

Supporting Information

The Enantioselectivity in Asymmetric Ketone Hydrogenation Catalyzed by RuH₂(diphosphine)(diamine) Complexes: Insights From a 3D-QSSR and DFT Study

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Figure S1. Two most likely coordinate modes for ketone with catalysts A and C. . . .	2
Figure S2. The structures of RuH ₂ (diphosphine)(diamine) catalyst molecules.	4
Table S1. Energies of stationary points along reaction pathways calculated at ωB97X-D/BSI level, including free energy (<i>G</i>), enthalpy(<i>H</i>), potential energy (<i>E</i>) with zero-point energy correction in gas phase (unit: a.u.)	5
Table S2. Relative energies of stationary points along reaction pathways calculated at ωB97X-D/BSI level, including free energy (<i>G</i>), enthalpy(<i>H</i>), potential energy (<i>E</i>) with zero-point energy (ZPE) correction in gas phase.(unit: kcal/mol)	6
Table S3. Calculated imaginary frequencies of all transition states in gas phase at ωB97X-D/BSI level.	7
Cartesian coordinates of the stationary points and transition states (optimized in gas phase at ωB97X-D/BSI level).	8
Cartesian coordinates of the RuH ₂ (diphosphine)(diamine) complexes in training set and test set (optimized in gas phase at B3LYP/BSI level).	69
The structure, steric and electrostatic contour maps from CoMFA of catalysts in training set.	127

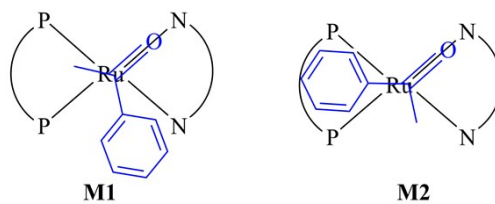


Figure S1. Two most likely coordinate modes for ketone with catalysts A and C.

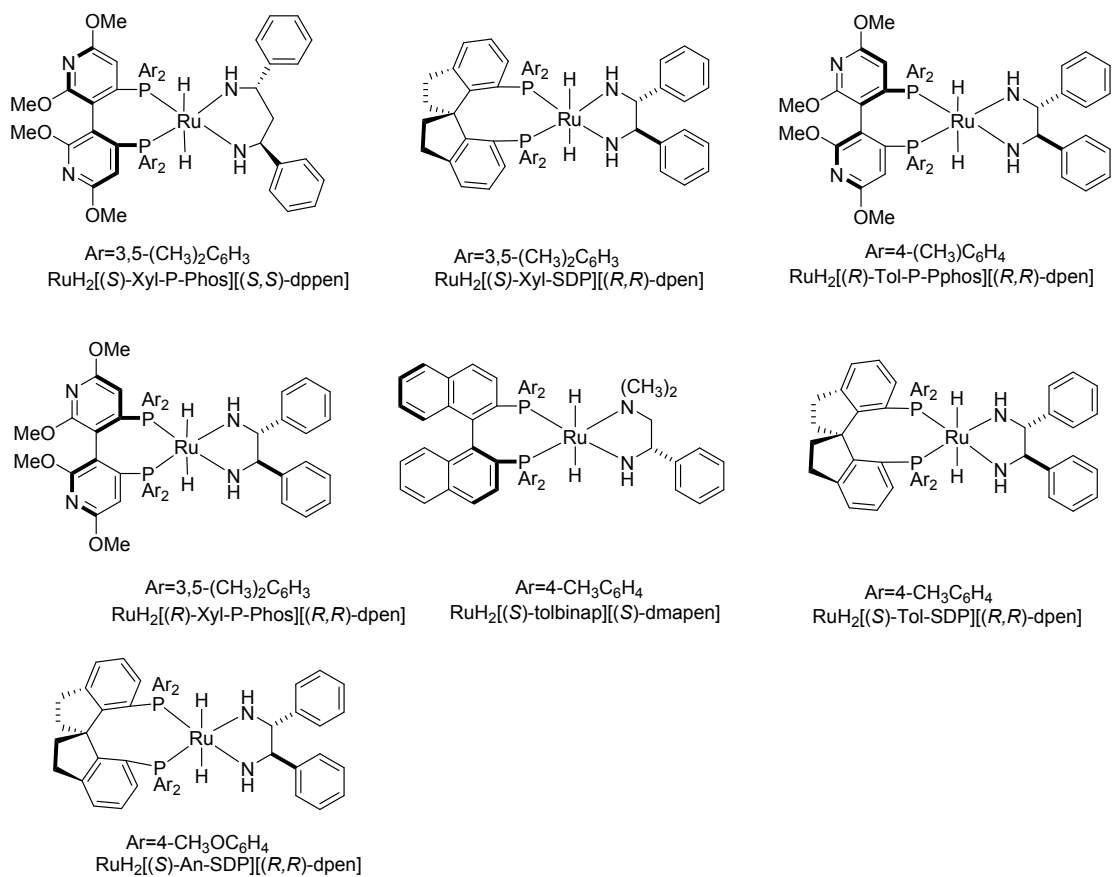


Figure S2. The structures of RuH₂(diphosphine)(diamine) catalyst molecules.

Table S1. Energies of stationary points along reaction pathways calculated at ω B97X-D/BSI level, including free energy (G), enthalpy(H), potential energy (E) with zero-point energy correction in gas phase (unit: a.u.)

	G	H	E
A1	-3281.9251	-3281.7709	-3281.8305
A2	-3666.5897	-3666.4143	-3666.4838
TSA2-3	-3666.5817	-3666.4101	-3666.4784
A3	-3666.5951	-3666.4239	-3666.4921
TSA3-4	-3666.5967	-3666.4240	-3666.4923
A4	-3666.5961	-3666.4213	-3666.4902
A2u	-3666.5848	-3666.4100	-3666.4791
TSAu2-3	-3666.5753	-3666.4047	-3666.4728
A3u	-3666.5910	-3666.4167	-3666.4854
TSAu3-4	-3666.5918	-3666.4169	-3666.4855
A4u	-3666.5897	-3666.4138	-3666.4829
A5	-3280.7436	-3280.5864	-3280.6464
C1	-3392.5708	-3392.4082	-3392.4714
C2	-3777.2334	-3777.0517	-3777.1242
TSC2-3	-3777.2269	-3777.0486	-3777.1200
C3	-3777.2394	-3777.0618	-3777.1329
TSC3-4	-3777.2380	-3777.0607	-3777.1317
C4	-3777.2375	-3777.0579	-3777.1295
C2u	-3777.2300	-3777.0484	-3777.1208
TSCu2-3	-3777.2204	-3777.0433	-3777.1144
C3u	-3777.2333	-3777.0536	-3777.1252
TSCu3-4	-3777.2327	-3777.0535	-3777.1249
C4u	-3777.2250	-3777.0470	-3777.1183
C5	-3391.3860	-3391.2234	-3391.2863

* All of the systems have three columns of data. G , H and E are the free energies, enthalpies and potential energies with zero-point energy correction in gas phase.

Table S2. Relative energies of stationary points along reaction pathways calculated at ω B97X-D/BSI level, including free energy (G), enthalpy(H), potential energy (E) with zero-point energy (ZPE) correction in gas phase.(unit: kcal/mol)

	A1	A2	TSA2-3	A3	TSA3-4	A4	A5+R	A2u	TSAu2-3	A3u	TSAu3-4	A4u	A5+S
G	0.0	-4.2	0.8	-7.7	-8.7	-8.3	3.7	-1.2	4.8	-5.1	-5.6	-4.2	3.7
H	0.0	-16.8	-14.1	-22.8	-22.9	-21.1	6.3	-14.0	-10.8	-18.3	-18.4	-16.5	6.3
E	0.0	-17.5	-14.1	-22.8	-22.9	-21.6	5.8	-14.6	-10.6	-18.6	-18.6	-17.0	5.8
	C1	C2	TSC2-3	C3	TSC3-4	C4	C5+R	C2u	TSCu2-3	C3u	TSCu3-4	C4u	C5+S
G	0.0	-3.0	1.1	-6.8	-5.9	-5.6	5.8	-0.9	5.2	-2.9	-2.5	2.3	5.8
H	0.0	-16.9	-14.9	-23.2	-22.5	-20.7	6.5	-14.8	-11.6	-18.1	-18.0	-13.9	6.5
E	0.0	-17.2	-14.6	-22.7	-22.0	-20.6	6.3	-15.1	-11.1	-17.9	-17.7	-13.6	6.3

* All of the systems have three rows of data. The data are energies of stationary points optimized in gas phase

Table S3. Calculated imaginary frequencies of all transition states in gas phase at ω B97X-D/BSI level.

TSA2-3	TSA3-4	TSAu2-3	TSAu3-4	TSC2-3	TSC3-4	TSCu2-3	TSCu3-4
338.80 <i>i</i>	865.91 <i>i</i>	496.30 <i>i</i>	783.26 <i>i</i>	360.81 <i>i</i>	859.78 <i>i</i>	487.99 <i>i</i>	691.42 <i>i</i>

Cartesian coordinates of the stationary points and transition states (optimized in gas phase at ω B97X-D/BSI level).

A1

Coordinates (Angstroms)			
X	Y	Z	

Ru	1.00114300	-0.00026200	0.00017000
P	-0.55756300	1.62458100	0.08694900
P	-0.55783200	-1.62484400	-0.08674400
C	-1.40780400	-2.29282900	1.40386100
C	-1.08308300	-1.79456000	2.66321000
C	-4.06663800	-0.34104500	-2.90752500
C	-2.03002500	-1.20812000	-1.13966300
C	-6.01441800	-1.02778500	3.37120800
C	-4.06693200	0.34232100	2.90763000
C	-2.81150800	-3.15435100	3.69075900
C	0.17449900	3.15296100	0.83953100
C	0.21067800	-4.38878800	-0.19122600
C	0.21278900	4.38803100	0.19020500
C	0.17374300	-3.15324100	-0.83970500
C	1.59376300	5.34932500	1.94504300
C	-1.40743100	2.29222800	-1.40384500
C	0.88051500	3.03084600	2.04902500
C	-2.02987900	1.20860500	1.13989300
C	-2.95803300	-0.27382300	-0.69939800
C	-2.13351600	-1.72164400	-2.45873600
C	-5.94363200	1.55426100	-2.06080500
C	-3.99389600	0.17715600	-1.58697100
C	1.56415400	-4.10892200	-2.59317500
C	-4.96225700	1.14278000	-1.19690800
C	-3.11090100	3.67477900	-2.42821900
C	0.91123000	-5.46556500	-0.73688400
C	-3.11423800	-1.30528900	-3.31479100
C	-5.94466500	-1.55219400	2.06081700
C	-5.08942300	-0.10482800	3.78401600
C	-2.43227400	-3.24093300	1.29890900
C	-1.78341300	-2.21776100	3.78976800
C	-3.11312900	-3.67364800	2.42752100
C	-2.13334000	1.72235800	2.45889200
C	-3.11421600	1.30627800	3.31494500
C	-3.99437300	-0.17584700	1.58702200
C	-2.81044000	3.15388700	-3.69107600
C	0.91377200	5.46468800	0.73557300
C	-2.43050800	3.24190000	-1.29940000
C	-5.08901100	0.10638800	-3.78390700
C	-2.95813300	0.27460900	0.69957800
C	1.59210900	-5.34983900	-1.94580200
C	0.88057100	-3.03078600	-2.04867900
C	-1.08395700	1.79221300	-2.66281000
C	-6.01368300	1.02969800	-3.37112400
C	-4.96320000	-1.14097800	1.19689700
C	1.56449200	4.10886800	2.59324100
C	-1.78396600	2.21547300	-3.78953300
H	-0.29948700	-1.04367900	2.73545000
H	-6.79775300	-1.35894300	4.04717400

H	-0.29920000	-4.52293400	0.75676300
H	-0.29639900	4.52191800	-0.75818300
H	0.91354900	2.05965200	2.53725700
H	-1.42222900	-2.46671600	-2.79558400
H	-6.66942400	2.29472000	-1.73789100
H	2.09302300	-3.98476100	-3.53612900
H	-4.91099600	1.56964400	-0.20193300
H	-3.91087400	4.40467600	-2.32757000
H	0.92484600	-6.41328800	-0.20366100
H	-3.17630400	-1.71811000	-4.31873300
H	-6.67067400	-2.29243300	1.73789900
H	-5.12730200	0.30553200	4.79015800
H	-2.71059700	-3.63068100	0.32209900
H	-1.53742000	-1.79471900	4.76106300
H	-3.91436700	-4.40208600	2.32642800
H	-1.42192300	2.46733600	2.79569500
H	-3.17620000	1.71915100	4.31887500
H	0.92840600	6.41203600	0.20170200
H	-2.70788500	3.63300400	-0.32285700
H	-5.12713600	-0.30409900	-4.78998700
H	0.91447800	-2.05929600	-2.53626600
H	-0.30158100	1.04000500	-2.73457400
H	-6.79701700	1.36097000	-4.04703900
H	-4.91212500	-1.56781800	0.20191900
H	2.09268600	3.98495900	3.53660600
H	-1.53896900	1.79112100	-4.76050700
H	1.12294700	-0.04161600	-1.71142600
H	1.12300600	0.04115400	1.71177100
C	-3.61419400	-3.56680800	4.89747500
H	-4.58119600	-3.04989100	4.90194200
H	-3.81395000	-4.64387000	4.89804300
H	-3.09699400	-3.31580700	5.82872200
C	2.34016900	-6.51265500	-2.54686700
H	2.32437300	-7.38331900	-1.88457100
H	1.89802000	-6.81138300	-3.50434500
H	3.38794200	-6.25445700	-2.73786000
C	2.34228900	6.51202000	2.54577100
H	3.38974800	6.25317900	2.73763400
H	2.32757800	7.38220700	1.88282100
H	1.89974000	6.81179300	3.50273900
C	-3.61281300	3.56651700	-4.89793800
H	-4.58080300	3.05142900	-4.90139200
H	-3.81052700	4.64395300	-4.89970400
H	-3.09649200	3.31342500	-5.82910500
N	2.69483700	-1.39274000	0.06333500
N	2.69489000	1.39207600	-0.06308600
C	3.93872300	0.67073700	-0.38145900
C	3.93866400	-0.67147700	0.38192800
H	2.53905700	-2.12101500	0.75504800
H	2.76053000	-1.86266300	-0.83641800
H	3.88541100	0.43890500	-1.45158100
H	2.76052500	1.86203900	0.83662100
H	2.53920000	2.12033200	-0.75485000
C	5.19562300	1.46981100	-0.09627000
C	6.19054900	1.59731300	-1.06463500
C	5.39715900	2.05681900	1.15612000
C	7.36257200	2.29763700	-0.79316500
H	6.05093100	1.13167000	-2.03681200
C	6.56514400	2.76002900	1.43054000
H	4.64045100	1.96466300	1.93296000

C	7.55219200	2.88235100	0.45526500
H	8.12794000	2.38518100	-1.55850800
H	8.46566800	3.42922400	0.66893200
C	5.19559400	-1.47050700	0.09678600
C	6.18975100	-1.59946600	1.06575500
C	5.39809200	-2.05568500	-1.15629600
C	7.36196600	-2.29944000	0.79416800
H	6.04938300	-1.13525400	2.03850700
C	6.56632600	-2.75840400	-1.43089000
H	4.64203300	-1.96225600	-1.93362200
C	7.55260100	-2.88220300	-0.45502900
H	8.12672400	-2.38816300	1.55998400
H	6.70793400	-3.20933700	-2.40870800
H	3.88521600	-0.43974300	1.45206100
H	6.70594000	3.21252900	2.40775100
H	8.46627100	-3.42869800	-0.66883000

A2

Coordinates (Angstroms)

X	Y	Z	
Ru	0.61902800	0.33203500	-0.12067400
P	-0.73554500	-1.36905900	-0.69720000
P	-1.11572300	1.70685500	0.30936100
C	-2.07053000	2.57505500	-1.00363900
C	-1.66616000	2.47492700	-2.33364800
C	-4.31825000	-0.69702400	2.73050300
C	-2.49530200	0.85531400	1.21606500
C	-6.61896800	1.26234200	-3.14168600
C	-4.49359700	0.09456600	-3.06603800
C	-3.59857800	3.75278600	-3.06031300
C	0.23429400	-2.48875300	-1.80634100
C	-0.86245200	4.44642000	1.16955000
C	0.70594100	-3.72377700	-1.35682700
C	-0.59533300	3.09841200	1.41742800
C	2.26699000	-3.88997500	-3.21145400
C	-1.45095500	-2.56107500	0.51356600
C	0.79239700	-1.97211700	-2.98783700
C	-2.28407500	-0.90270100	-1.60418500
C	-3.30698400	-0.06312700	0.56441100
C	-2.60611800	1.00690300	2.62385200
C	-5.90332400	-2.62385600	1.46414900
C	-4.22371300	-0.86923800	1.32332700
C	0.76926400	3.78280700	3.31282800
C	-5.03753800	-1.86583600	0.71878300
C	-2.79908600	-4.49955800	1.04775700
C	-0.32580100	5.44289000	1.98496400
C	-3.48963300	0.26536700	3.35687000
C	-6.56630600	1.42805600	-1.73893000
C	-5.60094000	0.61143500	-3.78766200
C	-3.24107200	3.28343300	-0.71032000
C	-2.42561900	3.05368800	-3.34631500
C	-3.98572300	3.87258300	-1.72287200
C	-2.38904700	-1.09249000	-3.00622700
C	-3.45009900	-0.60524900	-3.71665800
C	-4.43163400	0.26231200	-1.65670500

C	-2.66688400	-4.24936900	2.41696100
C	1.70954700	-4.40639900	-2.04476400
C	-2.21082400	-3.66261000	0.10821200
C	-5.22479300	-1.49207300	3.47768500
C	-3.30179000	-0.24266200	-0.92817800
C	0.49114700	5.13229800	3.07032700
C	0.24338500	2.78895300	2.50060900
C	-1.30807500	-2.31572800	1.87606700
C	-6.00746800	-2.43275600	2.86020700
C	-5.50396800	0.94615200	-1.01976200
C	1.77144300	-2.66881300	-3.68312000
C	-1.90844400	-3.14782700	2.81503300
H	-0.76554900	1.90811300	-2.55836200
H	-7.46561300	1.64957700	-3.70127400
H	-1.47984800	4.73598800	0.32602400
H	0.31343400	-4.15150700	-0.44049000
H	0.50958400	-0.97611300	-3.31502400
H	-1.97982700	1.73484600	3.12809400
H	-6.50975500	-3.38238500	0.97806800
H	1.42753900	3.50593700	4.13367900
H	-4.95685400	-2.03603500	-0.34853100
H	-3.39210800	-5.34836600	0.71507300
H	-0.54473400	6.48471300	1.76242900
H	-3.56668500	0.40860500	4.43206800
H	-7.37141500	1.94831800	-1.22832300
H	-5.62790500	0.47437200	-4.86600000
H	-3.58667200	3.35612300	0.31865400
H	-2.10813500	2.94360600	-4.38091500
H	-4.90167600	4.40440900	-1.47665700
H	-1.61627000	-1.64390800	-3.52841000
H	-3.50846700	-0.76018500	-4.79122800
H	2.07363200	-5.35243300	-1.65004300
H	-2.35126000	-3.86287100	-0.95166200
H	-5.28707000	-1.33933900	4.55243200
H	0.50573800	1.74814100	2.66910000
H	-0.75006200	-1.43016000	2.17183700
H	-6.70197000	-3.03449600	3.43975300
H	-5.46870900	1.09905000	0.05276600
H	2.18902700	-2.23811300	-4.59100400
H	-1.80827700	-2.92190100	3.87469000
H	0.68589400	-0.07902700	1.53313500
H	0.74045000	0.75648000	-1.77817400
C	-4.45660800	4.32079600	-4.16131200
H	-5.24572500	3.60820700	-4.42958700
H	-4.94324800	5.25160500	-3.85176400
H	-3.87094700	4.52554000	-5.06319700
C	1.06158300	6.20729800	3.96024600
H	0.94535200	7.19932900	3.51356900
H	0.55731600	6.21877300	4.93391800
H	2.12804100	6.04176000	4.14704600
C	3.40375400	-4.58040400	-3.91931000
H	4.34053700	-4.03109300	-3.76258000
H	3.54774000	-5.59949500	-3.54781700
H	3.22968900	-4.63417700	-4.99945200
C	-3.37774000	-5.10763700	3.43053500
H	-4.37114600	-4.69258700	3.63935900
H	-3.51381100	-6.13149600	3.06776100
H	-2.83079300	-5.14919400	4.37794800
N	2.19657400	1.81684800	0.23537400
N	2.46023800	-0.82881100	-0.44313600

C	3.68564400	-0.01226100	-0.32294400
C	3.35742000	1.46575800	-0.60151400
H	1.89739000	2.76695500	0.02969300
H	2.44923800	1.79394300	1.22320200
H	3.99354200	-0.06404700	0.72398300
H	2.39556900	-1.22869300	-1.37544000
H	2.52043000	-1.61686900	0.19718000
C	4.80824100	-0.52335900	-1.20101100
C	6.07394300	-0.77763900	-0.67455700
C	4.59163800	-0.73869000	-2.56497400
C	7.09885800	-1.25801600	-1.48554800
H	6.26104200	-0.58377200	0.37813200
C	5.61120200	-1.22313600	-3.37820300
H	3.61734500	-0.52557100	-2.99976000
C	6.86812600	-1.48912600	-2.83852500
H	8.07928200	-1.44858000	-1.05883500
H	7.66533700	-1.86580900	-3.47255900
C	4.57404400	2.34211800	-0.37962800
C	5.18600200	2.97754900	-1.45960200
C	5.12638300	2.49336000	0.89678500
C	6.32764800	3.75301900	-1.27558800
H	4.76843000	2.85423900	-2.45589300
C	6.26536100	3.27027400	1.08224300
H	4.67288500	1.99451700	1.75072100
C	6.86983900	3.90197400	-0.00283600
H	6.79323800	4.23925900	-2.12794800
H	6.68507400	3.38079300	2.07811800
H	3.01539200	1.55794200	-1.63724200
C	2.01897600	-2.68485200	2.63772400
C	2.32879600	-3.85632100	1.95534000
C	3.61754700	-4.05769800	1.46416800
C	4.60156100	-3.09189800	1.67128500
C	4.28643600	-1.91672900	2.34440600
C	2.98852400	-1.69447500	2.81357600
H	1.00596400	-2.52821200	2.98533000
H	1.55610400	-4.60280500	1.79861200
H	3.85576700	-4.96666500	0.91982400
H	5.60596800	-3.24539300	1.28933600
H	5.03690900	-1.14742500	2.50065300
C	2.65281500	-0.36842000	3.42137600
O	3.33290500	0.61493000	3.16970500
C	1.47943400	-0.28552100	4.36775100
H	0.55152300	-0.37549800	3.79232800
H	1.50887200	-1.09093900	5.10901800
H	1.49085400	0.68500700	4.86734700
H	5.42590900	-1.38651000	-4.43619900
H	7.76081600	4.50548300	0.14410600

TSA2-3

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.65452300	0.29015700	0.08310400
P	0.73132400	-1.42760400	0.62030900
P	1.10626600	1.71076300	-0.22009100
C	2.04118100	2.43708100	1.19129300

