524062000	1.323849000	1.952485000
C	-3.807799000	1.489859000	3.309086000
C	-2.821299000	1.944762000	4.185209000
C	-1.538860000	2.222121000	3.704028000
C	-1.247559000	2.052568000	2.351206000
C	-1.344509000	3.059280000	-0.901300000
C	-1.421129000	4.195551000	-0.084346000
C	-1.165319000	5.463803000	-0.611726000
C	-0.833671000	5.612452000	-1.958672000
C	-0.754404000	4.482980000	-2.777935000
C	-1.005118000	3.213979000	-2.256369000
H	-1.694167000	4.101607000	0.964972000
H	-1.236734000	6.337117000	0.036753000
H	-0.647912000	6.603949000	-2.371562000
H	-4.297333000	0.957873000	1.279317000
H	-4.805016000	1.256036000	3.680241000
H	-3.048127000	2.074372000	5.243315000
H	-0.760789000	2.566869000	4.383489000
H	-0.243488000	2.264507000	1.983124000
H	-4.181186000	2.984005000	-0.580244000
H	-6.338469000	2.658011000	-1.736602000
H	-6.754913000	0.579875000	-3.049862000
H	-4.981864000	-1.164577000	-3.193147000
H	-2.839111000	-0.860277000	-2.005301000
H	-0.507682000	4.589451000	-3.834158000
H	-0.947306000	2.340001000	-2.900411000