C	1.58989400	2.28097900	2.49967700
C	4.26269000	-0.56679800	-2.80904100
C	2.48211100	0.91292100	-1.17747800
C	6.65670700	1.03636000	3.14222700
C	4.51928100	-0.10543200	3.02607100
C	3.53862100	3.44285400	3.36323500
C	-0.24842700	-2.55627800	1.70751900
C	1.04291800	4.51943600	-0.90586300
C	-0.77765500	-3.74875000	1.20951100
C	0.65411300	3.21064000	-1.20297500
C	-2.33221400	-3.92508700	3.06951600
C	1.43950100	-2.58943700	-0.61824400
C	-0.77319000	-2.06858500	2.91633800
C	2.28471500	-1.00049600	1.53770800
C	3.29240700	-0.05116400	-0.59379700
C	2.57258600	1.14678100	-2.57575500
C	5.83170500	-2.59345900	-1.68545300
C	4.18711500	-0.82167800	-1.41318000
C	-0.69603400	4.08723900	-3.02619900
C	4.99186300	-1.86622200	-0.88199100
C	2.73866000	-4.54203800	-1.21198800
C	0.57601200	5.58944300	-1.66696200
C	3.43584600	0.43997500	-3.36456300
C	6.60207900	1.25841500	1.74723500
C	5.63451100	0.36943300	3.76446400
C	3.24778900	3.11629000	0.98016200
C	2.33325000	2.77417100	3.56906200
C	3.97712200	3.61915900	2.04749900
C	2.40425500	-1.26941900	2.92554300
C	3.47532200	-0.82740100	3.65028700
C	4.45084800	0.12675000	1.62634100
C	2.65356800	-4.21938700	-2.57033800
C	-1.80456400	-4.41589100	1.87800900
C	2.15123500	-3.73445200	-0.24675000
C	5.14337300	-1.33110200	-3.61653000
C	3.30463300	-0.32010000	0.88521700
C	-0.29281700	5.39484400	-2.74101600
C	-0.23492900	3.02002300	-2.26900300
C	1.34784700	-2.26890000	-1.96959800
C	5.91808500	-2.32038900	-3.06909600
C	5.53072600	0.82104300	1.01315000
C	-1.77959700	-2.74844800	3.58866100
C	1.94539900	-3.07357300	-2.93313200
H	0.66463900	1.73815000	2.66933400
H	7.50956300	1.39052500	3.71418100
H	1.69969300	4.72177700	-0.06712300
H	-0.41284000	-4.15357700	0.27079200
H	-0.43985500	-1.10623700	3.29283000
H	1.94551200	1.90958500	-3.02470700
H	6.43025300	-3.39138800	-1.25599000
H	-1.39989300	3.89250400	-3.83170100
H	4.92335000	-2.09840800	0.17459500
H	3.29103000	-5.42805100	-0.90752000
H	0.88921300	6.59877700	-1.40965200
H	3.49549900	0.64279300	-4.43113700
H	7.41330000	1.78642200	1.25456300
H	5.66372300	0.18798800	4.83606800
H	3.63689900	3.22736700	-0.02938500
H	1.97396100	2.61889900	4.58381400
H	4.92267300	4.12270900	1.86165900

H	1.63545000	-1.84579300	3.42563700
H	3.54124400	-1.03603300	4.71522600
H	-2.21329400	-5.32675600	1.44688900
H	2.25214600	-3.99249300	0.80502600
H	5.19040800	-1.11752000	-4.68159100
H	-0.60474700	2.02320300	-2.47998200
H	0.83147100	-1.35304400	-2.24306800
H	6.59182600	-2.89927900	-3.69452700
H	5.49620100	1.01703000	-0.05225600
H	-2.17353000	-2.33749200	4.51571200
H	1.88185600	-2.79070900	-3.98151700
H	-0.85982000	-0.13025800	-1.64112600
H	-0.70276700	0.67430400	1.70466500
C	4.37362500	3.93773800	4.51618500
H	5.32565300	3.39602800	4.55776000
H	4.60438500	5.00399000	4.41192100
H	3.86216400	3.79449500	5.47286300
C	-0.78576100	6.55234600	-3.57168000
H	-0.61442900	7.50923600	-3.06935700
H	-0.27043200	6.58721300	-4.53909900
H	-1.85774000	6.46240500	-3.77657800
C	-3.49346100	-4.59411900	3.75732900
H	-3.70276200	-5.57660800	3.32406400
H	-3.30161500	-4.72816600	4.82750600
H	-4.39861100	-3.98214900	3.65785300
C	3.36093000	-5.04987500	-3.60891600
H	4.35459600	-4.63051400	-3.80813800
H	3.49501200	-6.08427000	-3.27703700
H	2.81200600	-5.06180100	-4.55594200
N	-2.22503400	1.75336600	-0.24186800
N	-2.46721500	-0.86188400	0.49423200
C	-3.70827600	-0.06639600	0.37885900
C	-3.39573300	1.42518500	0.59195800
H	-1.94074500	2.71484300	-0.07020100
H	-2.46770400	1.68389900	-1.23861000
H	-4.04756900	-0.16956300	-0.65375800
H	-2.37239100	-1.21544500	1.44266300
H	-2.54907900	-1.68270500	-0.10347700
C	-4.78553600	-0.58064700	1.30869200
C	-6.01134700	-1.01763300	0.81044600
C	-4.55132300	-0.65338600	2.68531200
C	-6.98306200	-1.53003600	1.66635800
H	-6.20135600	-0.95551800	-0.25726800
C	-5.51774400	-1.16776600	3.54302600
H	-3.60284900	-0.30842400	3.09269800
C	-6.73730700	-1.61144100	3.03377600
H	-7.93268000	-1.86884900	1.26251000
H	-7.49345500	-2.01220300	3.70251500
C	-4.62202400	2.26615200	0.29580700
C	-5.08065800	2.42069700	-1.01674200
C	-5.33879000	2.85367600	1.33764600
C	-6.23358000	3.15552900	-1.27413700
H	-4.53357500	1.96688700	-1.84124800
C	-6.49424700	3.58664900	1.08059400
H	-4.99446200	2.72515500	2.36096200
C	-6.94377200	3.74015900	-0.22734600
H	-6.57890300	3.27281000	-2.29744100
H	-7.04124100	4.03814500	1.90320200
H	-3.08605800	1.57708800	1.63076700
C	-2.21266900	-2.52911600	-2.28634700

C	-2.98867500	-3.63825100	-1.96473200
C	-4.37779600	-3.58220000	-2.07987800
C	-4.98263400	-2.41121700	-2.52570100
C	-4.20527200	-1.29684200	-2.83419000
C	-2.81531400	-1.33972300	-2.70747800
H	-1.13575200	-2.56893900	-2.15826100
H	-2.50676500	-4.54636900	-1.61408900
H	-4.98215800	-4.44757300	-1.82434700
H	-6.06293100	-2.36114700	-2.63054100
H	-4.66694500	-0.37226700	-3.16721700
C	-2.04058200	-0.08962000	-3.07520800
O	-2.62652600	1.00819100	-3.02001600
C	-0.91068500	-0.27904800	-4.07552800
H	-0.40453700	-1.23889400	-3.96241700
H	-1.36178400	-0.24669900	-5.07631500
H	-0.18046900	0.52822300	-3.99808400
H	-7.84456300	4.31179100	-0.43140200
H	-5.32139700	-1.22030000	4.61029800

A3

Coordinates (Angstroms)

X	Y	Z
Ru	-0.64713100	0.32840600
P	0.72948800	-1.44420200
P	1.15708200	1.72619000
C	2.13749200	2.37224500
C	1.67322400	2.25556200
C	4.08672000	-0.68627000
C	2.45551100	0.86403400
C	6.80292600	0.86824000
C	4.63215300	-0.21478300
C	3.68547900	3.30044200
C	-0.25841800	-2.51631500
C	1.32592900	4.51168200
C	-0.84612900	-3.69206900
C	0.76187300	3.25433400
C	-2.37096200	-3.77797000
C	1.33920900	-2.62772300
C	-0.73537700	-1.99339000
C	2.31886400	-1.05084100
C	3.25696000	-0.13121700
C	2.47725600	1.09088800
C	5.64487700	-2.76204300
C	4.08005200	-0.93352000
C	-0.57023400	4.25839900
C	4.87718500	-2.00298000
C	2.54563700	-4.62645900
C	0.95285100	5.61612700
C	3.26723100	0.34696400
C	6.70528300	1.07378900
C	5.78646600	0.23667100
C	3.38740500	2.96968100
C	2.44058600	2.70839400
C	4.14093400	3.43546100
C	2.48240900	-1.31851900

C	3.59262000	-0.90136600	3.58106900
C	4.51849100	0.00766600	1.51256000
C	2.40102600	-4.31630600	-2.58925500
C	-1.88539900	-4.30730500	2.01353400
C	2.03237600	-3.79177400	-0.24974400
C	4.89242900	-1.48553300	-3.76793700
C	3.32966700	-0.40258400	0.82144500
C	0.00322400	5.51043200	-2.68499800
C	-0.20410700	3.15081200	-2.15852400
C	1.18827000	-2.32025500	-1.94959700
C	5.66091800	-2.49927000	-3.25862100
C	5.59586600	0.65992800	0.85085400
C	-1.75840300	-2.62080800	3.70231300
C	1.71068600	-3.15503900	-2.93153700
H	0.71580900	1.77842300	2.71253400
H	7.68538100	1.20497600	3.47200000
H	2.05372400	4.64778600	-0.11579600
H	-0.51936300	-4.12176700	0.37514800
H	-0.34633400	-1.04807200	3.37077300
H	1.85408200	1.87363400	-3.02045100
H	6.23960300	-3.57784700	-1.47005200
H	-1.33078500	4.13341400	-3.68019300
H	4.86155800	-2.22890900	0.03479500
H	3.08439200	-5.52644300	-0.94454200
H	1.40910500	6.58119900	-1.45893200
H	3.26959100	0.54040000	-4.50197700
H	7.51415900	1.57035800	1.01244600
H	5.85106600	0.06522100	4.67433700
H	3.79123300	3.04303100	0.00984400
H	2.06572200	2.58437400	4.61560500
H	5.11659300	3.87717300	1.89789600
H	1.71736400	-1.87172100	3.43304000
H	3.69353300	-1.10363800	4.64435400
H	-2.33959100	-5.20528900	1.60209200
H	2.17520100	-4.04116900	0.79910100
H	4.88474800	-1.27919300	-4.83527300
H	-0.73030700	2.21958900	-2.35887500
H	0.69083400	-1.39756500	-2.22987200
H	6.27786300	-3.10439200	-3.91679700
H	5.52884900	0.84176000	-0.21553200
H	-2.11514400	-2.18404000	4.63230300
H	1.59457200	-2.88412200	-3.97786800
H	-1.13689000	-0.15608400	-1.82329700
H	-0.55982100	0.68503500	1.69906500
C	4.54011300	3.76065900	4.55070400
H	5.48630200	3.20798900	4.56965300
H	4.78206600	4.82604500	4.46424400
H	4.03785300	3.60578100	5.51029000
C	-0.42158300	6.71668600	-3.48305700
H	0.34208100	7.50031200	-3.46140700
H	-0.61352300	6.45518900	-4.52854200
H	-1.34673900	7.14421600	-3.07782300
C	-3.55421700	-4.38373700	3.91520300
H	-4.46664900	-3.82479900	3.67172100
H	-3.71011600	-5.42538200	3.61960300
H	-3.42789400	-4.35219700	5.00244100
C	3.02427600	-5.18960000	-3.64595600
H	4.08467100	-4.93670900	-3.76706600
H	2.96305600	-6.25002700	-3.38035800
H	2.53865400	-5.05141900	-4.61659400

N	-2.18359500	1.79548400	-0.14002200
N	-2.45784200	-0.79414200	0.60720000
C	-3.69639600	-0.00138800	0.42760500
C	-3.38214100	1.48499600	0.66080200
H	-1.91598600	2.76678300	0.00179900
H	-2.40326100	1.66227100	-1.17912800
H	-3.97321500	-0.09944900	-0.62439900
H	-2.38429700	-1.09782000	1.57565000
H	-2.54507200	-1.64893300	0.05600900
C	-4.81232200	-0.53734200	1.29554800
C	-5.96932000	-1.05948200	0.72043000
C	-4.67717000	-0.56510400	2.68717600
C	-6.97292400	-1.60316900	1.51846100
H	-6.07568600	-1.04682400	-0.36072600
C	-5.67593000	-1.10974500	3.48710400
H	-3.78135200	-0.15961300	3.15390300
C	-6.82828700	-1.63276600	2.90244900
H	-7.86849100	-2.00811800	1.05649100
H	-7.61053200	-2.05724800	3.52499000
C	-4.58638700	2.33855900	0.31259700
C	-5.35007400	2.92399100	1.32167500
C	-4.97013900	2.50660500	-1.02280000
C	-6.48202300	3.67324400	1.01081800
H	-5.06333200	2.78299700	2.36135600
C	-6.09930500	3.25881200	-1.33078500
H	-4.37826200	2.04830500	-1.81559200
C	-6.85761100	3.84385200	-0.31819200
H	-7.06773500	4.12378100	1.80708800
H	-6.38732100	3.38960400	-2.37012900
H	-3.12554700	1.63521000	1.71640800
C	-2.38326900	-2.49842200	-2.11263800
C	-3.27116400	-3.56367500	-1.97072100
C	-4.60871400	-3.41039300	-2.32857700
C	-5.04517600	-2.18768100	-2.83579300
C	-4.15747800	-1.12150200	-2.95932500
C	-2.81816100	-1.26004700	-2.59315200
H	-1.34062800	-2.62603300	-1.82989900
H	-2.91593800	-4.51218100	-1.57566900
H	-5.30509500	-4.23633900	-2.21470200
H	-6.08581700	-2.06051600	-3.12391900
H	-4.48311400	-0.14924000	-3.31643800
C	-1.89187200	-0.03607700	-2.71725200
O	-2.53790400	1.13256600	-2.68821700
C	-1.00001000	-0.19247200	-3.96896400
H	-0.52803400	-1.17981000	-4.03984700
H	-1.62781700	-0.04512500	-4.85413500
H	-0.21857900	0.57457600	-3.96751300
H	-5.55679900	-1.12393200	4.56696700
H	-7.73873400	4.42965300	-0.56486300

TSA3-4

Coordinates (Angstroms)

X	Y	Z
Ru	-0.65701700	0.33306300
P	0.72741200	-1.43710100

P	1.13866500	1.74058400	-0.19559500
C	2.11192500	2.37638200	1.22942700
C	1.63977800	2.25465800	2.53519200
C	4.07056300	-0.67807400	-2.92011200
C	2.44487900	0.88020800	-1.20052000
C	6.80318600	0.88158200	2.92092100
C	4.63704500	-0.21116900	2.90180000
C	3.64956400	3.29128100	3.41663500
C	-0.26016200	-2.49848100	1.80136200
C	1.30067300	4.54051200	-0.85889100
C	-0.85827900	-3.67358200	1.33949900
C	0.76717400	3.27994400	-1.14583400
C	-2.38483000	-3.72842900	3.22993400
C	1.34002900	-2.64169100	-0.58428700
C	-0.73187100	-1.96169500	3.01084600
C	2.31899100	-1.04689700	1.51652500
C	3.24506000	-0.11698700	-0.65742300
C	2.46942600	1.10616600	-2.60343200
C	5.61581800	-2.76281400	-1.87361700
C	4.06375100	-0.92343400	-1.52034500
C	-0.50742300	4.29877700	-2.94593900
C	4.85477600	-1.99754400	-1.02832300
C	2.53764700	-4.65827000	-1.18026500
C	0.94144800	5.65404900	-1.61248300
C	3.25619000	0.35943300	-3.43464500
C	6.69681000	1.09526200	1.52729300
C	5.79395200	0.23994100	3.58932500
C	3.36194300	2.97588400	1.03205700
C	2.40149700	2.70134200	3.61120300
C	4.11079000	3.43552300	2.10571100
C	2.49112400	-1.32243900	2.89717500
C	3.60367900	-0.90574800	3.57327300
C	4.51449800	0.01997600	1.50544600
C	2.41007300	-4.36370200	-2.54272300
C	-1.90321600	-4.27324400	2.04153600
C	2.02091700	-3.80717300	-0.21409200
C	4.87069700	-1.48251300	-3.77141900
C	3.32350900	-0.39043200	0.81877700
C	0.03618400	5.55471300	-2.66987900
C	-0.15545300	3.18367200	-2.19578700
C	1.20659100	-2.35055200	-1.93900600
C	5.63253900	-2.50129800	-3.26225200
C	5.58574000	0.67991500	0.84145500
C	-1.76088600	-2.57319100	3.71505000
C	1.73299500	-3.20090800	-2.90568200
H	0.67855900	1.78264400	2.70776100
H	7.68667700	1.21977700	3.45441900
H	1.99431700	4.67107500	-0.03636800
H	-0.53482000	-4.11536000	0.40221300
H	-0.33317100	-1.01753000	3.37110500
H	1.85327700	1.89410000	-3.02272500
H	6.20470300	-3.58281900	-1.47337500
H	-1.23421500	4.18263400	-3.74613500
H	4.83811600	-2.22329900	0.03177800
H	3.06624800	-5.55872700	-0.87614000
H	1.37386400	6.62139200	-1.36714800
H	3.26123000	0.55495600	-4.50409200
H	7.50048800	1.59881400	0.99809500
H	5.86631800	0.06039700	4.65923000
H	3.76850600	3.05958800	0.02722000

H	2.01982500	2.57538100	4.62166400
H	5.08639400	3.88009400	1.92694500
H	1.73027300	-1.88110000	3.42933200
H	3.71125500	-1.11411000	4.63475900
H	-2.36513000	-5.17122800	1.63853500
H	2.15137300	-4.04507400	0.83899000
H	4.86386800	-1.27633700	-4.83883400
H	-0.64921700	2.24353100	-2.42293700
H	0.72455900	-1.42544900	-2.23850900
H	6.24506000	-3.11085800	-3.92047000
H	5.51201000	0.86677000	-0.22370100
H	-2.11447900	-2.12442700	4.64042700
H	1.63295500	-2.94091400	-3.95647600
H	-1.08972300	-0.26875500	-1.89615000
H	-0.57750400	0.70408800	1.66462600
C	4.50613100	3.71808600	4.58052200
H	5.31597800	2.99531900	4.73676500
H	4.96767100	4.69507400	4.40168300
H	3.92636700	3.77981600	5.50655400
C	-0.37623100	6.77060500	-3.45973200
H	0.39103200	7.55023400	-3.42366100
H	-0.56065100	6.52106600	-4.50945000
H	-1.30223200	7.19892600	-3.05724600
C	-3.57538400	-4.31475800	3.94194500
H	-4.48037500	-3.74435000	3.69725800
H	-3.74538400	-5.35581200	3.65186500
H	-3.44742800	-4.27947600	5.02889000
C	3.03811200	-5.25335200	-3.58280100
H	4.09878700	-5.00146500	-3.70386700
H	2.97674300	-6.30943600	-3.30061100
H	2.55649600	-5.13091900	-4.55758700
N	-2.19036600	1.72616800	-0.27505400
N	-2.46104200	-0.79788600	0.59665200
C	-3.70467300	-0.01015800	0.41516400
C	-3.36231200	1.48128900	0.57067700
H	-1.93710500	2.71021100	-0.21132500
H	-2.41211100	1.42504800	-1.55350800
H	-4.01407700	-0.15532200	-0.62191700
H	-2.37499000	-1.06982600	1.57352500
H	-2.55120800	-1.67261800	0.07913200
C	-4.79351900	-0.51255500	1.33508200
C	-5.95364100	-1.08423200	0.81532700
C	-4.62993000	-0.46282600	2.72327100
C	-6.93191500	-1.59883800	1.66279500
H	-6.08287700	-1.13383000	-0.26254500
C	-5.60311100	-0.97771900	3.57294500
H	-3.73127500	-0.01883800	3.14703900
C	-6.75915500	-1.54889100	3.04298700
H	-7.83035900	-2.04130600	1.24248100
H	-7.52192600	-1.94877200	3.70483200
C	-4.57309500	2.33095600	0.22420200
C	-5.32696900	2.92401700	1.23732900
C	-4.97978300	2.49454500	-1.10422800
C	-6.46479600	3.66924500	0.93870300
H	-5.02418400	2.79230300	2.27368200
C	-6.11513600	3.24112800	-1.40357400
H	-4.40142400	2.03874200	-1.90419200
C	-6.86143400	3.83102100	-0.38522600
H	-7.03862500	4.12453200	1.74109000
H	-6.41733300	3.36475400	-2.43999600

H	-3.10864600	1.66657400	1.62543400
C	-2.38349600	-2.57416400	-2.12133000
C	-3.28853000	-3.62192700	-1.96344900
C	-4.62612200	-3.44777900	-2.31094300
C	-5.04681300	-2.22264300	-2.82488900
C	-4.14220800	-1.17342000	-2.96795700
C	-2.80295200	-1.33426000	-2.61110800
H	-1.34143400	-2.71559700	-1.84310600
H	-2.94695000	-4.57233100	-1.56184600
H	-5.33581300	-4.25998000	-2.18266200
H	-6.08783300	-2.07889900	-3.10232200
H	-4.46343100	-0.20173500	-3.32971800
C	-1.84267800	-0.14951400	-2.74092100
O	-2.47872700	1.06147600	-2.66746900
C	-1.02375200	-0.25941800	-4.03377700
H	-0.55822700	-1.24564900	-4.14351000
H	-1.68748100	-0.09283900	-4.88850000
H	-0.24026700	0.50533000	-4.04529800
H	-5.46229600	-0.92871100	4.64914200
H	-7.74720200	4.41343000	-0.62325300

A4

Coordinates (Angstroms)

X	Y	Z
Ru	-0.65950400	0.33205800
P	0.73298600	-1.43561300
P	1.12237800	1.74439700
C	2.09293400	2.41140500
C	1.64264400	2.27682400
C	4.10160200	-0.66810500
C	2.44415400	0.89012800
C	6.77405200	0.95882900
C	4.61856600	-0.15497700
C	3.63904700	3.36173300
C	-0.25049800	-2.50233500
C	1.16057400	4.55297300
C	-0.84142900	-3.68034000
C	0.72532400	3.26642200
C	-2.38024800	-3.73793500
C	1.36634200	-2.64703000
C	-0.73116900	-1.96660500
C	2.31708200	-1.02637200
C	3.24624600	-0.09736500
C	2.48637200	1.10825800
C	5.64584400	-2.73709800
C	4.07972500	-0.90407100
C	-0.52082500	4.23409100
C	4.87154800	-1.97013000
C	2.58418300	-4.65857500
C	0.76871600	5.65466000
C	3.28814800	0.36217200
C	6.66946500	1.16871700
C	5.76875400	0.30940500
C	3.32311000	3.04398300
C	2.40869600	2.74112200

C	4.07626700	3.52029600	2.04746300
C	2.48644300	-1.29296500	2.90922400
C	3.59039400	-0.85939400	3.58897300
C	4.49851200	0.07049800	1.52213400
C	2.47092800	-4.37122900	-2.50604600
C	-1.88931400	-4.28251100	2.03815600
C	2.05053500	-3.80637200	-0.18471200
C	4.91621500	-1.47306600	-3.73359900
C	3.31631300	-0.35887400	0.83175700
C	-0.07361900	5.51693200	-2.70516900
C	-0.13676600	3.13158100	-2.27465400
C	1.24532700	-2.36474700	-1.92489800
C	5.67756300	-2.48446900	-3.20904600
C	5.56465300	0.74059100	0.86020800
C	-1.76231100	-2.58002900	3.70996100
C	1.78859300	-3.21541800	-2.88201600
H	0.69607600	1.78098500	2.69765500
H	7.65264000	1.30683800	3.47799800
H	1.80247100	4.71216800	0.01233500
H	-0.51075100	-4.12306800	0.40753200
H	-0.33859000	-1.02022800	3.37246300
H	1.87480600	1.89213600	-3.04120000
H	6.23439500	-3.55133400	-1.40660400
H	-1.19719800	4.08768100	-3.86573000
H	4.84448200	-2.18858600	0.07400500
H	3.11623200	-5.55341200	-0.82642300
H	1.12420200	6.64326000	-1.31950800
H	3.30776700	0.55417100	-4.49636900
H	7.46935700	1.67962100	1.02043600
H	5.83952800	0.13327400	4.68028000
H	3.70862100	3.14441500	-0.02756700
H	2.04538400	2.60517500	4.59319000
H	5.03712700	3.99075600	1.85531600
H	1.73086400	-1.85964900	3.44036900
H	3.69605600	-1.06313300	4.65159900
H	-2.34583400	-5.18253700	1.63341200
H	2.17111900	-4.03847000	0.87077700
H	4.92132700	-1.27310800	-4.80224800
H	-0.55156000	2.16399700	-2.53756700
H	0.76380800	-1.44251900	-2.23408100
H	6.30112200	-3.09472100	-3.85623800
H	5.49189800	0.92501300	-0.20540900
H	-2.12459400	-2.13018200	4.63151100
H	1.70098900	-2.95990400	-3.93514900
H	-1.06368900	-0.36284000	-1.99135000
H	-0.55823100	0.69294100	1.66305300
C	4.50167500	3.80652300	4.51755700
H	5.30597900	3.08062800	4.68732200
H	4.97035200	4.77578500	4.31714000
H	3.92469400	3.89214800	5.44346600
C	-0.52131200	6.71931200	-3.49654900
H	0.22431700	7.51989900	-3.46202600
H	-0.69956500	6.46372200	-4.54576300
H	-1.45800200	7.12286900	-3.09307300
C	-3.56956200	-4.32863500	3.93294500
H	-4.43961500	-3.66876500	3.82716500
H	-3.83655300	-5.30617700	3.52113500
H	-3.37573300	-4.45146600	5.00408400
C	3.12310400	-5.25641900	-3.53505600
H	4.17650700	-4.97578700	-3.65836700

H	3.09121000	-6.31025600	-3.23999400
H	2.63921800	-5.15889800	-4.51159200
N	-2.17677500	1.69573600	-0.30808900
N	-2.46094200	-0.79586800	0.61159300
C	-3.70245400	-0.00584300	0.42470300
C	-3.34361000	1.48563900	0.54468500
H	-1.92650400	2.68231800	-0.27728300
H	-2.40967200	1.29091300	-1.87357900
H	-4.02134200	-0.17075500	-0.60698100
H	-2.36998300	-1.05171900	1.59232100
H	-2.55460000	-1.68001100	0.11135600
C	-4.78628300	-0.48273100	1.36405300
C	-5.96352600	-1.04057600	0.86786600
C	-4.60480700	-0.41755500	2.74960300
C	-6.93902800	-1.52843800	1.73405200
H	-6.10928200	-1.09938500	-0.20732600
C	-5.57525700	-0.90545400	3.61833300
H	-3.69494400	0.01959800	3.15606400
C	-6.74726200	-1.46466700	3.11111800
H	-7.85024600	-1.96069700	1.33080400
H	-7.50757000	-1.84369000	3.78789500
C	-4.55084500	2.33398700	0.17866500
C	-5.30124200	2.95706200	1.17637600
C	-4.96084500	2.46930800	-1.15159300
C	-6.43519500	3.70156500	0.86136400
H	-4.99708100	2.84965100	2.21512200
C	-6.09248700	3.21362900	-1.46944000
H	-4.38903900	1.99219400	-1.94242100
C	-6.83398600	3.83312100	-0.46516800
H	-7.00476600	4.17990200	1.65340300
H	-6.39547200	3.31288800	-2.50833500
H	-3.10653500	1.68934300	1.60284300
C	-2.38480200	-2.66184800	-2.06296600
C	-3.30324200	-3.67975200	-1.81763800
C	-4.64887200	-3.49547200	-2.12825300
C	-5.06394500	-2.29238500	-2.69475100
C	-4.14527400	-1.27143700	-2.92788100
C	-2.79911300	-1.44248500	-2.60639200
H	-1.33602500	-2.80719900	-1.81285900
H	-2.96648900	-4.61334700	-1.37521800
H	-5.36912500	-4.28368200	-1.92979400
H	-6.11114400	-2.14180800	-2.94313400
H	-4.46382000	-0.31694300	-3.33470200
C	-1.80568400	-0.30696900	-2.82935500
O	-2.41558100	0.94247600	-2.84552700
C	-1.02417100	-0.50488400	-4.12824600
H	-0.58071500	-1.50490400	-4.18106800
H	-1.70190600	-0.38136100	-4.97918300
H	-0.22666600	0.24196400	-4.20247900
H	-5.42064600	-0.84283900	4.69197700
H	-7.71667600	4.41470200	-0.71631600

A2u

Coordinates (Angstroms)

X Y Z

Ru	-0.77439400	0.23955500	-0.46776900
P	0.80085100	1.74453200	0.09835100
P	0.76756900	-1.34603800	-0.89252900
C	1.75418100	-1.41529500	-2.44558400
C	1.52001800	-0.49178000	-3.46094100
C	3.97141600	-1.28917300	2.51745600
C	2.12988800	-1.38552600	0.36793200
C	6.56107900	0.25086300	-3.39555200
C	4.56448300	1.41692000	-2.66177300
C	3.34801000	-1.40795500	-4.77011500
C	0.12557000	3.45252800	-0.15660700
C	0.04116300	-3.91182400	-1.93939400
C	-0.01804700	4.38492000	0.87253500
C	-0.00629600	-3.02843300	-0.85881600
C	-1.25958600	5.89780600	-0.56979900
C	1.54399600	1.87128400	1.78046900
C	-0.45777900	3.76061500	-1.39789300
C	2.36415000	1.66467600	-0.90073500
C	3.10768800	-0.39880800	0.37781400
C	2.07327000	-2.32166600	1.43377800
C	5.93833500	0.69937400	2.59291600
C	4.04322200	-0.33379800	1.46772000
C	-1.55367200	-4.55282300	0.23084600
C	5.04849900	0.66833000	1.55020000
C	3.13286700	2.84786000	3.32553300
C	-0.69639900	-5.09576800	-1.93241300
C	2.96350600	-2.28130700	2.46879200
C	6.38103200	-0.68924300	-2.35570200
C	5.66600000	1.27721500	-3.54501900
C	2.78497200	-2.34847200	-2.60958200
C	2.31421000	-0.48747900	-4.60508000
C	3.56102500	-2.35073000	-3.75907600
C	2.58732700	2.60276600	-1.94069800
C	3.64586000	2.48426600	-2.79617300
C	4.37673800	0.47609600	-1.61342100
C	2.79908800	1.90656200	4.30458700
C	-0.70105900	5.58445700	0.66661100
C	2.52690700	2.82235300	2.07779300
C	4.90116900	-1.23152400	3.58703500
C	3.25306500	0.61082500	-0.72782200
C	-1.50104400	-5.43986700	-0.84975500
C	-0.83241000	-3.36748900	0.22597500
C	1.19638700	0.94239700	2.75653600
C	5.87188800	-0.26490200	3.62346500
C	5.31964500	-0.58249800	-1.49467400
C	-1.12435400	4.96070600	-1.60089100
C	1.82317500	0.95924100	3.99960200
H	0.73011200	0.24248300	-3.32061600
H	7.40530300	0.15605300	-4.07271100
H	0.64473100	-3.67656900	-2.80907700
H	0.39417700	4.18236100	1.85526400
H	-0.42016000	3.01696300	-2.18984000
H	1.30924600	-3.09017400	1.43035000
H	6.69676700	1.47569400	2.63019900
H	-2.18340400	-4.78861500	1.08494100
H	5.10187700	1.42568400	0.77673000
H	3.89968000	3.58946500	3.53703400
H	-0.64409600	-5.75814300	-2.79345100
H	2.90520800	-3.01715500	3.26744600
H	7.08650800	-1.50724400	-2.24250400

H	5.78778400	2.00700200	-4.34172500
H	2.99207300	-3.06954500	-1.82181000
H	2.13540500	0.25923900	-5.37546100
H	4.36601000	-3.07464500	-3.86276200
H	1.90544300	3.43649800	-2.05984500
H	3.79629800	3.21519100	-3.58698000
H	-0.79976800	6.28648700	1.49139300
H	2.82992700	3.54162600	1.32035000
H	4.83173400	-1.97649400	4.37616200
H	-0.92888300	-2.66771300	1.05305900
H	0.46668300	0.17833700	2.49663100
H	6.58750600	-0.23519500	4.44037500
H	5.18679400	-1.32428600	-0.71546700
H	-1.56211000	5.16933800	-2.57502100
H	1.57009700	0.20519800	4.74204100
H	-0.97040400	-0.40885600	1.10456400
H	-0.79552900	0.86396600	-2.06583400
C	4.24263500	-1.37626500	-5.98243900
H	5.24316500	-1.02255800	-5.70689200
H	4.35404200	-2.37204400	-6.42602300
H	3.85084100	-0.70368600	-6.75171000
C	-2.30150800	-6.71735400	-0.83392900
H	-2.22618800	-7.24743500	-1.78799300
H	-1.94960300	-7.39427000	-0.04644600
H	-3.36167400	-6.51735900	-0.64220400
C	-1.98325200	7.19957400	-0.80243900
H	-2.95009500	7.03435800	-1.29034900
H	-2.16514000	7.72888600	0.13757100
H	-1.39842600	7.86199400	-1.45166200
C	3.52012400	1.88890000	5.62708600
H	4.50949100	1.43062700	5.51110600
H	3.66637400	2.90074400	6.02005300
H	2.97092700	1.30909600	6.37560100
N	-2.49079300	-0.97558900	-1.09679700
N	-2.45516900	1.60434400	-0.06494000
C	-3.73210200	0.87116000	-0.14130800
C	-3.65120700	-0.09615600	-1.33534700
H	-2.28515000	-1.50931700	-1.93762700
H	-2.70785200	-1.65470000	-0.36984200
H	-3.78606000	0.25684200	0.76083000
H	-2.42108800	2.34669800	-0.76032700
H	-2.38514200	2.06588700	0.83843800
C	-4.94650100	1.77222700	-0.17955600
C	-5.95492000	1.60957300	0.77061700
C	-5.08517200	2.76445800	-1.15321300
C	-7.08180600	2.42722200	0.75286600
H	-5.85272000	0.82762000	1.51967500
C	-6.20957400	3.58292200	-1.17237400
H	-4.31296900	2.90145700	-1.90836400
C	-7.21074600	3.41654800	-0.21752700
H	-7.85981300	2.29023600	1.49825200
H	-8.08861400	4.05590800	-0.23238700
C	-4.94223000	-0.85326000	-1.56563000
C	-5.62717100	-0.71640800	-2.77178500
C	-5.46808000	-1.69363500	-0.57871400
C	-6.81597500	-1.40534400	-2.99828500
H	-5.22980100	-0.05712200	-3.53985500
C	-6.65469100	-2.38309800	-0.80404600
H	-4.96470700	-1.79642400	0.38043200
C	-7.33147400	-2.24252700	-2.01419800

H	-7.33730100	-1.28637200	-3.94362900
H	-7.05537600	-3.02938400	-0.02842700
H	-3.40417000	0.48692300	-2.23052200
C	-3.03385900	-0.83005800	3.11162400
O	-4.03538500	-1.17885300	2.50422400
H	-6.30615000	4.35053300	-1.93483100
H	-8.25981400	-2.77950000	-2.18581500
C	-2.74661900	0.63113700	3.36202700
H	-2.58305400	0.83120000	4.42622900
H	-1.83586200	0.90482200	2.81489200
H	-3.58992300	1.22881300	3.00852200
C	-2.06222500	-1.84976900	3.61189500
C	-0.86114200	-1.49008100	4.22693100
C	-2.35488500	-3.20288500	3.42016400
C	0.05211900	-2.46564300	4.60939600
H	-0.62454100	-0.44485600	4.39046800
C	-1.44865400	-4.17929100	3.81283700
H	-3.29472500	-3.46569000	2.94524200
C	-0.23808300	-3.81093500	4.39824600
H	0.99498400	-2.17507500	5.06247800
H	-1.67700800	-5.22886600	3.65352100
H	0.47686200	-4.57347700	4.69316300

TSAu2-3

Coordinates (Angstroms)

X	Y	Z
Ru	-0.88245600	-0.07857400
P	0.63837400	-1.71602100
P	0.71939000	1.24907200
C	1.50015400	0.90544000
C	0.99198900	-0.06850100
C	4.15758700	1.30359600
C	2.19918500	1.32417900
C	6.15413300	-1.08274400
C	4.16267600	-2.01391200
C	2.74671700	0.37272300
C	-0.29314300	-3.30942800
C	0.31700400	3.72635700
C	-0.66493500	-4.01372500
C	0.16260300	2.99542400
C	-2.28942000	-5.32931100
C	1.52238700	-1.88042600
C	-0.92808400	-3.65260300
C	2.09389400	-1.87664900
C	3.08499300	0.25710600
C	2.28868500	2.37830800
C	5.90439300	-0.86831400
C	4.07607300	0.22812200
C	-1.11051300	4.85287900
C	4.97348700	-0.86213300
C	3.05298400	-3.04151600
C	-0.23154300	5.00136000
C	3.24012300	2.37562200
C	6.14162400	-0.03600100
C	5.18455900	-2.04953400

C	2.63345700	1.62194400	3.09358900
C	1.61254600	-0.33205100	4.76441000
C	3.24030400	1.36551800	4.31392400
C	2.18110400	-2.95734400	1.74654200
C	3.17163300	-3.02042900	2.68578400
C	4.13311000	-0.95458000	1.80897200
C	3.04647400	-1.96662400	-4.27240500
C	-1.64825500	-5.00225600	-1.29269300
C	2.31466900	-2.99485600	-2.20299500
C	5.13148800	1.27220000	-3.12514500
C	3.06935400	-0.88779300	0.84676900
C	-0.94649200	5.58981400	1.56022000
C	-0.57959500	3.57702700	0.26002500
C	1.50175800	-0.81382400	-2.79957900
C	5.99316200	0.21334700	-3.24592300
C	5.16022600	0.02753900	1.87650000
C	-1.89237800	-4.65066900	1.05789300
C	2.26100000	-0.85636800	-3.96475900
H	0.11952500	-0.63440600	3.23241800
H	6.93362700	-1.11938900	4.53641500
H	0.85346800	3.30402600	3.31782200
H	-0.20699700	-3.77537600	-2.29610200
H	-0.70921000	-3.08463200	1.91059300
H	1.58404200	3.20114000	-0.95752100
H	6.57564700	-1.71545100	-2.44776500
H	-1.67419500	5.28036400	-0.44275000
H	4.90881900	-1.70692200	-0.65826200
H	3.66263700	-3.91535800	-3.59575100
H	-0.10141300	5.54300200	3.53565700
H	3.28448900	3.19137500	-2.69707200
H	6.91194300	0.72874800	2.86286200
H	5.18287200	-2.86282600	4.46100200
H	3.05653600	2.37686100	2.43494100
H	1.21245900	-1.11109600	5.40935700
H	4.13141900	1.92019900	4.59735900
H	1.44941000	-3.75503900	1.70145400
H	3.21017800	-3.84943900	3.38808400
H	-1.92977300	-5.51474600	-2.20958100
H	2.35888500	-3.82879700	-1.50613200
H	5.17762800	2.10643800	-3.82102200
H	-0.74869400	3.00302800	-0.64485600
H	0.92335900	0.06920400	-2.53798300
H	6.74039400	0.20005800	-4.03435400
H	5.15381000	0.84679100	1.16684400
H	-2.37119700	-4.88556100	2.00608200
H	2.27026200	0.00325900	-4.63093100
H	-0.89427900	0.72328900	-1.48402600
H	-1.11332700	-0.78610800	1.62831300
C	3.45192100	0.05806500	6.45941500
H	4.39954900	-0.45639600	6.26088500
H	3.68423300	0.97064300	7.01935600
H	2.84478700	-0.58855400	7.10043100
C	-1.54286400	6.96806200	1.69209400
H	-2.62702800	6.94378700	1.53409100
H	-1.35645900	7.39294500	2.68279500
H	-1.12125200	7.65344700	0.94766100
C	-3.41540500	-6.32896600	-0.05773900
H	-4.38184800	-5.81345000	-0.12507500
H	-3.35678900	-7.03814700	-0.88897100
H	-3.40998000	-6.89814800	0.87763900

C	3.91237600	-1.98022800	-5.50486400
H	4.86168800	-1.46934600	-5.30324900
H	4.14307900	-3.00163800	-5.82361900
H	3.43022400	-1.46225000	-6.34024500
N	-2.59017900	1.19150300	0.56507400
N	-2.57480300	-1.31672800	-0.50908000
C	-3.88538000	-0.65453100	-0.32654900
C	-3.77218500	0.35058500	0.83425600
H	-2.45463900	1.85281200	1.32610900
H	-2.74666100	1.72991100	-0.29803700
H	-4.07026500	-0.06288200	-1.22824700
H	-2.52951200	-2.15361600	0.06722700
H	-2.48924100	-1.64374400	-1.46808600
C	-5.00066800	-1.65718700	-0.12462800
C	-6.11958300	-1.65958100	-0.95571600
C	-4.91726600	-2.60860300	0.89683500
C	-7.13097200	-2.60144600	-0.78234600
H	-6.20067700	-0.91190100	-1.74045700
C	-5.92304100	-3.55303600	1.07095400
H	-4.05833700	-2.61628900	1.56522000
C	-7.03290800	-3.55382600	0.22761700
H	-7.99553800	-2.59100800	-1.43957300
H	-7.81886000	-4.29132900	0.36113400
C	-5.06032200	1.12828700	1.01239800
C	-5.85214600	0.91324000	2.13985500
C	-5.49154500	2.03868600	0.04166600
C	-7.05578600	1.59291600	2.30471800
H	-5.52722300	0.19779100	2.89139100
C	-6.69316500	2.72023500	0.20788100
H	-4.88897200	2.20800300	-0.84802600
C	-7.47832700	2.50002400	1.33801700
H	-7.66136600	1.41323600	3.18829400
H	-7.01911800	3.42607000	-0.55077100
H	-3.55322100	-0.20315500	1.75337900
C	-1.96729100	1.38165700	-2.74295300
O	-2.96041900	1.86620400	-2.15561200
H	-5.84285100	-4.28760100	1.86739200
H	-8.41696500	3.03217900	1.46284600
C	-2.12470600	0.06614700	-3.50037400
H	-1.22979400	-0.55911700	-3.46828100
H	-2.97415400	-0.48306500	-3.08977500
H	-2.35913400	0.29093400	-4.54936500
C	-0.92934000	2.33733500	-3.29442300
C	0.08351800	1.93854200	-4.16955700
C	-1.04705700	3.69355600	-2.98549300
C	0.99832700	2.86167400	-4.66536200
H	0.16108000	0.90156500	-4.47557900
C	-0.12957800	4.61889600	-3.46969800
H	-1.88383500	4.00248300	-2.36786100
C	0.90556600	4.20386700	-4.30505600
H	1.78514600	2.53090200	-5.33820000
H	-0.23074700	5.66815700	-3.20675800
H	1.62208000	4.92486800	-4.68861500

A3u

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.84689000	-0.17243800	0.09811500
P	0.73064200	-1.66987500	-0.66557500
P	0.73827100	1.04095200	1.23690900
C	1.50932300	0.40790900	2.77806700
C	1.00907100	-0.72623500	3.41360500
C	4.13892700	1.72460600	-1.89203300
C	2.20625800	1.33804200	0.14090000
C	6.23513600	-1.57374100	3.47249400
C	4.27414500	-2.38241000	2.29569200
C	2.74506900	-0.60817800	5.10395800
C	-0.12833400	-3.29288300	-0.83696500
C	0.30637700	3.25599800	3.01900400
C	-0.42106000	-3.84147800	-2.08692100
C	0.14484400	2.71064000	1.74218600
C	-1.96476000	-5.43966800	-1.09951600
C	1.55803300	-1.44990700	-2.28354500
C	-0.75862500	-3.85345200	0.28643600
C	2.19667500	-1.98357200	0.41924400
C	3.10586400	0.31804300	-0.14321100
C	2.28051900	2.55566700	-0.58532800
C	5.93995800	-0.32309200	-2.52129600
C	4.08652500	0.49771800	-1.17650700
C	-1.14796300	4.67434900	1.12775400
C	5.01352800	-0.52099400	-1.53074100
C	3.15724900	-2.09819900	-3.97512600
C	-0.24849600	4.49303500	3.33724300
C	3.21595600	2.74499700	-1.56368600
C	6.17759400	-0.37474700	2.72514700
C	5.30252800	-2.55431800	3.25883400
C	2.63014100	1.04013100	3.33115800
C	1.62253800	-1.22802800	4.55779100
C	3.23087800	0.54401500	4.47868500
C	2.32588800	-3.20624700	1.12715200
C	3.32182100	-3.39739700	2.04387800
C	4.20038700	-1.17284900	1.55440600
C	2.94125500	-0.90501900	-4.67322100
C	-1.32757900	-4.89480600	-2.21202800
C	2.48419300	-2.36664700	-2.79107400
C	5.10574700	1.90122800	-2.91559600
C	3.13259200	-0.97769400	0.61607400
C	-0.97412600	5.22735300	2.39888800
C	-0.61057900	3.43530100	0.81090700
C	1.32170500	-0.27448800	-2.98900300
C	5.99334000	0.90343600	-3.22204100
C	5.18942900	-0.17917200	1.79608000
C	-1.64465400	-4.91353100	0.15736300
C	2.00504600	-0.00278900	-4.16838200
H	0.14765100	-1.23161000	2.98997000
H	7.02073700	-1.71501500	4.20915700
H	0.85228800	2.71463300	3.78362000
H	0.03649900	-3.43035600	-2.98116900
H	-0.59039200	-3.41797300	1.26727200
H	1.57931100	3.35314000	-0.36877100
H	6.63493800	-1.11772600	-2.77590000
H	-1.71620500	5.20694500	0.37007400
H	4.97521600	-1.47369900	-1.01501800
H	3.88267200	-2.81410400	-4.35412200
H	-0.11396700	4.89164200	4.34017100

H	3.25085200	3.68789700	-2.10283100
H	6.92005900	0.39972700	2.89353900
H	5.33808200	-3.48445400	3.82063900
H	3.05088600	1.91631900	2.84383400
H	1.22671400	-2.12707800	5.02397900
H	4.11250600	1.03838800	4.87854600
H	1.62519600	-4.01040000	0.93732900
H	3.39668900	-4.33837500	2.58298400
H	-1.55133600	-5.28598100	-3.20140400
H	2.68867200	-3.28791300	-2.25044100
H	5.13011300	2.84823900	-3.44889500
H	-0.79428300	3.02752100	-0.17691500
H	0.61820000	0.44372900	-2.58171300
H	6.73643500	1.04981100	-4.00085500
H	5.14922300	0.75324400	1.24472000
H	-2.12301200	-5.32138300	1.04501800
H	1.81965000	0.93190600	-4.69284600
H	-1.15637400	1.20760500	-1.63183800
H	-0.96247100	-1.11834400	1.35724100
C	3.44583600	-1.17134700	6.31307400
H	4.43671500	-1.54972000	6.03591700
H	3.58931000	-0.40568900	7.08358600
H	2.88136700	-1.99693300	6.75665700
C	-1.54490500	6.58130900	2.73444000
H	-1.66860400	6.70928600	3.81417700
H	-0.88251800	7.38002500	2.37907300
H	-2.51983800	6.72911100	2.25922300
C	-3.01085700	-6.51476800	-1.23518000
H	-4.01190700	-6.08199000	-1.11463700
H	-2.96831300	-6.99622900	-2.21639000
H	-2.89157300	-7.28835500	-0.46910600
C	3.73735200	-0.58012900	-5.90976700
H	4.65767900	-0.05086100	-5.63417600
H	4.02373300	-1.48556600	-6.45413100
H	3.17381000	0.06590100	-6.58989600
N	-2.56860200	0.92836700	0.74787900
N	-2.49758300	-1.28969900	-0.79844400
C	-3.83941900	-0.77914800	-0.40636300
C	-3.70956700	0.00677200	0.91355000
H	-2.46630900	1.51248800	1.57463400
H	-2.79077200	1.54173400	-0.10152100
H	-4.11300300	-0.04670400	-1.17139700
H	-2.39007700	-2.25609700	-0.49800700
H	-2.44107100	-1.31341500	-1.81483000
C	-4.85827900	-1.89173100	-0.31435500
C	-6.04799700	-1.83398200	-1.03859500
C	-4.62243400	-2.99974700	0.50587000
C	-6.97838200	-2.86736600	-0.95798000
H	-6.24821200	-0.96626200	-1.66126200
C	-5.54501600	-4.03757100	0.58354700
H	-3.70727600	-3.05455600	1.09209800
C	-6.72686100	-3.97449800	-0.15244100
H	-7.90216900	-2.80657500	-1.52573100
H	-7.45209000	-4.78063600	-0.09153100
C	-5.01247500	0.70691200	1.24928900
C	-5.77909100	0.28456200	2.33500800
C	-5.47678200	1.76070500	0.45295000
C	-6.99194600	0.90179400	2.63177900
H	-5.42770100	-0.54133500	2.94950800
C	-6.68761000	2.37641900	0.75249900

H	-4.88685600	2.09122600	-0.40067000
C	-7.44823500	1.95122000	1.84024600
H	-7.57834500	0.56175700	3.48073000
H	-7.04071300	3.19334600	0.12929900
H	-3.46098900	-0.69348400	1.71961500
C	-1.95611300	1.79337300	-2.26258000
O	-3.11925000	1.90103200	-1.61679100
H	-5.34546100	-4.89188200	1.22485700
H	-8.39364600	2.43542900	2.06826400
C	-2.07180800	0.99809900	-3.58066800
H	-1.11261800	0.85752800	-4.09184000
H	-2.51014500	0.01266800	-3.38422100
H	-2.75209900	1.53407100	-4.25090500
C	-1.29570500	3.15744700	-2.55126300
C	0.00446100	3.29768600	-3.04058900
C	-2.04654000	4.31066200	-2.32305200
C	0.54424300	4.55700800	-3.28822800
H	0.61950400	2.41924900	-3.21248100
C	-1.51245700	5.57310700	-2.56959000
H	-3.05048700	4.17539000	-1.93350600
C	-0.21216600	5.70265800	-3.05160300
H	1.55805200	4.64404700	-3.67159100
H	-2.11215200	6.46079000	-2.38302500
H	0.20934000	6.68586300	-3.24130600

TSAu3-4

Coordinates (Angstroms)

X	Y	Z
Ru	-0.86582600	-0.18834400
P	0.72234500	-1.66936600
P	0.70250500	0.99590800
C	1.47617200	0.31000000
C	0.96870700	-0.83873900
C	4.10079500	1.77741000
C	2.17309600	1.32677500
C	6.23864100	-1.64733100
C	4.28105200	-2.44084600
C	2.70725800	-0.78026400
C	-0.13722100	-3.29016600
C	0.30686500	3.15912300
C	-0.44551600	-3.81362500
C	0.12644800	2.65462600
C	-1.99054700	-5.42078700
C	1.55396900	-1.43430100
C	-0.76001700	-3.86952500
C	2.19251300	-2.00726000
C	3.07661300	0.31882500
C	2.24391300	2.56467500
C	5.89529800	-0.25148300
C	4.05181500	0.53007800
C	-1.14066100	4.65718700
C	4.97586900	-0.47790400
C	3.15070300	-2.07976300
C	-0.22627000	4.39376300
C	3.17787400	2.78602700

C	6.16491300	-0.42650300	2.71817400
C	5.31621700	-2.63132100	3.18719800
C	2.60202300	0.91760100	3.37073200
C	1.58014600	-1.37728500	4.53317100
C	3.20048500	0.38552000	4.50363300
C	2.33671600	-3.24938000	1.04881200
C	3.33789100	-3.45753400	1.95620300
C	4.19100700	-1.20965400	1.53186000
C	2.95290800	-0.87488100	-4.69105000
C	-1.36010200	-4.85862600	-2.28528400
C	2.47021100	-2.35468300	-2.83012100
C	5.06175400	1.98433100	-2.85414500
C	3.11726900	-0.99756900	0.60437400
C	-0.95310700	5.16558900	2.59481900
C	-0.62537300	3.42076100	0.94742600
C	1.33537100	-0.24688600	-3.00338800
C	5.94605000	0.99551400	-3.19681100
C	5.17084800	-0.21353300	1.79928500
C	-1.65456000	-4.92102900	0.08598300
C	2.02623500	0.03191500	-4.17688400
H	0.10125600	-1.32386300	2.97013800
H	7.02851100	-1.80248800	4.15706200
H	0.85519500	2.58987000	3.88045400
H	0.00729000	-3.38938800	-3.03907200
H	-0.57799700	-3.45620400	1.21479500
H	1.54199400	3.35464700	-0.25471000
H	6.58705500	-1.03923700	-2.81626200
H	-1.70369700	5.22562900	0.57150300
H	4.94048700	-1.44541200	-1.05484600
H	3.86848500	-2.79982500	-4.39432100
H	-0.07289300	4.76020400	4.51318200
H	3.20910700	3.74460400	-1.97939700
H	6.89981400	0.35032800	2.90755100
H	5.36536400	-3.57836300	3.71901800
H	3.02813700	1.80459800	2.90831700
H	1.17740700	-2.28520000	4.97575300
H	4.08509200	0.86332500	4.91673800
H	1.64310700	-4.05435400	0.83685100
H	3.42475700	-4.41322900	2.46689300
H	-1.59519400	-5.22970700	-3.27987900
H	2.66133400	-3.28557700	-2.30128000
H	5.08379500	2.94706200	-3.35869000
H	-0.82289500	3.04743700	-0.05022500
H	0.64440300	0.47941600	-2.58878200
H	6.68441400	1.16476700	-3.97549400
H	5.11822200	0.73442900	1.27617300
H	-2.12647900	-5.34310100	0.97044700
H	1.85701300	0.97623100	-4.68955300
H	-1.05254200	1.32389400	-1.66250500
H	-0.98522700	-1.16009400	1.32899100
C	3.40743900	-1.38948100	6.28302800
H	4.33392200	-1.88137700	5.96409500
H	3.67815200	-0.62774500	7.02186200
H	2.78155800	-2.13740700	6.77909400
C	-1.55382900	6.48875300	2.99479900
H	-1.09656900	6.87787200	3.90961000
H	-1.42740900	7.23686100	2.20514600
H	-2.63009800	6.38566700	3.17772200
C	-3.04468000	-6.48667700	-1.32385300
H	-4.04281400	-6.04755700	-1.20178400

H	-3.00383000	-6.96081100	-2.30876300
H	-2.93275000	-7.26711400	-0.56370500
C	3.76031800	-0.54028300	-5.91757500
H	4.67508300	-0.00812900	-5.62885800
H	4.05671000	-1.44142900	-6.46358700
H	3.20162500	0.10709200	-6.60055200
N	-2.56428500	0.92323100	0.66402100
N	-2.50606100	-1.28975300	-0.84635300
C	-3.84976000	-0.77268100	-0.46717500
C	-3.70629000	0.02155400	0.84800300
H	-2.47857900	1.52762500	1.47837900
H	-2.78598900	1.62148000	-0.44067100
H	-4.13121700	-0.05218600	-1.23974300
H	-2.40293300	-2.25079200	-0.52696500
H	-2.43887300	-1.34042800	-1.86117000
C	-4.87295500	-1.88141100	-0.37730500
C	-6.06861300	-1.81408700	-1.09097000
C	-4.63870900	-2.99340600	0.43812700
C	-7.00554900	-2.84114200	-1.00627600
H	-6.27050300	-0.94240300	-1.70782000
C	-5.56766800	-4.02522400	0.51958100
H	-3.72115900	-3.05519200	1.01958400
C	-6.75491600	-3.95267600	-0.20670100
H	-7.93387200	-2.77147600	-1.56556600
H	-7.48484600	-4.75427800	-0.14239800
C	-5.01028800	0.72431100	1.18582200
C	-5.80017000	0.26742500	2.24140500
C	-5.46028400	1.81084200	0.42722800
C	-7.01486700	0.87869300	2.54255500
H	-5.46263500	-0.58304400	2.82954200
C	-6.67302000	2.42219500	0.72846600
H	-4.85951900	2.17654100	-0.40150500
C	-7.45447900	1.96029500	1.78568400
H	-7.61606400	0.50905400	3.36860500
H	-7.01062200	3.26539800	0.13193400
H	-3.49412300	-0.69906800	1.65156100
C	-1.82317800	1.93095900	-2.23722500
O	-2.97745000	2.04583900	-1.51214300
H	-5.36861800	-4.88247000	1.15709000
H	-8.40096000	2.44088900	2.01701500
C	-2.06514200	1.18572600	-3.55747800
H	-1.14487000	1.04335300	-4.13451600
H	-2.50550700	0.20333000	-3.35516500
H	-2.77559900	1.75515400	-4.16529100
C	-1.17505800	3.29244600	-2.51171900
C	0.10439100	3.41372300	-3.05738000
C	-1.88968300	4.45492200	-2.22240900
C	0.65932600	4.66611000	-3.30427800
H	0.68922300	2.52451300	-3.27539500
C	-1.33743600	5.71005800	-2.46556800
H	-2.87801200	4.34253000	-1.78916200
C	-0.05945000	5.82162700	-3.00712600
H	1.65615700	4.73955100	-3.73171800
H	-1.90703500	6.60558800	-2.23038100
H	0.37457400	6.79949600	-3.19511500

A4u

Coordinates (Angstroms)

X	Y	Z	

Ru	-0.87949300	-0.19918700	0.10410300
P	0.70979600	-1.66995000	-0.71362700
P	0.68643600	0.97578900	1.29682500
C	1.45196500	0.28668800	2.81751000
C	0.94354500	-0.86540300	3.41390300
C	4.12389000	1.76739200	-1.77705800
C	2.16928000	1.30911000	0.22439500
C	6.18877200	-1.71892100	3.45987300
C	4.23682300	-2.49036900	2.24313500
C	2.67484400	-0.81124000	5.11262200
C	-0.15700300	-3.28424200	-0.93879500
C	0.28198500	3.13684900	3.15350400
C	-0.47112900	-3.78273800	-2.20480100
C	0.11727000	2.63860000	1.85834100
C	-2.02826700	-5.39529600	-1.26223500
C	1.56502600	-1.43090900	-2.32091900
C	-0.78415800	-3.87932300	0.16876800
C	2.16842000	-2.02917800	0.36945000
C	3.06846900	0.29797800	-0.09284300
C	2.26026000	2.55493200	-0.45126800
C	5.90380200	-0.27110300	-2.48799500
C	4.05561000	0.51247000	-1.11366100
C	-1.11794200	4.65797900	1.30456500
C	4.97293300	-0.50015000	-1.50845300
C	3.16674600	-2.08465100	-4.01150200
C	-0.24113900	4.37698400	3.51112400
C	3.20712400	2.78012300	-1.41105900
C	6.12638500	-0.49041300	2.76260500
C	5.26332600	-2.69570700	3.20189700
C	2.57404600	0.89385900	3.39429000
C	1.55099100	-1.40764100	4.54246400
C	3.16859400	0.35794200	4.52746400
C	2.30226800	-3.27907700	1.02752600
C	3.29286100	-3.50037200	1.94357300
C	4.15810100	-1.25152700	1.55270800
C	2.99839100	-0.86817100	-4.68088300
C	-1.39436400	-4.81761500	-2.36006400
C	2.46932100	-2.36113200	-2.84314400
C	5.09687700	1.97733700	-2.78843600
C	3.09418600	-1.02564600	0.61699200
C	-0.93872600	5.16334000	2.59449300
C	-0.61361800	3.41537800	0.95012200
C	1.37788000	-0.23041500	-2.99984400
C	5.97397000	0.98359500	-3.13533000
C	5.14022900	-0.26298300	1.83870000
C	-1.68704600	-4.92111900	0.00956000
C	2.08504600	0.05009200	-4.16311700
H	0.07855000	-1.34983800	2.97352400
H	6.97235700	-1.88579600	4.19328700
H	0.80719500	2.55617900	3.90339000
H	-0.01579700	-3.34654100	-3.08844300
H	-0.59926600	-3.48581300	1.16411000
H	1.56481300	3.34935900	-0.20666100
H	6.58985800	-1.06255500	-2.77475400
H	-1.66756600	5.23325200	0.56408300
H	4.92318900	-1.47281800	-1.03292500
H	3.87443200	-2.81349900	-4.39944700

H	-0.10373300	4.73593800	4.52851500
H	3.25435800	3.74544100	-1.90802500
H	6.86323900	0.28097600	2.96606900
H	5.30367300	-3.64840400	3.72427700
H	3.00011900	1.78394700	2.93778700
H	1.14758900	-2.31781600	4.97977600
H	4.05033000	0.83566800	4.94679900
H	1.60950400	-4.08000600	0.79823200
H	3.37134900	-4.46203000	2.44438000
H	-1.63325700	-5.16815900	-3.36125800
H	2.63719900	-3.30237500	-2.32486500
H	5.13418900	2.94609500	-3.28045400
H	-0.80529700	3.04300000	-0.04890500
H	0.69994900	0.50563700	-2.58111900
H	6.72128100	1.15477000	-3.90501900
H	5.09598200	0.69067300	1.32529600
H	-2.16129800	-5.35542100	0.88685300
H	1.93995800	1.00420300	-4.66510900
H	-1.01805300	1.35666600	-1.71059200
H	-0.97415400	-1.19735400	1.31298400
C	3.37092700	-1.42503700	6.29968100
H	4.29266000	-1.92548200	5.98024400
H	3.64904000	-0.66486700	7.03734900
H	2.73904300	-2.16695900	6.79720700
C	-1.47508600	6.52011600	2.97304400
H	-1.58990500	6.61885300	4.05677000
H	-0.79669600	7.31390000	2.63720900
H	-2.44951000	6.70399500	2.50922000
C	-3.09066800	-6.45046900	-1.42601200
H	-4.08568200	-6.00522400	-1.30044600
H	-3.05092400	-6.91196300	-2.41699100
H	-2.98697400	-7.24169600	-0.67595400
C	3.82191500	-0.53371500	-5.89671800
H	4.73608900	-0.00743200	-5.59584200
H	4.11960500	-1.43451000	-6.44253300
H	3.27481000	0.11912300	-6.58395300
N	-2.55275900	0.90804800	0.67421400
N	-2.52657400	-1.28141000	-0.85341800
C	-3.86494500	-0.75795900	-0.46439300
C	-3.70271200	0.02459900	0.85649200
H	-2.46411100	1.50579900	1.49310800
H	-2.79468600	1.70852500	-0.65512900
H	-4.14701700	-0.03179700	-1.23161400
H	-2.42742200	-2.24507500	-0.54065200
H	-2.46386400	-1.32816500	-1.86862000
C	-4.89734400	-1.85877900	-0.38109900
C	-6.10486300	-1.76350600	-1.07155700
C	-4.66337600	-2.98940700	0.40841100
C	-7.05300300	-2.78041800	-0.99022800
H	-6.30742700	-0.87702700	-1.66683000
C	-5.60324400	-4.01171600	0.48558300
H	-3.73735800	-3.07382200	0.97311700
C	-6.80214800	-3.91082500	-0.21768900
H	-7.99027900	-2.68783800	-1.53097900
H	-7.54033500	-4.70507100	-0.15658600
C	-4.99880500	0.74101600	1.20155400
C	-5.82062300	0.25358200	2.21893700
C	-5.41534100	1.86892500	0.48648300
C	-7.03022900	0.87317900	2.52288700
H	-5.51124700	-0.62929600	2.77378500

C	-6.62291300	2.48991300	0.78909200
H	-4.79627600	2.26209800	-0.31424500
C	-7.43502900	1.99605000	1.80774200
H	-7.65543500	0.47782000	3.31871400
H	-6.93210100	3.36544100	0.22447800
H	-3.51557100	-0.71568500	1.65203400
C	-1.74814100	1.96091500	-2.31245000
O	-2.94908500	2.05743700	-1.62612400
H	-5.40315400	-4.88421200	1.10173300
H	-8.37739200	2.48350600	2.04147400
C	-1.95923100	1.23012600	-3.64087800
H	-1.02525300	1.11267500	-4.20000700
H	-2.38162100	0.23679900	-3.45610500
H	-2.66758100	1.79396000	-4.25605200
C	-1.11534900	3.33253900	-2.54213600
C	0.17959400	3.46480000	-3.04769900
C	-1.84264900	4.48761300	-2.25513900
C	0.73721100	4.72203400	-3.25870200
H	0.77292500	2.58007400	-3.26123200
C	-1.28645000	5.74764900	-2.46269400
H	-2.84390700	4.37290700	-1.85392700
C	0.00608300	5.87065800	-2.96487100
H	1.74584500	4.80477400	-3.65521300
H	-1.86540600	6.63757800	-2.23000100
H	0.44210700	6.85242400	-3.12534000

A5

Coordinates (Angstroms)

X	Y	Z
Ru	1.02474400	0.03784400
P	-0.42530500	-1.66326100
P	-0.63979200	1.60841600
C	-1.78229500	1.95730400
C	-1.59438800	1.35380600
C	-3.42555000	0.52845400
C	-1.86219600	1.25372000
C	-6.54363800	0.21161900
C	-4.44655600	-0.97377700
C	-3.61622200	2.38559000
C	0.20983100	-3.30520800
C	-0.25152100	4.43447000
C	0.34491500	-4.41991600
C	0.00908900	3.28530100
C	1.41655300	-5.69830000
C	-0.83609700	-1.99164700
C	0.71584400	-3.40455900
C	-2.10013900	-1.49728800
C	-2.78318900	0.21940100
C	-1.75293600	1.94526700
C	-5.28961000	-1.54924500
C	-3.59095300	-0.14852700
C	1.52781000	4.59961200
C	-4.55039500	-1.19749100
C	-2.12365100	-3.07464700
C	0.36254400	5.64624100

C	-2.49629100	1.59211400	3.34187300
C	-6.30955900	0.90013200	-1.40135300
C	-5.62635100	-0.70093200	-3.06497300
C	-2.88975300	2.79627100	-1.57318200
C	-2.50521600	1.56227800	-4.02096700
C	-3.78439600	3.01417000	-2.60985000
C	-2.38173000	-2.19725300	-2.02773700
C	-3.50665400	-1.93940300	-2.75940300
C	-4.20062800	-0.27839000	-1.11182100
C	-1.47846000	-2.31982900	4.44575300
C	0.93898800	-5.59312800	-0.24955000
C	-1.81492300	-2.90857200	2.11842000
C	-4.19497300	0.13602400	4.39572200
C	-2.99783400	-0.54121200	-0.37168500
C	1.25806100	5.75221800	0.70062000
C	0.92325600	3.39071600	1.13375500
C	-0.17590200	-1.25432700	2.70029300
C	-5.10935600	-0.88016900	4.30226500
C	-5.16916200	0.66757400	-0.67744900
C	1.29574400	-4.57843200	-2.38410500
C	-0.49630400	-1.41499500	4.04529500
H	-0.74309300	0.69670100	-3.13172900
H	-7.45002900	0.40549800	-3.17955900
H	-0.92990500	4.39542500	-1.51967800
H	-0.00230400	-4.37971000	1.24052100
H	0.66588000	-2.53634000	-2.57557300
H	-1.06461000	2.77712200	2.33514700
H	-6.01615700	-2.35314500	2.99622500
H	2.24304200	4.64359500	2.26372200
H	-4.68936300	-1.73283700	1.03896200
H	-2.90371700	-3.77465900	3.74957900
H	0.14140000	6.52358200	-0.96440400
H	-2.38264300	2.13178500	4.27882900
H	-7.03458600	1.62671900	-1.04663900
H	-5.79190900	-1.23684600	-3.99634100
H	-3.06315800	3.26806100	-0.60900100
H	-2.35313800	1.06288900	-4.97480800
H	-4.64738500	3.65562100	-2.44849200
H	-1.68950300	-2.95506500	-2.37584400
H	-3.69706800	-2.48408800	-3.68089900
H	1.03288700	-6.44051500	0.42551300
H	-2.35982500	-3.47681800	1.36807100
H	-4.04601500	0.66147200	5.33584000
H	1.19040100	2.49960800	1.69363400
H	0.56874100	-0.52223800	2.39468800
H	-5.69814800	-1.17012000	5.16791900
H	-4.99468400	1.21851900	0.23959700
H	1.67325000	-4.62502400	-3.40336700
H	0.01232100	-0.81042500	4.79236700
H	0.50755100	-0.36624200	-2.00016500
C	-4.63398200	2.57385400	-4.94275400
H	-5.56947100	2.06435600	-4.68342100
H	-4.86485500	3.63370200	-5.09660900
H	-4.27999300	2.16199000	-5.89279700
C	1.94256500	7.05426400	1.03033800
H	1.59083700	7.86571500	0.38637900
H	1.76034500	7.34456000	2.07120700
H	3.02745200	6.96751500	0.90080500
C	2.04349400	-6.97013700	-2.06527100
H	3.01981000	-6.77572400	-2.52269900

H	2.18620200	-7.69807600	-1.26123000
H	1.41242800	-7.43708000	-2.83055500
C	-1.86863500	-2.46773500	5.89388200
H	-2.91489100	-2.17466000	6.03847300
H	-1.76611700	-3.50542600	6.23125300
H	-1.24928900	-1.83966000	6.54134500
N	2.53186700	1.33160300	-0.35090100
N	2.77862100	-1.24094000	-0.80347800
C	3.96240200	-0.58456400	-0.20513800
C	3.88990000	0.90448600	-0.60039400
H	2.45459800	2.33836300	-0.46332700
H	3.80990400	-0.62861400	0.87890700
H	2.89121200	-1.31663200	-1.81282100
H	2.68805600	-2.19529300	-0.46001100
C	5.27660200	-1.24769700	-0.55584200
C	6.18888800	-1.56850300	0.44960300
C	5.62847400	-1.50477300	-1.88413300
C	7.42056200	-2.13906100	0.14125700
H	5.93653600	-1.35342800	1.48475400
C	6.85629900	-2.07856200	-2.19753700
H	4.94599600	-1.24280400	-2.68994500
C	7.75656500	-2.39878200	-1.18406100
H	8.11890800	-2.37918000	0.93755100
H	8.71588300	-2.84609100	-1.42678800
C	4.92977600	1.70142300	0.17382800
C	6.20458100	1.91932900	-0.35066900
C	4.63058600	2.20179400	1.44250900
C	7.16284900	2.62109000	0.37510200
H	6.44967900	1.52554000	-1.33431100
C	5.58496300	2.90580900	2.17080800
H	3.63327600	2.03701200	1.83966100
C	6.85512500	3.11814600	1.63889600
H	8.14991300	2.78214100	-0.04921100
H	5.33728800	3.29280600	3.15585800
H	4.15985100	0.96674000	-1.67338600
H	7.11206500	-2.27088100	-3.23551400
H	7.59954100	3.67098500	2.20504300

C1

Coordinates (Angstroms)

X	Y	Z
Ru	-0.73690900	-0.00615100
P	0.83135500	-1.62491400
P	0.81345800	1.62722600
C	1.68712700	2.25719500
C	1.39918100	1.70780000
C	4.27734500	0.43192800
C	2.27032500	1.24522500
C	6.31699500	0.98091000
C	4.37534100	-0.39386200
C	3.15429300	3.02986200
C	0.12845800	-3.18266000
C	0.02460000	4.38485600
C	0.11466700	-4.40662300
C	0.06416700	3.17371300

C	-1.23668300	-5.42949000	1.84755200
C	1.66154100	-2.24610800	-1.46852200
C	-0.57470900	-3.09805400	1.99028500
C	2.31872000	-1.22789500	1.09440100
C	3.21157300	0.30534100	-0.71948200
C	2.34675700	1.79114200	-2.42649700
C	6.18190400	-1.47063900	-2.18009000
C	4.23345700	-0.11710100	-1.63669000
C	-1.37059600	4.17468600	-2.41881100
C	5.21608400	-1.08415100	-1.28787300
C	3.35768900	-3.58369500	-2.56340500
C	-0.70012700	5.47097900	-0.52633800
C	3.31216000	1.40024800	-3.31136500
C	6.23465200	1.52741500	2.02998500
C	5.40240500	0.04299200	3.73208800
C	2.70401900	3.21402400	1.36791300
C	2.13185600	2.08610300	3.83180800
C	3.41699800	3.60224500	2.49308000
C	2.44059200	-1.77038000	2.40022300
C	3.43058000	-1.36976300	3.25318500
C	4.28528800	0.15238700	1.54764700
C	3.01932500	-3.04272900	-3.80648400
C	-0.55940800	-5.50820400	0.63367300
C	2.69917300	-3.18214600	-1.40884500
C	5.28440400	0.00986600	-3.85246200
C	3.23823900	-0.28058000	0.66401400
C	-1.40429900	5.38985900	-1.72459700
C	-0.66216600	3.08685600	-1.92758300
C	1.30076900	-1.72492300	-2.70977300
C	6.22153300	-0.91797300	-3.47997200
C	5.24680800	1.12859700	1.16729500
C	-1.23245400	-4.20054000	2.51768400
C	1.97745600	-2.11601000	-3.86070300
H	0.62451700	0.94680400	2.77243600
H	7.10148600	1.30660500	4.00747500
H	0.54843200	4.49130900	0.90956200
H	0.62160900	-4.51233700	-0.84796200
H	-0.62536400	-2.13634600	2.49582000
H	1.62579000	2.54054200	-2.73153400
H	6.91807200	-2.21373200	-1.88820800
H	-1.91780300	4.07694100	-3.35442400
H	5.18744000	-1.53277500	-0.30168700
H	4.16961900	-4.30400200	-2.49657800
H	-0.71733000	6.39779500	0.04250900
H	3.35193800	1.83655500	-4.30649900
H	6.95462500	2.27677300	1.71428100
H	5.45108000	-0.38608600	4.72997400
H	2.95676900	3.64020900	0.39947200
H	1.92187400	1.61626700	4.79001800
H	4.21843800	4.33117200	2.39718800
H	1.73428700	-2.52351100	2.72971500
H	3.50509700	-1.80294700	4.24774200
H	-0.55537400	-6.44606300	0.08289800
H	3.00699200	-3.58895700	-0.44797000
H	5.29998000	0.44349300	-4.84950900
H	-0.69579300	2.13243500	-2.44787600
H	0.50666500	-0.98268300	-2.74633900
H	6.99149900	-1.23117400	-4.17937000
H	5.18425900	1.57462400	0.18148000
H	-1.76027900	-4.10462100	3.46457800

H	1.70257800	-1.67682300	-4.81719100
H	-0.88788300	0.08382800	-1.66900100
H	-0.83100600	-0.09523100	1.75068400
C	3.96602800	3.42105500	4.94979700
H	5.02236900	3.54404600	4.68913800
H	3.61533100	4.36959500	5.37540800
H	3.90053800	2.65968300	5.73305900
C	-2.18579200	6.56163000	-2.26218000
H	-2.19257900	7.39504800	-1.55353700
H	-1.75503600	6.92492500	-3.20266300
H	-3.22642900	6.28434800	-2.46481300
C	-1.95621000	-6.61959700	2.42997100
H	-3.00356100	-6.38196600	2.64857600
H	-1.94118400	-7.47084200	1.74277600
H	-1.49141800	-6.93936000	3.36990600
C	3.79568300	-3.40978100	-5.04503800
H	4.60253200	-2.68556200	-5.21060500
H	4.25297000	-4.40031700	-4.95405000
H	3.15793200	-3.40726800	-5.93526100
N	-2.42951800	1.37822800	0.16378500
N	-2.42947000	-1.39614200	-0.03762800
C	-3.67364700	-0.67016200	-0.35268000
C	-3.68389000	0.65354600	0.44087400
H	-2.27713100	2.07609300	0.88699900
H	-2.49399700	1.89055000	-0.71274800
H	-3.60639000	-0.41336300	-1.41650300
H	-2.50126100	-1.87239900	0.85838500
H	-2.27714700	-2.12170700	-0.73312500
C	-4.92988500	-1.47791300	-0.10346500
C	-5.91327200	-1.60192200	-1.08350200
C	-5.16497900	-2.08311800	1.13354900
C	-7.08641600	-2.30695400	-0.84882700
H	-5.76479800	-1.12728700	-2.05027000
C	-6.33118800	-2.79286400	1.38188900
H	-4.42823900	-2.00326000	1.93104400
C	-7.31334600	-2.91672200	0.39049500
H	-7.83862800	-2.38204000	-1.63025500
C	-4.92729000	1.46701600	0.15054800
C	-5.93889200	1.60334800	1.09951300
C	-5.11985300	2.06579000	-1.09697100
C	-7.10083200	2.31169500	0.82376700
H	-5.82399900	1.13241900	2.07260600
C	-6.27445100	2.77891500	-1.38594400
H	-4.36011100	1.97514200	-1.87161600
C	-7.28716000	2.91201500	-0.42679400
H	-7.87199100	2.40316400	1.58458000
H	-6.39567500	3.24215800	-2.36220300
H	-3.65419200	0.39634800	1.50659600
N	-8.42777200	3.66937700	-0.69484800
H	-8.66509600	3.74452300	-1.67424900
H	-9.23539700	3.42766200	-0.13763200
H	-6.48914700	-3.25227300	2.35466400
N	-8.51132800	-3.58348700	0.65159700
H	-8.98094100	-3.94244900	-0.16817300
H	-8.45498200	-4.28363800	1.37818600

Coordinates (Angstroms)			
X	Y	Z	
Ru	0.41317200	0.27342300	-0.08624500
P	-0.98517900	-1.41267000	-0.60051200
P	-1.28856100	1.72797200	0.20273300
C	-2.16180700	2.55204900	-1.19365900
C	-1.69638900	2.37703000	-2.49530900
C	-4.66078500	-0.42713600	2.63035800
C	-2.72907400	0.97471300	1.10253200
C	-6.65238500	1.28528500	-3.45234400
C	-4.57749000	0.05096800	-3.21329400
C	-3.55455500	3.66603100	-3.37794200
C	-0.02645400	-2.64065000	-1.60015200
C	-1.01245400	4.50165300	0.94719200
C	0.36127100	-3.87197600	-1.06861900
C	-0.76610900	3.16217700	1.25492800
C	1.98698600	-4.21324600	-2.84186200
C	-1.79046800	-2.49362800	0.65713300
C	0.60520900	-2.21680200	-2.78134500
C	-2.47844000	-0.94582700	-1.59689100
C	-3.55523800	0.05474500	0.47159100
C	-2.87590100	1.19954100	2.49736600
C	-6.29544900	-2.33907800	1.40364900
C	-4.53046400	-0.67248100	1.23688600
C	0.57097400	3.90729500	3.14651300
C	-5.37180500	-1.65855200	0.65338000
C	-3.24664300	-4.32523600	1.27695200
C	-0.47939200	5.52430200	1.73165700
C	-3.80992700	0.52920100	3.23649800
C	-6.66133500	1.51966500	-2.05850200
C	-5.62932500	0.56740700	-4.01393800
C	-3.32543200	3.30284500	-0.99342100
C	-2.38837100	2.92534000	-3.57088500
C	-4.00398900	3.85986300	-2.06896300
C	-2.52741500	-1.20868200	-2.98991200
C	-3.53312600	-0.72043900	-3.77569300
C	-4.57497100	0.29099000	-1.81323600
C	-3.13279600	-3.99519500	2.63081000
C	1.35600600	-4.63919500	-1.67638200
C	-2.59586300	-3.57982400	0.30192200
C	-5.62559100	-1.14450700	3.38348200
C	-3.49823000	-0.21120900	-1.00665200
C	0.31457000	5.24875700	2.84331100
C	0.04637700	2.88725100	2.36665900
C	-1.66491800	-2.17057500	2.00499800
C	-6.43260800	-2.07705800	2.78523200
C	-5.65184000	1.04111600	-1.26463200
C	1.57403900	-2.99653900	-3.39684800
C	-2.32757400	-2.90988600	2.97870600
H	-0.80249800	1.77711900	-2.64800500
H	-7.45610400	1.67202900	-4.07250600
H	-1.60879300	4.76333400	0.07972800
H	-0.09070000	-4.23162600	-0.15038800
H	0.38767400	-1.22736200	-3.17158200
H	-2.23443200	1.92538300	2.98563200
H	-6.92316900	-3.09031800	0.93354300
H	1.21083500	3.65593000	3.98983100
H	-5.26683000	-1.88181100	-0.40198000

H	-3.87610700	-5.16204600	0.98295800
H	-0.68161700	6.55866100	1.46316200
H	-3.91157500	0.72526500	4.30137500
H	-7.47136800	2.09080400	-1.61434500
H	-5.60839800	0.37741600	-5.08437200
H	-3.72067900	3.43294300	0.01188900
H	-2.02182000	2.75976200	-4.58156300
H	-4.91750900	4.42342600	-1.89455400
H	-1.75448400	-1.81665700	-3.44431300
H	-3.54629400	-0.92863600	-4.84276700
H	1.65392700	-5.57991300	-1.21852000
H	-2.72370700	-3.83855900	-0.74675300
H	-5.71312000	-0.93881500	4.44768100
H	0.28774300	1.84998900	2.58252100
H	-1.06865700	-1.29695800	2.25859600
H	-7.17262100	-2.61767100	3.36875800
H	-5.66486300	1.24591300	-0.20026200
H	2.05001700	-2.63573300	-4.30641000
H	-2.23904000	-2.62190800	4.02437400
H	0.42251400	-0.02939000	1.59354500
H	0.59724700	0.58419200	-1.76189900
C	-4.34056600	4.20024600	-4.54758500
H	-5.14219600	3.50076400	-4.81379100
H	-4.80679300	5.16313800	-4.31384000
H	-3.70684800	4.33322300	-5.43015800
C	0.88727500	6.35267600	3.69558900
H	0.76380800	7.33034500	3.22020300
H	0.39148000	6.39206600	4.67292900
H	1.95600000	6.19676900	3.87798200
C	3.11647900	-4.99190300	-3.46484900
H	4.06526100	-4.45799700	-3.32790700
H	3.22055300	-5.98211400	-3.01078600
H	2.96462600	-5.12616100	-4.54151500
C	-3.90745900	-4.75018400	3.67945600
H	-4.88858000	-4.28299900	3.82874600
H	-4.07510400	-5.79189200	3.38745900
H	-3.38841600	-4.74445900	4.64337700
N	2.02199300	1.73097700	0.21438800
N	2.22129600	-0.96071300	-0.27346500
C	3.47057500	-0.17930100	-0.14678300
C	3.20882600	1.28474300	-0.54113300
H	1.76572000	2.67046200	-0.07894600
H	2.23970200	1.78669400	1.20938400
H	3.71910100	-0.16704000	0.91726900
H	2.18151200	-1.40719100	-1.18555800
H	2.23264200	-1.71713600	0.40687200
C	4.61777600	-0.79231000	-0.91879700
C	5.85538100	-1.02311700	-0.32077100
C	4.47412400	-1.13150400	-2.26597400
C	6.90663900	-1.59629400	-1.02493500
H	6.00565500	-0.73793800	0.71710700
C	5.51402000	-1.70936000	-2.98223400
H	3.53149800	-0.94369000	-2.77565700
C	6.74928700	-1.95624100	-2.36861800
H	7.86343100	-1.75867100	-0.53436400
C	4.43744000	2.14000500	-0.32218400
C	5.09777600	2.72645200	-1.40015500
C	4.97093100	2.32999900	0.95651900
C	6.25063700	3.48038900	-1.22081200
H	4.70931600	2.58215200	-2.40555400

C	6.12133900	3.08179900	1.14772400
H	4.49034100	1.87757800	1.82198000
C	6.78133000	3.66905200	0.05988000
H	6.74329500	3.93012700	-2.07957300
H	6.51548400	3.22132400	2.15177500
H	2.91814600	1.31373400	-1.59633100
C	1.64784900	-2.61428600	2.86627100
C	1.97161900	-3.82330300	2.25963600
C	3.28189300	-4.07221200	1.85472000
C	4.27203100	-3.11511800	2.07071500
C	3.94344700	-1.90217300	2.66570800
C	2.62665700	-1.63409800	3.04948000
H	0.61967200	-2.42272900	3.14585200
H	1.19402100	-4.56251200	2.09382500
H	3.53077100	-5.01058000	1.36824400
H	5.29304900	-3.30406900	1.75447200
H	4.69819700	-1.13744100	2.82326300
C	2.28837200	-0.27365600	3.57600500
O	3.00137600	0.68316500	3.31470200
N	7.91044400	4.46767600	0.25650200
H	8.43016400	4.25928600	1.09787600
H	8.52260400	4.53304000	-0.54514500
C	1.07146800	-0.12553600	4.45822500
H	0.17214300	-0.21080500	3.83852800
H	1.04033400	-0.90497800	5.22670900
H	1.08524400	0.86165700	4.92394500
H	5.37517900	-1.95675000	-4.03235200
N	7.81457000	-2.48937400	-3.09683700
H	8.51118300	-2.96463300	-2.54011100
H	7.54389000	-3.04232300	-3.89810600

TSC2-3

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.45108000	0.22990200	0.05401200
P	0.98673700	-1.48565100	0.45949600
P	1.24535000	1.74748900	-0.00595900
C	2.11680900	2.31967500	1.51287000
C	1.65287800	1.96372900	2.77683700
C	4.54065000	-0.05645100	-2.78081600
C	2.67632600	1.14081900	-1.01845500
C	6.77363500	0.90536300	3.34398900
C	4.69991700	-0.32044700	3.05611500
C	3.52406600	3.09131100	3.83584100
C	0.02084600	-2.73179200	1.42207100
C	1.01426100	4.61214900	-0.26811400
C	-0.48864700	-3.87993300	0.81128700
C	0.74612700	3.34466400	-0.79050200
C	-2.05378300	-4.24448400	2.63477200
C	1.75881800	-2.50667500	-0.86364700
C	-0.51857200	-2.36346200	2.66569100
C	2.51358300	-1.11147100	1.44270300
C	3.50508500	0.13377700	-0.54383200
C	2.79670000	1.56586000	-2.36850800
C	6.12645400	-2.18679800	-1.90136300

C	4.43860800	-0.49917100	-1.43425200
C	-0.55320400	4.40918400	-2.54922600
C	5.25353600	-1.59085400	-1.02775400
C	3.10080300	-4.37606300	-1.61210000
C	0.51299000	5.75680900	-0.88552400
C	3.70249400	0.99771500	-3.21897400
C	6.71691200	1.29991800	1.98772000
C	5.78471200	0.11174800	3.86283000
C	3.28851700	3.08183600	1.42465600
C	2.35228800	2.34110800	3.92029000
C	3.97337200	3.46921600	2.56706200
C	2.64168900	-1.55626900	2.78400800
C	3.69011100	-1.16722200	3.56993100
C	4.62853600	0.08475500	1.69650300
C	3.09233200	-3.89290800	-2.92445800
C	-1.51111600	-4.61860100	1.40790100
C	2.45530000	-3.68848800	-0.59172000
C	5.45901900	-0.68453000	-3.66021600
C	3.50811900	-0.31432100	0.89137800
C	-0.27253800	5.67867200	-2.03501900
C	-0.06097200	3.26729300	-1.93419500
C	1.74612700	-2.02590500	-2.16994800
C	6.24143500	-1.72504300	-3.23199900
C	5.67549500	0.90388700	1.18985200
C	-1.52074600	-3.11372600	3.26434800
C	2.40197800	-2.70962200	-3.18732000
H	0.75326700	1.35930600	2.84792100
H	7.60183600	1.22833900	3.96836000
H	1.60460500	4.72113400	0.63479800
H	-0.11263200	-4.18983100	-0.15891700
H	-0.20021800	-1.43588200	3.13088300
H	2.16066400	2.36684500	-2.72937200
H	6.73041300	-3.02612500	-1.56924700
H	-1.18393600	4.30119300	-3.42829100
H	5.16381600	-1.96968800	-0.01600700
H	3.63652600	-5.29495500	-1.38498500
H	0.73365800	6.73031100	-0.45362300
H	3.78607400	1.34808900	-4.24494000
H	7.50063100	1.93020100	1.57772300
H	5.81655500	-0.20300100	4.90310300
H	3.68537900	3.35267400	0.44893100
H	1.98512700	2.03032900	4.89583900
H	4.89305500	4.04150600	2.47303800
H	1.89767000	-2.22761900	3.19576900
H	3.76272700	-1.51271500	4.59826500
H	-1.90510100	-5.49161400	0.89294700
H	2.49633700	-4.07326300	0.42478100
H	5.52801400	-0.32445900	-4.68384500
H	-0.34238200	2.29583700	-2.32571600
H	1.24002000	-1.08420300	-2.36233500
H	6.94458700	-2.19881700	-3.91125100
H	5.63647200	1.23262200	0.15779100
H	-1.92797600	-2.79367300	4.22094400
H	2.39931500	-2.30010000	-4.19493500
H	-0.55421100	-0.00848700	-1.71175300
H	-0.59220200	0.44452000	1.70181300
C	4.31427300	3.46116800	5.06477700
H	5.27480400	2.93286000	5.07294300
H	4.52785500	4.53559700	5.09459900
H	3.77722000	3.19794800	5.98122800

C	-0.83589600	6.91559500	-2.68742100
H	-1.91851000	6.98379600	-2.52743900
H	-0.38124900	7.82465900	-2.28219200
H	-0.66718100	6.90441600	-3.76970600
C	-3.21594100	-4.98274700	3.24572400
H	-3.36480800	-5.95881600	2.77408200
H	-3.06817500	-5.14177300	4.31938900
H	-4.13896100	-4.40265600	3.11964100
C	3.85689100	-4.59561400	-4.01563300
H	4.84416800	-4.13361100	-4.13897500
H	4.00914500	-5.65499700	-3.78653100
H	3.33902000	-4.52405400	-4.97748800
N	-2.06734200	1.64935500	-0.20175700
N	-2.22511600	-1.03000100	0.26381900
C	-3.50111200	-0.28019800	0.18472400
C	-3.26850400	1.20196700	0.52928700
H	-1.83729300	2.60095700	0.07481400
H	-2.25273400	1.67131800	-1.21278800
H	-3.81314800	-0.30982700	-0.86101400
H	-2.15112900	-1.47615500	1.17426800
H	-2.25189600	-1.78801100	-0.41626900
C	-4.57158600	-0.91950400	1.03816700
C	-5.76405000	-1.38161500	0.48579300
C	-4.37511400	-1.09393800	2.41072500
C	-6.72728600	-2.00723700	1.26730700
H	-5.94128400	-1.24985600	-0.57812500
C	-5.32684300	-1.72087400	3.20298300
H	-3.45683500	-0.73878400	2.87527400
C	-6.52119200	-2.19156200	2.63955400
H	-7.65204300	-2.35393300	0.81249200
C	-4.51154800	2.01183300	0.22270700
C	-4.88249100	2.28679500	-1.09751600
C	-5.35270400	2.44875100	1.24444600
C	-6.04708800	2.98577200	-1.38210900
H	-4.25126900	1.95574400	-1.92029100
C	-6.52312700	3.14525200	0.96993800
H	-5.09618500	2.23192900	2.27872200
C	-6.88708000	3.42705500	-0.35152400
H	-6.31356200	3.18927000	-2.41679900
H	-7.16547700	3.46923100	1.78535200
H	-3.02709200	1.28326200	1.59404500
C	-1.76845800	-2.35931100	-2.70038800
C	-2.51792500	-3.51910000	-2.53330100
C	-3.90416100	-3.48902000	-2.68896500
C	-4.53179600	-2.29221800	-3.01962500
C	-3.78047300	-1.12902400	-3.17522900
C	-2.39466700	-1.14736800	-3.00666200
H	-0.69553100	-2.38300300	-2.54119200
H	-2.01797300	-4.44799200	-2.27374500
H	-4.48772900	-4.39494600	-2.55426500
H	-5.60965400	-2.25999900	-3.15297400
H	-4.26084600	-0.18534300	-3.41474700
C	-1.64534200	0.15540500	-3.20188100
O	-2.26947400	1.22520400	-3.07122700
C	-0.45116700	0.10738600	-4.14356600
H	0.07106300	-0.85004000	-4.11621600
H	-0.84003600	0.25499900	-5.16000400
H	0.25378300	0.91015100	-3.92085800
N	-8.08645600	4.08402700	-0.63983800
H	-8.42764400	4.67720000	0.10406300

H	-8.09357000	4.57011900	-1.52607500
H	-5.15237100	-1.84062600	4.26983500
N	-7.50379900	-2.77705000	3.43979100
H	-8.13909800	-3.39023800	2.94844200
H	-7.16024900	-3.20387200	4.28880200

C3

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.44704400	0.25023600	0.12755000
P	0.99050800	-1.50802700	0.50459400
P	1.29270200	1.75535400	-0.00141400
C	2.21201900	2.27787400	1.50289000
C	1.74261000	1.97357400	2.77959900
C	4.40567100	-0.19207800	-2.88513900
C	2.65771800	1.07839000	-1.05796300
C	6.91672500	0.79623600	3.15079700
C	4.80304400	-0.37861000	2.95584600
C	3.68176800	3.01851800	3.79946500
C	0.01796600	-2.70156700	1.51971200
C	1.26792400	4.61502300	-0.31720200
C	-0.54380600	-3.84227500	0.94171500
C	0.84098300	3.36554500	-0.78096600
C	-2.08744100	-4.10993200	2.80029700
C	1.67672200	-2.55106000	-0.83962200
C	-0.48034400	-2.29039300	2.76712900
C	2.54838500	-1.14369300	1.43187600
C	3.48388300	0.05837800	-0.60480100
C	2.71583900	1.47330900	-2.42121600
C	5.99604500	-2.33357200	-2.04112100
C	4.36133400	-0.60799100	-1.52673900
C	-0.47228800	4.51086000	-2.47183200
C	5.17642700	-1.70647500	-1.13860800
C	2.94751100	-4.45478300	-1.62205700
C	0.83802600	5.78660200	-0.93179800
C	3.56530600	0.86775200	-3.30369900
C	6.82568400	1.16540500	1.78907700
C	5.92572700	0.03883300	3.71747400
C	3.42373600	2.97052100	1.39131000
C	2.47077500	2.33580700	3.90908400
C	4.13912200	3.34348000	2.52014000
C	2.70972300	-1.57133500	2.77470700
C	3.79119300	-1.19095900	3.51902300
C	4.69587100	0.00530700	1.59225400
C	2.88417400	-3.98963900	-2.93985200
C	-1.58023900	-4.53014200	1.57296300
C	2.36267100	-3.74278800	-0.58295100
C	5.26895000	-0.85382400	-3.79563200
C	3.53738400	-0.37414100	0.83431900
C	-0.03077300	5.75684200	-2.02448300
C	-0.05069400	3.33508700	-1.86153900
C	1.60574900	-2.09055800	-2.15186600
C	6.05344000	-1.89955600	-3.38494200
C	5.74750000	0.78421200	1.03418500
C	-1.50002400	-2.98891200	3.39871300

C	2.19954600	-2.80044600	-3.18849700
H	0.81077900	1.42779200	2.88346700
H	7.77398100	1.10818000	3.74029900
H	1.92554600	4.68877100	0.54129200
H	-0.20137100	-4.18471800	-0.02986800
H	-0.11048200	-1.37418500	3.21775100
H	2.07385700	2.27618100	-2.76712400
H	6.60195900	-3.17643700	-1.72196800
H	-1.17958300	4.44179700	-3.29439600
H	5.13220700	-2.06378700	-0.11618900
H	3.47810500	-5.37937400	-1.40726900
H	1.18031500	6.74374700	-0.54439600
H	3.59772600	1.19114300	-4.34106500
H	7.61393600	1.76237000	1.33996000
H	5.98603800	-0.25961400	4.76129900
H	3.82762100	3.19824800	0.40792100
H	2.09310400	2.07046900	4.89378900
H	5.08744100	3.86205200	2.40505800
H	1.96633900	-2.22128700	3.22063700
H	3.89029500	-1.51950400	4.55056200
H	-2.01579300	-5.39726600	1.08280400
H	2.44386800	-4.11400600	0.43607800
H	5.29255600	-0.51571100	-4.82861700
H	-0.48779900	2.40539500	-2.22333600
H	1.11266700	-1.14562300	-2.35511900
H	6.71436300	-2.39926600	-4.08745900
H	5.68438000	1.09175100	-0.00316100
H	-1.87493800	-2.63607700	4.35692000
H	2.14692900	-2.40690500	-4.20053800
H	-0.81703300	-0.06046400	-1.90253400
H	-0.43843800	0.46833700	1.69869100
C	4.50393300	3.35766600	5.01589900
H	5.30498800	2.62002500	5.14667400
H	4.97539300	4.34110400	4.91803300
H	3.89607200	3.35914800	5.92602600
C	-0.47374400	7.03014900	-2.69908200
H	-0.55223300	7.85461300	-1.98305400
H	0.24436700	7.33241100	-3.47120200
H	-1.44629100	6.90465100	-3.18463500
C	-3.26807000	-4.79085100	3.44120600
H	-4.17336800	-4.18842000	3.29323200
H	-3.44617400	-5.77815700	3.00482200
H	-3.12220600	-4.91461500	4.51958600
C	3.58911900	-4.71723600	-4.05412900
H	4.57627900	-4.27024200	-4.22469100
H	3.73667000	-5.77564000	-3.81811200
H	3.03104400	-4.64944900	-4.99329700
N	-2.02776800	1.67577800	-0.10526300
N	-2.22551300	-0.97572200	0.40632600
C	-3.49242900	-0.21859300	0.25142400
C	-3.25050800	1.25741700	0.60769200
H	-1.80657800	2.64062400	0.13052400
H	-2.19391900	1.63199500	-1.16053100
H	-3.73311600	-0.24342700	-0.81375300
H	-2.17323800	-1.35901600	1.34747700
H	-2.26108600	-1.78265700	-0.21788300
C	-4.61351000	-0.85975600	1.03329400
C	-5.75250600	-1.34415100	0.39292900
C	-4.52289400	-1.02071100	2.41820100
C	-6.76653700	-1.97368400	1.10313700

H	-5.84330200	-1.23083500	-0.68383600
C	-5.52693200	-1.65190100	3.14035400
H	-3.65029000	-0.64847800	2.95248800
C	-6.66788200	-2.14135500	2.48953600
H	-7.64776600	-2.33762900	0.58052400
C	-4.46850900	2.08889000	0.26196800
C	-5.32566000	2.55409100	1.25685100
C	-4.79356300	2.35560000	-1.07314800
C	-6.47313000	3.27331800	0.94385400
H	-5.10150700	2.34396600	2.30037400
C	-5.93545100	3.07602800	-1.39268600
H	-4.13926400	1.99863000	-1.86906600
C	-6.79358400	3.54696800	-0.39010200
H	-7.13071200	3.62017700	1.73756900
H	-6.17042200	3.27404000	-2.43621800
H	-3.05017200	1.33571700	1.68342900
C	-1.95081000	-2.40953200	-2.45297900
C	-2.79805000	-3.51607000	-2.43458900
C	-4.13145000	-3.38027100	-2.81541200
C	-4.60307400	-2.13333200	-3.22142500
C	-3.75523700	-1.02791800	-3.22406700
C	-2.42174600	-1.14957100	-2.83282900
H	-0.91216700	-2.52230700	-2.15009400
H	-2.41517300	-4.48321200	-2.11810400
H	-4.79695400	-4.23880400	-2.79739400
H	-5.64052100	-2.01866600	-3.52587400
H	-4.11053000	-0.04006200	-3.50095600
C	-1.53643700	0.11061800	-2.81942900
O	-2.22002600	1.25275400	-2.72765800
C	-0.58612300	0.08186500	-4.03719200
H	-0.09044600	-0.88676200	-4.17263900
H	-1.17787000	0.29594800	-4.93356600
H	0.17803700	0.85979700	-3.93275200
N	-7.97019700	4.22784900	-0.71938400
H	-8.31102400	4.84500700	0.00502700
H	-7.93939800	4.69938200	-1.61306500
H	-5.43584400	-1.75777800	4.21905300
N	-7.70456000	-2.73042900	3.21535600
H	-8.29761200	-3.34813600	2.67898700
H	-7.42449600	-3.15266200	4.08955100

TSC3-4

Coordinates (Angstroms)

X	Y	Z
Ru	-0.46039200	0.25386100
P	0.98497400	-1.50370400
P	1.26955300	1.76825100
C	2.17112100	2.28273000
C	1.68950400	1.96755800
C	4.41413100	-0.17257100
C	2.65193400	1.09776900
C	6.88025200	0.82394500
C	4.77757700	-0.36761800
C	3.61610500	3.00807600
C	0.00969300	-2.69776100

C	1.24357900	4.63300600	-0.29045300
C	-0.55385000	-3.83820500	0.93247300
C	0.84131600	3.38618900	-0.78053300
C	-2.11175500	-4.09073900	2.78145000
C	1.68548400	-2.55623900	-0.83766300
C	-0.49429800	-2.28046000	2.75254500
C	2.53725200	-1.14224300	1.43554300
C	3.47539100	0.07659100	-0.58888100
C	2.72527200	1.49595500	-2.40756800
C	5.99223900	-2.31926600	-2.01106200
C	4.35887500	-0.58952900	-1.50575600
C	-0.39988800	4.54043400	-2.52076400
C	5.16893400	-1.69030300	-1.11318700
C	2.96051600	-4.46804700	-1.59789000
C	0.83753100	5.80813300	-0.91528100
C	3.58041400	0.89101100	-3.28508500
C	6.79388300	1.19955500	1.82926100
C	5.89271700	0.05478000	3.74647200
C	3.38184300	2.97973000	1.42328000
C	2.40572700	2.32159400	3.92592000
C	4.08509300	3.34512000	2.56217200
C	2.69603700	-1.57809200	2.77620900
C	3.77012700	-1.19296100	3.52884300
C	4.67448000	0.02372900	1.61477100
C	2.91632100	-4.00856500	-2.91813800
C	-1.59810800	-4.51848900	1.55943100
C	2.36442100	-3.74944100	-0.56953700
C	5.28175900	-0.83547700	-3.76874500
C	3.52271400	-0.36003200	0.84915700
C	0.01477700	5.78453000	-2.04242100
C	-0.00276900	3.36306200	-1.89859800
C	1.63328700	-2.10258000	-2.15394400
C	6.05999900	-1.88427700	-3.35410100
C	5.72305200	0.81345900	1.06634600
C	-1.52182700	-2.97103500	3.37988000
C	2.23846500	-2.81832000	-3.18012400
H	0.75677600	1.42122100	2.87747200
H	7.73141000	1.13999200	3.78567800
H	1.86827600	4.70180900	0.59269100
H	-0.20632100	-4.18607200	-0.03551400
H	-0.12212700	-1.36474700	3.20262800
H	2.09354000	2.30524500	-2.75675700
H	6.59342200	-3.16427300	-1.68859200
H	-1.06237000	4.48037300	-3.38065200
H	5.11713900	-2.04823700	-0.09136400
H	3.48587800	-5.39299100	-1.37187800
H	1.16569200	6.76317800	-0.51098500
H	3.62471600	1.21986300	-4.32040000
H	7.57957100	1.80567600	1.38793800
H	5.95007900	-0.24927600	4.78887900
H	3.79420300	3.21764000	0.44583500
H	2.01827200	2.04792000	4.90449700
H	5.03303300	3.86721400	2.46074200
H	1.95583400	-2.23761400	3.21360600
H	3.86702100	-1.52791700	4.55857100
H	-2.03493900	-5.38537500	1.06979100
H	2.43182000	-4.11637100	0.45202700
H	5.31409200	-0.49565500	-4.80096900
H	-0.40496200	2.42763900	-2.27835600
H	1.15066700	-1.15473500	-2.36968700

H	6.72425600	-2.38520500	-4.05261000
H	5.66282400	1.12576000	0.03015500
H	-1.90250800	-2.61167300	4.33331100
H	2.20333700	-2.42805600	-4.19424300
H	-0.76156700	-0.16564800	-1.99305600
H	-0.46357400	0.47896300	1.66091800
C	4.42512100	3.33914800	5.06147400
H	5.22458100	2.60051000	5.19628100
H	4.89780200	4.32305400	4.97497800
H	3.80724900	3.33507300	5.96484800
C	-0.44981900	7.06290800	-2.69256600
H	-0.64599600	6.91788900	-3.75942800
H	-1.37962100	7.41821600	-2.23201600
H	0.29496700	7.85833700	-2.58700100
C	-3.30123200	-4.76126400	3.41695600
H	-4.19758400	-4.14355800	3.27787300
H	-3.49436600	-5.74129800	2.97064400
H	-3.15510000	-4.89867400	4.49374100
C	3.63427800	-4.74173200	-4.02040500
H	4.62308500	-4.29513600	-4.18245000
H	3.77972300	-5.79874100	-3.77702600
H	3.08689200	-4.67959600	-4.96626400
N	-2.02804300	1.61581900	-0.24914400
N	-2.23273500	-0.98383100	0.37370400
C	-3.50385800	-0.22859000	0.22456500
C	-3.22904100	1.25706600	0.51325300
H	-1.81987800	2.59872600	-0.08466900
H	-2.17477000	1.42901300	-1.56908000
H	-3.77869200	-0.29574000	-0.83022200
H	-2.17214800	-1.35160000	1.32047600
H	-2.26953400	-1.80351900	-0.23275000
C	-4.59823900	-0.84308500	1.06315900
C	-5.74938000	-1.36655800	0.47735000
C	-4.46708300	-0.94695300	2.45058200
C	-6.73501700	-1.97860500	1.24147300
H	-5.87294300	-1.29785100	-0.60024000
C	-5.44157600	-1.56026600	3.22648100
H	-3.58444900	-0.54237200	2.94275400
C	-6.59434200	-2.08925400	2.62975100
H	-7.62635900	-2.37353100	0.75993700
C	-4.45397200	2.08642800	0.17290300
C	-5.30993500	2.53983500	1.17548300
C	-4.79381900	2.36826600	-1.15414500
C	-6.46356900	3.25607600	0.87830100
H	-5.07666100	2.32283200	2.21558300
C	-5.94216500	3.08527400	-1.46150400
H	-4.14788900	2.02714400	-1.95939000
C	-6.79596900	3.54161100	-0.44979600
H	-7.11611700	3.59276400	1.68072700
H	-6.18467600	3.29221300	-2.50176000
H	-3.03333300	1.36496700	1.59127200
C	-1.93169300	-2.49443400	-2.49935200
C	-2.79096800	-3.59077400	-2.46948000
C	-4.13007300	-3.43776200	-2.82207400
C	-4.59709600	-2.18437400	-3.21216800
C	-3.73742000	-1.08849500	-3.23004400
C	-2.39800500	-1.22919400	-2.86687800
H	-0.88928500	-2.61909500	-2.21487100
H	-2.41311400	-4.56305500	-2.16398400
H	-4.80486100	-4.28849100	-2.79318500

H	-5.63977200	-2.05580400	-3.49076900
H	-4.09605000	-0.09834600	-3.49306900
C	-1.48399300	-0.00153900	-2.85662700
O	-2.16749400	1.17607700	-2.70956500
C	-0.60939500	0.02614900	-4.11687600
H	-0.11220900	-0.93474500	-4.29126900
H	-1.24143400	0.25160400	-4.98210100
H	0.15225500	0.80807600	-4.02686500
N	-7.98007200	4.22037200	-0.76431300
H	-8.31450900	4.82828800	-0.02887800
H	-7.95054300	4.70950700	-1.64876400
H	-5.31819200	-1.62184200	4.30546100
N	-7.60186300	-2.66136800	3.40966500
H	-8.19941300	-3.30997200	2.91627900
H	-7.28863400	-3.04508200	4.29037800

C4

Coordinates (Angstroms)

X	Y	Z
Ru	-0.45789500	0.25855800
P	0.99733700	-1.49661300
P	1.26131800	1.77866500
C	2.17226600	2.31653500
C	1.71688300	1.99329100
C	4.40171200	-0.17778500
C	2.64374900	1.10841200
C	6.88971700	0.89148000
C	4.79472500	-0.31679500
C	3.63904800	3.07282500
C	0.03144600	-2.68610300
C	1.12750700	4.64118600
C	-0.53545700	-3.83045800
C	0.80912100	3.38660300
C	-2.08443000	-4.07130400
C	1.70134600	-2.56964500
C	-0.46523300	-2.26269900
C	2.55228500	-1.11975500
C	3.47137900	0.09303400
C	2.71533700	1.49573400
C	5.98223800	-2.31661800
C	4.35276300	-0.58022200
C	-0.42904800	4.51368900
C	5.16529300	-1.67628100
C	2.97825600	-4.49202700
C	0.68113600	5.80750900
C	3.56737400	0.88291200
C	6.79103900	1.26092300
C	5.91167100	0.11744300
C	3.36593600	3.03897800
C	2.44397900	2.36272300
C	4.08003200	3.41913500
C	2.72257200	-1.54648300
C	3.79740300	-1.14806500
C	4.67968300	0.06748700
C	2.93676200	-4.05047600

C	-1.57697500	-4.50651600	1.60591900
C	2.38012000	-3.75945100	-0.52733900
C	5.26356100	-0.85162800	-3.77692500
C	3.52735500	-0.33106100	0.84278700
C	-0.10013500	5.76676100	-2.03968100
C	0.00686200	3.34592800	-1.94676600
C	1.65127800	-2.13528400	-2.13464500
C	6.04214000	-1.89736200	-3.35524900
C	5.71802600	0.86345300	1.04105100
C	-1.48971000	-2.94928900	3.41701100
C	2.25871300	-2.86447100	-3.15028700
H	0.79607500	1.42970800	2.87315800
H	7.74259800	1.21637500	3.74497900
H	1.71637800	4.72212000	0.63662800
H	-0.19128800	-4.18539300	0.00327000
H	-0.08993100	-1.34524600	3.22399600
H	2.08644000	2.30440200	-2.78086000
H	6.58438600	-3.15863900	-1.67829300
H	-1.05558500	4.43962400	-3.44544700
H	5.11875300	-2.02230800	-0.08502300
H	3.50409200	-5.41329400	-1.30480900
H	0.94139200	6.76907300	-0.44747900
H	3.60955900	1.20402200	-4.33945000
H	7.56873900	1.87166800	1.34597900
H	5.97819900	-0.18127500	4.76653800
H	3.75426800	3.28879300	0.39162700
H	2.07793900	2.08253900	4.87968800
H	5.01411900	3.96270300	2.38705800
H	1.99102200	-2.21067000	3.22451600
H	3.90292700	-1.47691400	4.55535100
H	-2.01612200	-5.37672100	1.12412100
H	2.44605300	-4.11222700	0.49925000
H	5.29050200	-0.52357100	-4.81312700
H	-0.32662000	2.39774900	-2.35722200
H	1.17203500	-1.18895500	-2.36421100
H	6.70114800	-2.40754600	-4.05203300
H	5.64799400	1.17139500	0.00415100
H	-1.86437400	-2.58446200	4.37079600
H	2.22738400	-2.48716300	-4.16949000
H	-0.71875500	-0.23556800	-2.07821200
H	-0.43379400	0.47719600	1.67237200
C	4.46081900	3.41961400	4.99737800
H	5.26340900	2.68415400	5.13099100
H	4.93002800	4.40364700	4.89520900
H	3.85318400	3.42344800	5.90769500
C	-0.61440200	7.03336500	-2.67540400
H	0.08010800	7.86617900	-2.52549900
H	-0.76781400	6.90512400	-3.75141400
H	-1.57737500	7.32323600	-2.23782500
C	-3.27209900	-4.73625100	3.47265400
H	-4.16841100	-4.11847800	3.33328600
H	-3.46827100	-5.71895600	3.03354000
H	-3.12196600	-4.86699900	4.54969900
C	3.65933400	-4.79726600	-3.96122500
H	4.66016600	-4.37124800	-4.10443100
H	3.77847700	-5.85740500	-3.71706000
H	3.13113000	-4.72214300	-4.91690500
N	-2.01651600	1.59210300	-0.25563500
N	-2.22259900	-0.98468400	0.40791300
C	-3.49518000	-0.23651600	0.24289500

C	-3.21601900	1.25300900	0.50811700
H	-1.81636100	2.58064000	-0.11548400
H	-2.14626800	1.34230300	-1.85241100
H	-3.76549900	-0.32059500	-0.81215500
H	-2.15721900	-1.32477900	1.36473200
H	-2.25775900	-1.82274400	-0.17238100
C	-4.59203000	-0.83966000	1.08701700
C	-5.75451100	-1.34606300	0.50860400
C	-4.45756500	-0.94134500	2.47447700
C	-6.74651700	-1.94055800	1.27852300
H	-5.88330100	-1.27579500	-0.56820800
C	-5.43804100	-1.53759200	3.25632000
H	-3.56834300	-0.54636000	2.96247700
C	-6.60155400	-2.05007900	2.66634100
H	-7.64663300	-2.32149000	0.80195600
C	-4.44127100	2.07539300	0.14650900
C	-5.31715400	2.52604200	1.13338800
C	-4.76431300	2.35376000	-1.18477900
C	-6.47055900	3.23444700	0.81668000
H	-5.09875300	2.31236300	2.17737400
C	-5.91228100	3.06219900	-1.51363500
H	-4.10721600	2.01511300	-1.98039700
C	-6.78445900	3.51577100	-0.51669800
H	-7.13759600	3.56849800	1.60829500
H	-6.13970300	3.26465900	-2.55821400
H	-3.04316500	1.37352000	1.59158100
C	-1.95027700	-2.56067900	-2.44033500
C	-2.84162600	-3.62581000	-2.33500000
C	-4.18090200	-3.45215000	-2.67791200
C	-4.61645700	-2.21103000	-3.13630700
C	-3.72508900	-1.14475400	-3.23078200
C	-2.38629800	-1.30601600	-2.87553600
H	-0.90787700	-2.69828600	-2.16089000
H	-2.48919800	-4.58896700	-1.97541200
H	-4.88078700	-4.27777300	-2.58772000
H	-5.65902200	-2.06678300	-3.40682600
H	-4.06183800	-0.16287800	-3.54790200
C	-1.42892300	-0.12026000	-2.93923500
O	-2.08415400	1.10219400	-2.85879200
C	-0.58320200	-0.15848100	-4.21246100
H	-0.10949200	-1.13643200	-4.34912300
H	-1.22443600	0.03992900	-5.07744500
H	0.19511700	0.61063400	-4.16777300
N	-7.96809500	4.18710700	-0.85131400
H	-8.31667600	4.79373800	-0.12129500
H	-7.92466400	4.67838600	-1.73406800
H	-5.31130300	-1.59702100	4.33507800
N	-7.61518300	-2.60318100	3.45270300
H	-8.22408800	-3.24467200	2.96387800
H	-7.30345300	-2.98960600	4.33280300

C2u

Coordinates (Angstroms)

X	Y	Z
Ru	-0.49830200	0.24861200
	-0.50222600	

P	1.08656800	1.75589100	0.03264800
P	1.02796600	-1.38460100	-0.80415700
C	2.02524700	-1.55698400	-2.34309300
C	1.81331600	-0.68103500	-3.40512300
C	4.23187500	-1.21026700	2.60480800
C	2.38549900	-1.38145300	0.46221100
C	6.85430400	0.02386300	-3.33721500
C	4.87002000	1.25184800	-2.67428100
C	3.63418200	-1.68989200	-4.65393500
C	0.45030600	3.46678600	-0.28863100
C	0.25349500	-3.98589500	-1.70658200
C	0.32933400	4.44502600	0.70006700
C	0.22081300	-3.04604900	-0.67400700
C	-0.86438900	5.92852100	-0.81097800
C	1.80279200	1.91792700	1.72421800
C	-0.12046100	3.73703700	-1.54421400
C	2.65999100	1.61343200	-0.94309200
C	3.36955000	-0.40167500	0.43255100
C	2.33203200	-2.28089200	1.55951600
C	6.20262200	0.77598800	2.60205700
C	4.30511100	-0.29671200	1.51886500
C	-1.36423000	-4.47866100	0.48557400
C	5.31409800	0.70432600	1.56048900
C	3.37398600	2.88847800	3.28978300
C	-0.50970700	-5.15129700	-1.64253000
C	3.22565700	-2.20532800	2.59060700
C	6.64893200	-0.86776500	-2.26020400
C	5.97754400	1.05700000	-3.53932300
C	3.04162600	-2.51294400	-2.45315200
C	2.61406400	-0.74569600	-4.54206600
C	3.82494300	-2.58444500	-3.59635100
C	2.90615900	2.49949500	-2.02333400
C	3.96947300	2.32653500	-2.86320400
C	4.65788400	0.36111800	-1.58768100
C	2.99129500	1.97851300	4.28085900
C	-0.31969700	5.65276400	0.44059100
C	2.80066900	2.85129200	2.02633300
C	5.16138800	-1.11197100	3.67185500
C	3.53053700	0.55473300	-0.71722800
C	-1.32952600	-5.41898200	-0.54940000
C	-0.61478900	-3.31170700	0.42463300
C	1.40898000	1.02089700	2.71201300
C	6.13291800	-0.14556200	3.67087800
C	5.58218200	-0.70642000	-1.41465300
C	-0.75213000	4.94567800	-1.80112700
C	2.00026600	1.04802700	3.97139600
H	1.03418200	0.07151600	-3.30698800
H	7.70327600	-0.11372800	-4.00093000
H	0.86734800	-3.81168800	-2.58336000
H	0.73054500	4.27120400	1.69279200
H	-0.09916100	2.95914600	-2.30355500
H	1.56996700	-3.05135800	1.57937600
H	6.96295000	1.55128100	2.60869000
H	-1.99890900	-4.65370200	1.34993200
H	5.37053000	1.42946600	0.75690600
H	4.15361600	3.61537100	3.50567900
H	-0.46624300	-5.86029800	-2.46615200
H	3.17798400	-2.91960100	3.40972800
H	7.33902800	-1.69203300	-2.10536700
H	6.11903200	1.75047500	-4.36473500

H	3.23153500	-3.19892800	-1.63046000
H	2.45215400	-0.03510800	-5.34955000
H	4.61749400	-3.32649200	-3.65886200
H	2.23856800	3.33744300	-2.18637300
H	4.13831900	3.01961000	-3.68381500
H	-0.40312400	6.39089600	1.23497400
H	3.14215100	3.54592200	1.26207600
H	5.09051300	-1.82531100	4.48954200
H	-0.69730900	-2.57206300	1.21831800
H	0.66788100	0.27184600	2.44391500
H	6.84745600	-0.08417900	4.48695100
H	5.42908100	-1.41174900	-0.60588300
H	-1.18162900	5.12475100	-2.78475400
H	1.70464700	0.31729800	4.72230500
H	-0.74951300	-0.32156600	1.09234100
H	-0.47027700	0.79589400	-2.12629200
C	4.54065600	-1.72356600	-5.85746600
H	5.48287800	-1.20782800	-5.63621400
H	4.78592700	-2.75160600	-6.14518400
H	4.08238500	-1.22849400	-6.71933000
C	-2.18212400	-6.66088400	-0.48828900
H	-1.88112500	-7.39074100	-1.24576000
H	-2.11171500	-7.14254100	0.49315100
H	-3.23811000	-6.41963600	-0.65907600
C	-1.55148800	7.23885600	-1.10031500
H	-2.50815400	7.08090400	-1.61007800
H	-1.74651700	7.79875800	-0.18074400
H	-0.93472000	7.87027700	-1.75109500
C	3.67491900	1.97744000	5.62341600
H	4.66699000	1.51790700	5.54156900
H	3.81048800	2.99432000	6.00737200
H	3.10399000	1.40746600	6.36303200
N	-2.20366000	-0.98865900	-1.10051500
N	-2.17479600	1.63778000	-0.21582100
C	-3.45222100	0.89728100	-0.20300500
C	-3.40337500	-0.15310800	-1.32591400
H	-2.00248900	-1.52289700	-1.94215500
H	-2.39277000	-1.67502500	-0.37230200
H	-3.47278400	0.35391600	0.74473400
H	-2.15801700	2.30730900	-0.98203100
H	-2.10187900	2.19148300	0.63451500
C	-4.66843900	1.79225000	-0.26857300
C	-5.64447300	1.72388900	0.72592000
C	-4.85483100	2.70112500	-1.31224800
C	-6.76822100	2.53916400	0.68608000
H	-5.52020400	1.01422200	1.54085500
C	-5.97233800	3.52284800	-1.36066500
H	-4.11718700	2.77668300	-2.10966800
C	-6.94859600	3.45392400	-0.35782700
H	-7.51893800	2.46457600	1.46931200
C	-4.67153900	-0.97069800	-1.42513900
C	-5.36685300	-1.07097800	-2.62819700
C	-5.17142900	-1.66465000	-0.31830100
C	-6.52251700	-1.83533400	-2.73604200
H	-5.00352300	-0.53560000	-3.50253100
C	-6.32394100	-2.42948800	-0.41376900
H	-4.67572500	-1.59427000	0.64779700
C	-7.02003100	-2.52652300	-1.62637600
H	-7.04349400	-1.89902200	-3.68828200
H	-6.69632900	-2.95394800	0.46297700

H	-3.23031400	0.37130900	-2.27361200
C	-3.05430400	-0.50833300	3.23489600
O	-4.18255100	-0.71666800	2.81225200
N	-8.15380200	-3.33510400	-1.73389400
H	-8.64770900	-3.47844600	-0.86366300
H	-8.78909700	-3.06894300	-2.47374100
C	-2.49394900	0.89053800	3.29718200
H	-2.09845300	1.12828100	4.29001300
H	-1.66635000	0.95344400	2.57568700
H	-3.27886700	1.60281400	3.03336400
C	-2.19015200	-1.65209300	3.65871500
C	-0.85711500	-1.47161100	4.03363300
C	-2.72948800	-2.94195800	3.64414700
C	-0.06444600	-2.56518100	4.36360800
H	-0.42722100	-0.47782600	4.05433900
C	-1.94442000	-4.03326200	3.99424400
H	-3.76718900	-3.06823200	3.35275300
C	-0.60654600	-3.84737500	4.34185500
H	0.97820400	-2.41162900	4.62301900
H	-2.37055900	-5.03228900	3.98578100
H	0.01119700	-4.70327600	4.59773800
H	-6.09732200	4.22154300	-2.18460200
N	-8.09978600	4.24174300	-0.42845700
H	-8.54976300	4.40680100	0.46129500
H	-7.99105600	5.10112000	-0.94910800

TSCu2-3

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.67017800	-0.05441500	0.10506700
P	0.84203000	-1.71259200	-0.29521000
P	0.92755700	1.25933200	1.04824800
C	1.65843300	0.91953100	2.70355600
C	1.10995200	-0.03691800	3.55436200
C	4.46439000	1.22689400	-1.99794300
C	2.44158600	1.29941700	-0.02131400
C	6.24119700	-1.15181700	3.95431600
C	4.26267000	-2.05036700	2.87580800
C	2.82877400	0.38785800	5.21660800
C	-0.10575600	-3.29833600	-0.21870100
C	0.55316800	3.76910400	2.42182900
C	-0.43761200	-3.99961800	-1.37992200
C	0.39591100	3.01844000	1.25231200
C	-2.11710200	-5.30433600	-0.20266500
C	1.77722900	-1.88704600	-1.86785500
C	-0.78944600	-3.63681900	0.96136100
C	2.25792400	-1.88890600	0.88766200
C	3.31447000	0.21970700	-0.05533100
C	2.57480600	2.33937300	-0.97976700
C	6.19150300	-0.96869600	-2.15800100
C	4.33856900	0.16475200	-1.06198100
C	-0.83274300	4.88403500	0.29597600
C	5.22669200	-0.93854400	-1.18417700
C	3.35993300	-3.04915400	-3.28208900
C	0.02867700	5.05445000	2.51920600

C	3.55683900	2.31134700	-1.92818000
C	6.27508200	-0.10900200	3.00038700
C	5.25511800	-2.10047600	3.88898200
C	2.79386500	1.61858400	3.13134300
C	1.69324600	-0.30020400	4.79155000
C	3.36271100	1.36360200	4.37002900
C	2.29675300	-2.96446600	1.81140800
C	3.25637100	-3.03952000	2.78133700
C	4.28019500	-0.99528400	1.92444400
C	3.37931900	-1.97700400	-4.18176400
C	-1.42941100	-4.98154300	-1.36957200
C	2.58341500	-3.00080900	-2.13368600
C	5.47077200	1.16935200	-2.99564300
C	3.24860700	-0.91593300	0.92882000
C	-0.66893200	5.63680400	1.46021000
C	-0.32339200	3.59495500	0.19995800
C	1.78048800	-0.82661800	-2.76658200
C	6.32301700	0.09892600	-3.07389200
C	5.32255900	-0.03151600	2.01815900
C	-1.76072100	-4.62809900	0.97012300
C	2.57921100	-0.87067200	-3.90629300
H	0.23626800	-0.59010000	3.22208700
H	6.99905300	-1.20003300	4.73090900
H	1.07577200	3.35325400	3.27530600
H	0.05699000	-3.76314200	-2.31678700
H	-0.60326400	-3.06746800	1.86668600
H	1.87892400	3.17096300	-0.96772900
H	6.85567900	-1.82508900	-2.23051700
H	-1.37743000	5.30771400	-0.54450600
H	5.12987100	-1.77395600	-0.50050600
H	3.98159700	-3.92049800	-3.47556400
H	0.16331700	5.61230200	3.44325100
H	3.63423600	3.11665200	-2.65329400
H	7.05778100	0.64210200	3.05156800
H	5.21814500	-2.91043800	4.61334100
H	3.25005300	2.35785800	2.47703600
H	1.26251000	-1.06653800	5.43199300
H	4.25613300	1.90451300	4.67213400
H	1.55320500	-3.74982300	1.74816500
H	3.25909900	-3.86517900	3.48861900
H	-1.68020500	-5.49024800	-2.29738200
H	2.60830400	-3.83086800	-1.43127000
H	5.54898200	1.99271200	-3.70156200
H	-0.49206500	3.01015300	-0.69808800
H	1.18884600	0.05390900	-2.52768100
H	7.09356600	0.06544900	-3.83888900
H	5.35191000	0.78491300	1.30582200
H	-2.27944900	-4.85781800	1.89849000
H	2.60702300	-0.01391200	-4.57505900
H	-0.62009700	0.74720500	-1.52677800
H	-0.94827800	-0.75628700	1.58268000
C	3.49425500	0.07367900	6.53184800
H	4.44425600	-0.44680900	6.36235700
H	3.71554500	0.98704300	7.09509100
H	2.86542600	-0.56719700	7.15758000
C	-1.26415800	7.01607300	1.58818000
H	-2.25628800	6.96962300	2.05352000
H	-0.63947500	7.66401000	2.21147900
H	-1.38153400	7.49322700	0.61022000
C	-3.24728900	-6.30004300	-0.19873400

H	-3.28919800	-6.86290400	-1.13597900
H	-3.14863900	-7.01625400	0.62443400
H	-4.20609300	-5.78099000	-0.07457900
C	4.28750500	-2.00115700	-5.38315600
H	5.31607700	-1.76400800	-5.08533500
H	4.29877700	-2.98700500	-5.86003200
H	3.98138900	-1.26310400	-6.13064700
N	-2.36829400	1.23974900	0.47077000
N	-2.36108100	-1.26930200	-0.58351100
C	-3.67483600	-0.60056200	-0.42880900
C	-3.58062000	0.43019100	0.71127900
H	-2.24521600	1.90690800	1.22884800
H	-2.48997700	1.77570800	-0.39942300
H	-3.84863100	-0.02916100	-1.34574800
H	-2.33847400	-2.10684600	-0.00740700
H	-2.25991200	-1.60002600	-1.53980700
C	-4.79326100	-1.59619100	-0.22202800
C	-5.91481700	-1.61314600	-1.04898300
C	-4.72844400	-2.53715400	0.80924300
C	-6.93079100	-2.54381500	-0.87086700
H	-6.00028700	-0.87768100	-1.84493400
C	-5.73345700	-3.47600900	0.99625400
H	-3.87608700	-2.54551400	1.48637000
C	-6.85281100	-3.49575900	0.15246200
H	-7.79727600	-2.53071600	-1.52750800
C	-4.85237400	1.24422200	0.81628000
C	-5.22642200	2.13330900	-0.19705900
C	-5.70569500	1.09781400	1.90842200
C	-6.40810900	2.85517600	-0.11168500
H	-4.58734200	2.26266300	-1.06776100
C	-6.89251600	1.81427500	2.00197700
H	-5.44354100	0.40130400	2.70150500
C	-7.26108600	2.70786800	0.99049400
H	-6.68143300	3.53910600	-0.91200900
H	-7.54362600	1.67553000	2.86177300
H	-3.41210300	-0.10571500	1.65157400
C	-1.64034900	1.42759600	-2.82087000
O	-2.62819000	1.95114000	-2.26036600
N	-8.47591800	3.39525400	1.04864300
H	-8.83967000	3.52701000	1.98231400
H	-8.49430100	4.25847400	0.52328200
C	-0.56196100	2.34477300	-3.36108400
C	0.45016000	1.90873200	-4.21900200
C	-0.64211700	3.70650100	-3.06401100
C	1.39916600	2.80031000	-4.70882400
H	0.50012000	0.86751200	-4.51643400
C	0.31001400	4.59989800	-3.54070600
H	-1.48000100	4.04556700	-2.46434600
C	1.34315500	4.14716600	-4.35889500
H	2.18361100	2.44178800	-5.37018300
H	0.23717000	5.65362100	-3.28629800
H	2.08595100	4.84338300	-4.73827600
C	-1.82289400	0.10810000	-3.56480600
H	-2.03666300	0.32637800	-4.61964800
H	-0.94626200	-0.54134500	-3.51218900
H	-2.69247800	-0.41142300	-3.15836800
H	-5.66137800	-4.19422100	1.80998400
N	-7.88942800	-4.40472100	0.36646100
H	-8.45964700	-4.59724800	-0.44506900
H	-7.61820800	-5.25547800	0.83921300

C3u

Coordinates (Angstroms)

X	Y	Z	
Ru	0.63427400	0.10782500	0.05203000
P	-0.90521800	1.70593200	-0.57637000
P	-0.95732600	-1.09669300	1.19064900
C	-1.64943800	-0.51124500	2.78728100
C	-1.07693400	0.56511500	3.46141500
C	-4.47989700	-1.50408900	-1.84800200
C	-2.47287800	-1.28303100	0.13596400
C	-6.27589400	1.59881700	3.73321000
C	-4.32248800	2.39474100	2.53490800
C	-2.76266400	0.43775200	5.20146200
C	0.01603100	3.29982800	-0.68869400
C	-0.57726500	-3.42401500	2.83772700
C	0.30180600	3.89526800	-1.91847900
C	-0.41929400	-2.81347100	1.59109200
C	1.95097500	5.36316500	-0.90134800
C	-1.79418200	1.61423600	-2.17348300
C	0.70385600	3.77223500	0.44160700
C	-2.32202000	2.01721600	0.57267500
C	-3.33831400	-0.21662700	-0.07562400
C	-2.62102600	-2.46489500	-0.63603400
C	-6.20246900	0.64396300	-2.34625800
C	-4.35424700	-0.31123800	-1.08569300
C	0.76500600	-4.79451500	0.83166000
C	-5.24448800	0.76024000	-1.37266600
C	-3.40638400	2.42971300	-3.77798900
C	-0.07400800	-4.70213400	3.07047000
C	-3.59368900	-2.57548400	-1.58923900
C	-6.29164200	0.44220700	2.92010800
C	-5.31170600	2.55287900	3.54047700
C	-2.77981600	-1.12051100	3.34590000
C	-1.63012200	1.03393900	4.64949400
C	-3.32076100	-0.65799900	4.53658500
C	-2.37906700	3.20361600	1.34833200
C	-3.33727200	3.38357300	2.30653000
C	-4.32198600	1.22628400	1.72718800
C	-3.27710400	1.26363400	-4.54033900
C	1.25640300	4.90801700	-2.01951500
C	-2.68512800	2.60216900	-2.60463900
C	-5.47941500	-1.59678700	-2.85060500
C	-3.29217500	1.04020000	0.74561300
C	0.59786400	-5.41042200	2.07484700
C	0.27938000	-3.51642400	0.60002800
C	-1.64401400	0.46500100	-2.94300800
C	-6.32830300	-0.54925000	-3.09376700
C	-5.34267800	0.26048500	1.94837100
C	1.63845300	4.79225100	0.33773600
C	-2.37669600	0.28914500	-4.11081400
H	-0.20646000	1.05213300	3.03469800
H	-7.03141700	1.72979400	4.50250500
H	-1.08425300	-2.90650000	3.64448400
H	-0.19897700	3.55108300	-2.81782400

H	0.54209400	3.29651500	1.40457000
H	-1.94647300	-3.29828000	-0.47778200
H	-6.86650800	1.47862400	-2.55076700
H	1.28362900	-5.31008600	0.02777300
H	-5.15022800	1.68895900	-0.82158500
H	-4.10352700	3.20032500	-4.09820600
H	-0.20906400	-5.15403000	4.05041700
H	-3.68580800	-3.49337900	-2.16347900
H	-7.05883000	-0.31139500	3.07156700
H	-5.29134400	3.45113900	4.15287800
H	-3.25461200	-1.95177600	2.83040100
H	-1.17851000	1.88918100	5.14650700
H	-4.21120900	-1.13273200	4.94068900
H	-1.65125800	3.98807600	1.17860300
H	-3.35508200	4.29515100	2.89869100
H	1.47298500	5.33616800	-2.99507400
H	-2.82344700	3.50457200	-2.01369000
H	-5.55938200	-2.51950100	-3.41984500
H	0.45261100	-3.06468200	-0.37039800
H	-0.96854400	-0.30913700	-2.59391500
H	-7.09564600	-0.63026400	-3.85842500
H	-5.35893900	-0.64037100	1.34572100
H	2.16305900	5.12889100	1.22909000
H	-2.25825500	-0.62669300	-4.68542500
H	0.82768900	-1.19886500	-1.74569000
H	0.83546200	0.98923600	1.34733700
C	-3.39757100	0.97189100	6.45922500
H	-4.35196600	1.45853900	6.22602300
H	-3.60483500	0.16886100	7.17494900
H	-2.75483600	1.70750500	6.95214700
C	1.15893900	-6.78611300	2.32903700
H	0.76083400	-7.21814800	3.25225900
H	0.92275800	-7.46739000	1.50476600
H	2.25098500	-6.75007600	2.42056900
C	3.04784400	6.38905600	-1.01432600
H	4.02554000	5.90386500	-0.89966400
H	3.03167200	6.89058000	-1.98627500
H	2.96374500	7.15300000	-0.23381300
C	-4.12810600	1.04398200	-5.76323400
H	-5.06786800	0.55314400	-5.48190500
H	-4.37929200	1.98918100	-6.25476600
H	-3.62418900	0.40140400	-6.49175900
N	2.32668600	-1.08921900	0.58256100
N	2.29474700	1.19678600	-0.85352400
C	3.63185300	0.62164300	-0.53114600
C	3.51261000	-0.22464700	0.75121300
H	2.22861000	-1.70885300	1.38358000
H	2.49425200	-1.67138700	-0.29969200
H	3.85843800	-0.07884300	-1.34009000
H	2.24299600	2.15327800	-0.51007500
H	2.20600100	1.26876500	-1.86524900
C	4.68607100	1.69598600	-0.41971700
C	5.83430100	1.67418900	-1.20952200
C	4.53803100	2.75038400	0.48549900
C	6.79549700	2.67284000	-1.11476100
H	5.98232000	0.85566700	-1.90907300
C	5.48648000	3.75887200	0.58672800
H	3.66230500	2.79124400	1.13060900
C	6.63411100	3.73526900	-0.21754800
H	7.68589700	2.62695800	-1.73710400

C	4.79229400	-0.98817600	1.01695200
C	5.62118100	-0.63372000	2.07945300
C	5.19635100	-2.03580800	0.18067200
C	6.81751400	-1.29945200	2.31829100
H	5.33270000	0.18658000	2.73313500
C	6.38811200	-2.70716400	0.41490600
H	4.56945300	-2.32430300	-0.66190900
C	7.21763100	-2.35047200	1.48667800
H	7.45094000	-0.99877900	3.14969100
H	6.68872900	-3.51561800	-0.24799100
H	3.31646000	0.44560200	1.59667400
C	1.57493000	-1.78867200	-2.43619700
O	2.75091200	-1.98931600	-1.84047900
N	8.44341200	-2.99431600	1.68525800
H	8.78164200	-2.96203000	2.63726900
H	8.48232800	-3.93512000	1.31755600
C	1.68378700	-0.92825300	-3.71386300
H	0.71575400	-0.71937000	-4.18352100
H	2.17227700	0.02512800	-3.48158300
H	2.31745100	-1.45620400	-4.43442800
C	0.83546100	-3.10083700	-2.77527500
C	-0.48344000	-3.15253100	-3.23056100
C	1.53495900	-4.29923000	-2.63319400
C	-1.08984700	-4.36960700	-3.53040200
H	-1.05883800	-2.23784000	-3.33752800
C	0.93409000	-5.51963100	-2.93100600
H	2.55534200	-4.23105800	-2.26931300
C	-0.38386900	-5.56091800	-3.37964300
H	-2.11710800	-4.38698300	-3.88675400
H	1.49457500	-6.44380300	-2.81168900
H	-0.85741500	-6.51121400	-3.61018000
H	5.35082000	4.56262000	1.30726300
N	7.61849800	4.71561000	-0.08265400
H	8.21165400	4.83437000	-0.89198000
H	7.28834000	5.60355900	0.26842700

TSCu3-4

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.65655000	-0.12206700	0.07232800
P	0.88189300	-1.71646500	-0.59225300
P	0.92994200	1.05466400	1.24073400
C	1.63404000	0.42294800	2.81477600
C	1.05895800	-0.66520800	3.46728200
C	4.42693900	1.51782600	-1.82730300
C	2.44042500	1.25804600	0.17601400
C	6.27897300	-1.68945300	3.68295500
C	4.31767900	-2.46515700	2.48379500
C	2.76061300	-0.59327800	5.19522100
C	-0.04712200	-3.30609300	-0.72085400
C	0.62127000	3.35365100	2.94709500
C	-0.34371300	-3.88669200	-1.95530700
C	0.42478800	2.77099900	1.69230800
C	-2.00306300	-5.34953700	-0.94723300
C	1.76535800	-1.62272300	-2.19669000

C	-0.73351800	-3.78613000	0.40733200
C	2.30575900	-2.05499800	0.54004700
C	3.30577500	0.19696800	-0.06504200
C	2.58083200	2.45353600	-0.57722000
C	6.14657500	-0.61890500	-2.38144700
C	4.31066000	0.31181800	-1.08446500
C	-0.72081700	4.79842000	0.99630300
C	5.19980700	-0.75294100	-1.39919500
C	3.37480700	-2.43663000	-3.80712300
C	0.15759300	4.63965100	3.21478300
C	3.54299200	2.58325200	-1.53888000
C	6.28728300	-0.51726300	2.89228400
C	5.31459500	-2.64101700	3.47880100
C	2.77533900	1.00819800	3.37722300
C	1.61927600	-1.16763100	4.63845300
C	3.32241000	0.51350300	4.55188200
C	2.37039000	-3.25663300	1.29143700
C	3.33377700	-3.45207600	2.24161200
C	4.30941100	-1.28074500	1.69955100
C	3.23816700	-1.27374600	-4.57276800
C	-1.30844900	-4.88926200	-2.06324300
C	2.65854200	-2.60769500	-2.63041600
C	5.41492700	1.62892800	-2.83966700
C	3.27181900	-1.07721800	0.72993100
C	-0.51260900	5.38633700	2.24640400
C	-0.27630000	3.51191800	0.73160000
C	1.60549300	-0.47872700	-2.97277200
C	6.26208500	0.58673300	-3.11060100
C	5.33056700	-0.31801600	1.93155000
C	-1.67911300	-4.79542400	0.29658500
C	2.33301300	-0.30329900	-4.14421800
H	0.17962500	-1.13365900	3.03786200
H	7.04016400	-1.83427900	4.44417800
H	1.12880300	2.80773100	3.73440200
H	0.15747400	-3.53895000	-2.85316300
H	-0.56052200	-3.32488300	1.37536500
H	1.90949000	3.28472800	-0.39545800
H	6.80955300	-1.44894400	-2.60727300
H	-1.24314700	5.34421300	0.21479800
H	5.11360300	-1.69030700	-0.86158700
H	4.07472800	-3.20505700	-4.12664500
H	0.32250300	5.06771500	4.20085900
H	3.62601100	3.51142300	-2.09770300
H	7.05481700	0.23422000	3.05246200
H	5.30009900	-3.55113400	4.07360700
H	3.25348100	1.84660800	2.87660300
H	1.16517900	-2.03107100	5.11869600
H	4.22066200	0.97082500	4.95884500
H	1.64332000	-4.03933600	1.10982600
H	3.35744200	-4.37480400	2.81602400
H	-1.53259700	-5.30564800	-3.04228500
H	2.80353500	-3.50710700	-2.03650300
H	5.48813400	2.56181100	-3.39317100
H	-0.48973300	3.08070300	-0.23858500
H	0.92828300	0.29480800	-2.62575700
H	7.02103800	0.68193700	-3.88204000
H	5.34094100	0.59415800	1.34584700
H	-2.20200500	-5.13755200	1.18691800
H	2.20883100	0.60896500	-4.72346900
H	-0.72929500	1.32011300	-1.76208100

H	-0.85501800	-1.02469700	1.34492700
C	3.39825600	-1.15751400	6.43849400
H	4.37890500	-1.58719800	6.20316400
H	3.55241300	-0.38053100	7.19558700
H	2.78215500	-1.94507500	6.88274900
C	-1.02967500	6.77163900	2.53877600
H	-0.80220700	7.46036400	1.71816500
H	-2.11887500	6.76208000	2.66497500
H	-0.59186500	7.17876900	3.45532500
C	-3.10960000	-6.36441600	-1.06640600
H	-4.08298100	-5.87156700	-0.94790100
H	-3.09871200	-6.85949400	-2.04178500
H	-3.03187000	-7.13445800	-0.29127700
C	4.08775800	-1.05201000	-5.79623700
H	4.33338000	-1.99584200	-6.29324200
H	3.58638700	-0.40281500	-6.52068100
H	5.03051800	-0.56761100	-5.51354100
N	-2.31307100	1.08425600	0.53754700
N	-2.31201500	-1.19190400	-0.87316700
C	-3.64388600	-0.59476500	-0.56923700
C	-3.50483600	0.24639500	0.71559500
H	-2.22394200	1.71027100	1.33506600
H	-2.46489000	1.77661300	-0.60425600
H	-3.86402300	0.10480800	-1.38091700
H	-2.27406100	-2.13700800	-0.49720800
H	-2.21589700	-1.30849500	-1.88032500
C	-4.71633600	-1.65332000	-0.47593400
C	-5.86582500	-1.60314500	-1.26243000
C	-4.58629300	-2.72049100	0.41726500
C	-6.84459100	-2.58575000	-1.17719100
H	-6.00328400	-0.77359700	-1.95133900
C	-5.55219900	-3.71298000	0.50903600
H	-3.71239700	-2.78353300	1.06281400
C	-6.70073300	-3.66090700	-0.29248800
H	-7.73553600	-2.51636300	-1.79656000
C	-4.78180200	1.01734200	0.99055900
C	-5.63079400	0.62988800	2.02632400
C	-5.17114500	2.10055300	0.19510600
C	-6.82569000	1.29426600	2.27664500
H	-5.35642800	-0.21725500	2.65128900
C	-6.36201100	2.77160500	0.43794200
H	-4.53537800	2.42433800	-0.62519100
C	-7.20842900	2.38005300	1.48300400
H	-7.47119100	0.96589300	3.08816100
H	-6.64719600	3.60866400	-0.19599200
H	-3.35124300	-0.45281500	1.55159300
C	-1.44758100	1.94520600	-2.38040400
O	-2.58784500	2.20548200	-1.66847500
N	-8.43353000	3.02575800	1.69102200
H	-8.78101900	2.95708800	2.63797900
H	-8.45356500	3.98401700	1.36919000
C	-1.75234500	1.13363100	-3.64819200
H	-0.84705600	0.87805800	-4.21039600
H	-2.27196600	0.20699400	-3.38187300
H	-2.41447000	1.71711600	-4.29597600
C	-0.69301800	3.22721700	-2.74833600
C	0.59250800	3.20585200	-3.29233100
C	-1.31502300	4.46080400	-2.55587900
C	1.24171300	4.38792900	-3.63648900
H	1.10786700	2.26029300	-3.43253500

C	-0.66768300	5.64637800	-2.89458000
H	-2.30978700	4.45945800	-2.12272100
C	0.61425500	5.61530300	-3.43751500
H	2.24141000	4.34836100	-4.06184300
H	-1.16635100	6.59889400	-2.73485400
H	1.12112600	6.53890500	-3.70248600
H	-5.42943400	-4.52605500	1.22135100
N	-7.70196400	-4.62542900	-0.16627100
H	-8.29738300	-4.72612600	-0.97638900
H	-7.38640100	-5.52234600	0.17537800

C4u

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.37984900	0.63221500	-0.62230000
P	1.36455400	1.75921000	0.35265200
P	0.95674200	-1.16127600	-1.13041100
C	2.20302800	-1.07941400	-2.47759100
C	2.23137800	-0.00302400	-3.36110000
C	3.24468600	-2.10456200	2.84809300
C	1.99774200	-1.62154400	0.34552300
C	7.31629400	-0.58729700	-2.21631400
C	5.48924700	0.91691900	-1.68072400
C	4.14263800	-0.94343100	-4.52308400
C	1.13506800	3.58996700	0.23583300
C	0.20278800	-3.37315200	-2.79101100
C	1.11616200	4.44536700	1.33903000
C	0.02984500	-2.69438500	-1.58176400
C	0.54747200	6.34793800	-0.06283400
C	1.64091300	1.49305200	2.14697800
C	0.83182500	4.13777500	-1.02092400
C	3.06575900	1.45713800	-0.32155800
C	3.09661600	-0.85630600	0.71831200
C	1.53361500	-2.63738700	1.22492000
C	5.50891600	-0.63739900	3.59007900
C	3.75052600	-1.10626300	1.97368700
C	-1.84629300	-4.16759700	-1.09664800
C	4.90198400	-0.38151500	2.38817300
C	2.98191700	1.71673900	4.14991500
C	-0.63080300	-4.43423500	-3.13947200
C	2.12195700	-2.86186400	2.43789700
C	6.75195600	-1.56157600	-1.36146100
C	6.69490000	0.62413600	-2.37019900
C	3.14727600	-2.10031500	-2.64145000
C	3.19175900	0.06354400	-4.36654100
C	4.09554200	-2.03546800	-3.65155400
C	3.68222300	2.43141200	-1.14938000
C	4.84784300	2.17088300	-1.81400200
C	4.91058300	-0.06220200	-0.82997400
C	2.10675900	0.88817800	4.85816300
C	0.82424100	5.80059000	1.18806900
C	2.76060200	2.00448300	2.81116600
C	3.88106700	-2.33751400	4.09476800
C	3.67250000	0.21849100	-0.15983500
C	-1.66463900	-4.84980800	-2.30207600

C	-1.02098800	-3.10784000	-0.75185000
C	0.74074000	0.70108200	2.85958200
C	4.99319400	-1.62462100	4.45972300
C	5.58272400	-1.30846200	-0.69306900
C	0.55909200	5.49038400	-1.16869900
C	0.98225500	0.39568400	4.19630800
H	1.50725700	0.79593400	-3.24252800
H	8.24194900	-0.79997600	-2.74337400
H	0.98134200	-3.07303000	-3.48288200
H	1.32185800	4.05808400	2.33132100
H	0.80334300	3.48355500	-1.88881800
H	0.69646800	-3.25821200	0.92868700
H	6.38875600	-0.07078000	3.88067400
H	-2.65296800	-4.44873800	-0.42658600
H	5.29961300	0.39245500	1.74201500
H	3.86611700	2.11009000	4.64555700
H	-0.47353100	-4.93995400	-4.08946800
H	1.74190900	-3.64147300	3.09389500
H	7.24498900	-2.52158200	-1.23985100
H	7.11765400	1.38423600	-3.02275500
H	3.14858300	-2.94712900	-1.95938300
H	3.20672100	0.92228400	-5.03362700
H	4.83170100	-2.82955400	-3.74773800
H	3.21873400	3.40506300	-1.26027600
H	5.29699100	2.92911700	-2.45065700
H	0.81445200	6.44173100	2.06655600
H	3.47790200	2.61365900	2.26595000
H	3.47314500	-3.10131100	4.75228100
H	-1.22563000	-2.56875800	0.16480400
H	-0.14748900	0.31483200	2.36317000
H	5.48021200	-1.81633900	5.41158900
H	5.15410800	-2.07280400	-0.05504000
H	0.34223600	5.88869900	-2.15743800
H	0.29165200	-0.25104600	4.73082400
H	-1.00141700	-1.82708800	2.49108700
H	0.11561400	1.33577500	-1.94738100
C	5.21981500	-0.84896800	-5.57266100
H	6.17717800	-0.58299600	-5.10897800
H	5.35945600	-1.80480800	-6.08904600
H	4.98484500	-0.08761400	-6.32257200
C	-2.58685300	-5.98062700	-2.68094800
H	-2.26563800	-6.47048400	-3.60512900
H	-2.62769000	-6.73735500	-1.88978100
H	-3.60931600	-5.61417600	-2.83133200
C	0.21523200	7.80935500	-0.22574900
H	-0.86019900	7.95073500	-0.38708000
H	0.49614400	8.38432900	0.66177800
H	0.73343700	8.24119200	-1.08850300
C	2.39952400	0.51139600	6.28734300
H	3.18242000	-0.25549700	6.32226200
H	2.75354900	1.37236800	6.86439100
H	1.51262100	0.10772500	6.78518200
N	-2.15784400	-0.31283400	-0.85840700
N	-1.81595900	2.25629700	-0.35843300
C	-3.21062300	1.74628300	-0.22163800
C	-3.31943600	0.52948000	-1.14914200
H	-2.22453700	-1.17227500	-1.39546700
H	-2.34838500	-0.65837800	0.90937700
H	-3.28269500	1.37816600	0.80714300
H	-1.74644200	2.81295700	-1.20958200

H	-1.61509200	2.90386200	0.40200000
C	-4.22120800	2.85209100	-0.42935700
C	-4.78416400	3.49726800	0.67383200
C	-4.58313500	3.31037700	-1.69892500
C	-5.67496900	4.55223800	0.52687200
H	-4.52396700	3.16078600	1.67567500
C	-5.47157100	4.36442500	-1.86133200
H	-4.17239200	2.83561300	-2.58608900
C	-6.03385800	5.00380400	-0.74884700
H	-6.10570800	5.02510500	1.40616400
C	-4.60953200	-0.26691200	-1.01207700
C	-4.80550300	-1.33704300	-1.89174100
C	-5.57439700	-0.06790300	-0.02560800
C	-5.89040100	-2.19216400	-1.77885200
H	-4.07771100	-1.51929200	-2.68016600
C	-6.67513300	-0.91242800	0.09403300
H	-5.47807100	0.74826800	0.68197000
C	-6.84360300	-1.99572600	-0.77200400
H	-6.00490200	-3.01885800	-2.47638800
H	-7.40951100	-0.73022000	0.87516700
H	-3.26882700	0.89483600	-2.19180500
C	-2.08799600	-1.67149100	2.62180900
O	-2.51574800	-0.55354300	1.89018800
N	-7.95998100	-2.83464100	-0.66968700
H	-7.82295600	-3.75998800	-1.05297800
H	-8.36519100	-2.87929100	0.25545100
C	-2.35532500	-1.35725400	4.09327100
H	-1.97206600	-2.14857500	4.74584400
H	-1.88115400	-0.40753700	4.35865200
H	-3.43358200	-1.26010100	4.25656100
C	-2.79612900	-2.96173400	2.23084800
C	-2.21831700	-4.19754900	2.53137400
C	-4.04707600	-2.93323400	1.61630700
C	-2.88637600	-5.38437100	2.24564400
H	-1.23280700	-4.22820700	2.99336400
C	-4.71867800	-4.11936200	1.32819500
H	-4.48772500	-1.97702200	1.35838300
C	-4.14515500	-5.34805200	1.64686600
H	-2.42203700	-6.33772600	2.48157700
H	-5.69157800	-4.07458400	0.84613900
H	-4.66737300	-6.27363900	1.42085700
H	-5.74426700	4.69098500	-2.86213200
N	-6.97063300	6.02462900	-0.90940200
H	-7.04371700	6.66196900	-0.12884600
H	-6.91387100	6.51882400	-1.78881200

C5

Coordinates (Angstroms)

X	Y	Z
Ru	0.73223000	-0.00983600
P	-0.60731100	-1.66190600
P	-0.96190000	1.53352500
C	-2.25952600	1.65336800
C	-2.17545200	0.89346400
C	-3.29316100	0.87844600

C	-2.01764900	1.33281000	0.89012400
C	-7.05101400	-0.27044300	-1.98651800
C	-4.89251300	-1.36392000	-1.80739400
C	-4.31829700	1.74286700	-3.86031400
C	0.02220000	-3.34515700	-0.40943500
C	-0.72459800	4.28968400	-1.40883800
C	0.30207100	-4.34582700	0.52624000
C	-0.35565000	3.27579400	-0.52002800
C	1.21547100	-5.79752400	-1.19624400
C	-0.80936000	-1.78920000	1.86155000
C	0.37671700	-3.58803400	-1.74495200
C	-2.36543600	-1.63381600	-0.55404500
C	-2.90713900	0.27279300	1.02013800
C	-1.80177700	2.18527400	2.00559300
C	-5.09217800	-1.24387800	3.67464100
C	-3.56866600	0.03850400	2.27421900
C	1.19425200	4.84036600	0.51657800
C	-4.49088000	-1.02903800	2.46185000
C	-1.86643900	-2.69123600	3.84352900
C	-0.15104100	5.55527000	-1.32602300
C	-2.40410000	1.96377600	3.21156700
C	-6.70011500	0.57651200	-0.91112400
C	-6.16137100	-1.21630400	-2.42511200
C	-3.37710900	2.47599900	-1.75201700
C	-3.19579100	0.93623600	-4.04474000
C	-4.38392300	2.52663900	-2.70482300
C	-2.76046900	-2.48887200	-1.61708500
C	-3.97464600	-2.35561300	-2.22939500
C	-4.53083400	-0.51143900	-0.73074100
C	-1.13271000	-1.82617900	4.66066300
C	0.89081100	-5.54626100	0.13700400
C	-1.71413600	-2.66872000	2.46431000
C	-3.92017900	0.62673300	4.63342200
C	-3.24011900	-0.64983700	-0.11543300
C	0.81424600	5.85498200	-0.36367100
C	0.62699100	3.57469900	0.43413700
C	-0.05931800	-0.94100400	2.67444100
C	-4.80296100	-0.41063800	4.77929000
C	-5.47544600	0.46308300	-0.30627600
C	0.94907300	-4.79431700	-2.13123500
C	-0.22272100	-0.95864000	4.05626400
H	-1.31542800	0.24827000	-3.24576700
H	-8.02316100	-0.16979300	-2.46063600
H	-1.46269200	4.09718500	-2.17979400
H	0.07821200	-4.18837800	1.57546600
H	0.22191300	-2.80523900	-2.48293300
H	-1.14846500	3.04202200	1.90261800
H	-5.79304500	-2.06559900	3.78975500
H	1.96179900	5.03073900	1.26296300
H	-4.71081300	-1.69141100	1.63241300
H	-2.58977800	-3.36704700	4.29304400
H	-0.46050200	6.32386600	-2.03077700
H	-2.21190400	2.63060600	4.04855600
H	-7.40372700	1.32899400	-0.56742300
H	-6.41739700	-1.87638800	-3.25037700
H	-3.46876200	3.06784800	-0.84435600
H	-3.12202600	0.31884300	-4.93694100
H	-5.25224800	3.15858800	-2.53531900
H	-2.08483600	-3.26770000	-1.95135200
H	-4.25356800	-3.02165200	-3.04226600

H	1.10595500	-6.30021700	0.89081100
H	-2.32364800	-3.32258200	1.84474800
H	-3.68879800	1.28010400	5.47123300
H	0.97445600	2.79299600	1.10168100
H	0.63141700	-0.24113100	2.20774100
H	-5.28375900	-0.59212900	5.73623300
H	-5.21371300	1.13496400	0.50310700
H	1.20562900	-4.95307100	-3.17611800
H	0.35576200	-0.27515400	4.67323300
H	0.11620500	-0.61623900	-2.13113200
C	-5.45380400	1.73851800	-4.85069700
H	-6.24756700	1.06310800	-4.50949500
H	-5.89359800	2.73502300	-4.96367400
H	-5.12478700	1.39650800	-5.83705900
C	1.45158700	7.22016200	-0.30444900
H	0.71506100	8.01130400	-0.48020000
H	1.91962400	7.40017900	0.66815200
H	2.23022900	7.32070200	-1.07023600
C	1.82607300	-7.11165900	-1.61228900
H	2.33838500	-7.02672900	-2.57538100
H	2.55057200	-7.46610400	-0.87200200
H	1.05532800	-7.88535700	-1.71368300
C	-1.36211500	-1.80418900	6.14997100
H	-2.29085500	-1.26857900	6.38029700
H	-1.45710000	-2.81650300	6.55723400
H	-0.54416300	-1.30113300	6.67496700
N	2.21852200	1.31233500	-0.72907400
N	2.50482800	-1.26724700	-1.00295100
C	3.66347900	-0.57594000	-0.39162300
C	3.59821400	0.89460100	-0.84864800
H	2.13812400	2.31079300	-0.89562700
H	3.46854800	-0.57846800	0.68672600
H	2.63884300	-1.35682300	-2.00897400
H	2.42872900	-2.21728800	-0.64382900
C	4.99471500	-1.23942000	-0.65733200
C	5.85585100	-1.54819400	0.39537700
C	5.43384400	-1.51464800	-1.95488600
C	7.10358600	-2.11516500	0.17194300
H	5.55130600	-1.32444500	1.41474000
C	6.67666600	-2.08471800	-2.19412200
H	4.80318300	-1.26948800	-2.80741600
C	7.53393300	-2.39440500	-1.13012000
H	7.75197400	-2.34626100	1.01364300
C	4.54716000	1.74135700	-0.01486700
C	5.83846700	2.04326400	-0.44420800
C	4.15014000	2.21476100	1.23687200
C	6.70389000	2.79859000	0.33914100
H	6.17911500	1.67568500	-1.40970000
C	5.00311300	2.97064200	2.02970400
H	3.14471500	1.98581000	1.57896800
C	6.29663300	3.27756700	1.58914100
H	7.70716300	3.01830200	-0.01931200
H	4.66895000	3.32696900	3.00215400
H	3.95632000	0.92786300	-1.89661300
N	7.17786000	4.00034200	2.40354200
H	7.89790700	4.49502200	1.89456400
H	6.71915500	4.61448100	3.06292200
H	6.98942100	-2.29320700	-3.21457100
N	8.76390200	-3.01421900	-1.36053600
H	9.15666200	-2.84199500	-2.27570200

H	9.45068600	-2.86578500	-0.63402000
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Cartesian coordinates of the RuH₂(diphosphine)(diamine) complexes in training set and test set (optimized in gas phase at B3LYP/BSI level).

RuH₂[(*R*)-P-Phos][(*R,R*)-dpen]

Coordinates (Angstroms)

X	Y	Z	

Ru	0.99430000	-0.00010000	-0.00150000
P	-0.56310000	1.62500000	0.36240000
P	-0.56340000	-1.62530000	-0.36380000
O	-3.49260000	3.16020000	-3.64520000
O	-4.92910000	-0.59360000	-1.37470000
O	-4.92720000	0.59370000	1.37870000
O	-3.48680000	-3.15890000	3.64860000
N	2.71840000	1.32620000	0.41990000
H	2.79880000	2.01290000	-0.32890000
H	2.56210000	1.85460000	1.27600000
N	2.71870000	-1.32570000	-0.42460000
H	2.79870000	-2.01390000	0.32290000
H	2.56230000	-1.85240000	-1.28180000
N	-4.21910000	1.27250000	-2.51870000
N	-4.21530000	-1.27180000	2.52240000
C	-2.07560000	1.54470000	-0.73040000
C	-2.25690000	2.44880000	-1.77950000
H	-1.58890000	3.28120000	-1.95170000
C	-3.34170000	2.26420000	-2.63930000
C	-4.04520000	0.42170000	-1.50970000
C	-3.00040000	0.49110000	-0.56090000
C	-2.99960000	-0.49100000	0.56250000
C	-2.07450000	-1.54460000	0.73090000
C	-2.25410000	-2.44830000	1.78070000
H	-1.58580000	-3.28050000	1.95210000
C	-3.33760000	-2.26340000	2.64200000
C	-4.04300000	-0.42140000	1.51280000
C	-4.59750000	2.97270000	-4.52640000
H	-4.53140000	3.78740000	-5.25050000
H	-5.54950000	3.02350000	-3.98770000
H	-4.53800000	2.00660000	-5.03840000
C	-5.96420000	-0.69720000	-2.34820000
H	-6.55730000	-1.56280000	-2.04530000
H	-5.54820000	-0.85570000	-3.34810000
H	-6.58840000	0.20190000	-2.36300000
C	-4.59020000	-2.97100000	4.53160000
H	-4.52330000	-3.78580000	5.25550000
H	-5.54320000	-3.02150000	3.99430000
H	-4.52950000	-2.00510000	5.04350000
C	-5.96040000	0.69800000	2.35420000
H	-6.55420000	1.56330000	2.05160000
H	-5.54240000	0.85760000	3.35310000
H	-6.58440000	-0.20120000	2.37110000
C	-1.36800000	1.91180000	2.01990000
C	-2.47560000	2.76420000	2.16840000
H	-2.90920000	3.24640000	1.29680000
C	-3.02960000	2.99480000	3.42820000

H	-3.88420000	3.65960000	3.52860000
C	-2.48900000	2.37130000	4.55670000
C	-1.39520000	1.51570000	4.41680000
H	-0.97680000	1.01900000	5.28890000
C	-0.83790000	1.28690000	3.15580000
H	-0.00160000	0.60350000	3.02560000
C	0.15490000	3.31640000	0.00910000
C	0.15990000	4.36400000	0.94300000
H	-0.33460000	4.24100000	1.89990000
C	0.79800000	5.57630000	0.66010000
H	0.79070000	6.37030000	1.40270000
C	1.43540000	5.76980000	-0.56460000
C	1.44320000	4.73470000	-1.50390000
H	1.93680000	4.87230000	-2.46310000
C	0.82200000	3.51860000	-1.21610000
H	0.85920000	2.70090000	-1.93110000
C	-1.37010000	-1.91160000	-2.02060000
C	-2.47940000	-2.76190000	-2.16800000
H	-2.91370000	-3.24250000	-1.29580000
C	-3.03450000	-2.99230000	-3.42730000
H	-3.89050000	-3.65530000	-3.52680000
C	-1.39740000	-1.51750000	-4.41780000
H	-0.97830000	-1.02230000	-5.29050000
C	-0.83910000	-1.28870000	-3.15720000
H	-0.00150000	-0.60670000	-3.02790000
C	-2.49300000	-2.37090000	-4.55660000
C	0.15400000	-3.31720000	-0.01140000
C	0.82450000	-3.51880000	1.21200000
H	0.86480000	-2.70020000	1.92590000
C	1.44470000	-4.73540000	1.49960000
H	1.94120000	-4.87240000	2.45740000
C	1.43220000	-5.77180000	0.56180000
C	0.79110000	-5.57910000	-0.66110000
H	0.78000000	-6.37430000	-1.40250000
C	0.15420000	-4.36610000	-0.94380000
H	-0.34300000	-4.24370000	-1.89930000
C	3.97340000	0.54060000	0.55290000
H	3.89470000	0.02600000	1.51710000
C	3.97400000	-0.54030000	-0.55590000
H	3.89670000	-0.02570000	-1.52030000
C	5.21950000	1.41300000	0.55620000
C	5.54140000	2.22190000	-0.54440000
H	4.90650000	2.21920000	-1.42830000
C	6.67270000	3.03720000	-0.52430000
H	6.90590000	3.65720000	-1.38590000
C	7.50350000	3.05680000	0.59860000
H	8.38470000	3.69240000	0.61470000
C	7.19390000	2.25700000	1.69900000
H	7.83310000	2.26620000	2.57790000
C	6.05980000	1.44280000	1.67520000
H	5.82450000	0.82110000	2.53600000
C	5.21990000	-1.41290000	-0.55740000
C	6.06190000	-1.44290000	-1.67520000
H	5.82810000	-0.82120000	-2.53640000
C	7.19600000	-2.25730000	-1.69710000
H	7.83660000	-2.26660000	-2.57490000
C	7.50380000	-3.05700000	-0.59610000
H	8.38490000	-3.69260000	-0.61080000
C	6.67110000	-3.03720000	0.52550000
H	6.90290000	-3.65710000	1.38750000

C	5.54000000	-2.22170000	0.54370000
H	4.90370000	-2.21870000	1.42660000
H	1.12340000	-0.48570000	1.64420000
H	1.12160000	0.48540000	-1.64720000
H	1.92130000	-6.71720000	0.78210000
H	-2.92690000	-2.54970000	-5.53750000
H	1.92540000	6.71470000	-0.78510000
H	-2.92210000	2.55020000	5.53800000

RuH₂[(*R*)-P-Phos][(*S,S*)-dppen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.05860000	-0.00050000	0.00050000
P	0.50440000	1.61850000	0.37230000
P	0.50470000	-1.61910000	-0.37150000
N	-2.74430000	1.48390000	0.17620000
H	-2.99030000	1.62790000	1.15490000
H	-2.36980000	2.37380000	-0.14670000
N	-2.74400000	-1.48510000	-0.17570000
H	-2.98860000	-1.63010000	-1.15450000
H	-2.36980000	-2.37460000	0.14860000
C	1.31060000	2.58730000	-1.00210000
C	0.76980000	2.52530000	-2.29280000
H	-0.07320000	1.86040000	-2.46810000
C	1.32400000	3.27870000	-3.33120000
C	2.42510000	4.10210000	-3.09200000
H	2.85560000	4.68910000	-3.89970000
C	2.97680000	4.16540000	-1.80900000
C	2.42590000	3.41150000	-0.77200000
H	2.86780000	3.46220000	0.21920000
C	-0.20410000	2.99960000	1.41930000
C	-0.87730000	2.66040000	2.61050000
H	-0.93100000	1.61450000	2.90050000
C	-1.48500000	3.64030000	3.39620000
C	-1.45930000	4.97990000	2.99740000
H	-1.93880000	5.74290000	3.60540000
C	-0.81800000	5.32710000	1.80950000
C	-0.19210000	4.34820000	1.03010000
H	0.30610000	4.64550000	0.11440000
C	1.31200000	-2.58690000	1.00290000
C	2.42800000	-3.40990000	0.77270000
H	2.86980000	-3.46040000	-0.21850000
C	2.98000000	-4.16310000	1.80970000
C	2.42850000	-4.10000000	3.09290000
H	2.85980000	-4.68650000	3.90060000
C	1.32650000	-3.27780000	3.33210000
C	0.77140000	-2.52520000	2.29360000
H	-0.07230000	-1.86120000	2.46900000
C	-0.20390000	-3.00080000	-1.41740000
C	-0.19210000	-4.34900000	-1.02720000
H	0.30620000	-4.64580000	-0.11140000
C	-0.81830000	-5.32850000	-1.80550000
C	-1.45990000	-4.98220000	-2.99360000
H	-1.93970000	-5.74560000	-3.60090000
C	-1.48540000	-3.64290000	-3.39340000

C	-0.87740000	-2.66250000	-2.60860000
H	-0.93110000	-1.61680000	-2.89940000
C	2.94350000	-0.20130000	-0.71880000
C	2.01390000	-1.07400000	-1.32530000
C	2.19210000	-1.43760000	-2.66220000
H	1.52040000	-2.11100000	-3.17610000
C	3.28080000	-0.90820000	-3.35810000
N	4.16230000	-0.06890000	-2.82240000
C	3.98920000	0.26670000	-1.54620000
O	3.43130000	-1.28640000	-4.65090000
C	4.54100000	-0.74590000	-5.36430000
H	4.47400000	-1.17040000	-6.36810000
H	5.49030000	-1.02940000	-4.89770000
H	4.48850000	0.34680000	-5.41170000
O	4.87310000	1.12620000	-0.98920000
C	5.91840000	1.62390000	-1.81990000
H	6.50230000	2.28790000	-1.17890000
H	5.51400000	2.17990000	-2.67140000
H	6.54860000	0.81140000	-2.19540000
C	2.94390000	0.20120000	0.71800000
C	3.99000000	-0.26700000	1.54480000
N	4.16390000	0.06870000	2.82090000
C	3.28280000	0.90790000	3.35720000
C	2.19350000	1.43720000	2.66200000
H	1.52210000	2.11060000	3.17630000
C	2.01460000	1.07360000	1.32520000
O	4.87340000	-1.12650000	0.98720000
C	5.91960000	-1.62390000	1.81710000
H	6.50310000	-2.28790000	1.17570000
H	5.51610000	-2.17980000	2.66920000
H	6.55000000	-0.81110000	2.19180000
O	3.43410000	1.28610000	4.64990000
C	4.54400000	0.74520000	5.36270000
H	4.47720000	1.16900000	6.36680000
H	5.49320000	1.02920000	4.89610000
H	4.49170000	-0.34750000	5.40930000
C	-3.93460000	1.14390000	-0.64410000
H	-3.51550000	0.78950000	-1.59020000
C	-3.93520000	-1.14430000	0.64260000
H	-3.51760000	-0.78860000	1.58900000
C	-4.82950000	-2.34210000	0.94180000
C	-5.36010000	-3.13690000	-0.08570000
H	-5.12930000	-2.90780000	-1.12400000
C	-6.17820000	-4.22830000	0.20480000
H	-6.57610000	-4.83480000	-0.60460000
C	-6.48650000	-4.54080000	1.53140000
H	-7.12450000	-5.39080000	1.75810000
C	-5.96680000	-3.75750000	2.56230000
H	-6.19670000	-3.99500000	3.59770000
C	-5.14250000	-2.66930000	2.26690000
H	-4.73300000	-2.06720000	3.07510000
C	-4.82770000	2.34260000	-0.94300000
C	-5.36620000	3.13180000	0.08460000
H	-5.14370000	2.89700000	1.12350000
C	-6.18220000	4.22470000	-0.20620000
H	-6.58660000	4.82660000	0.60340000
C	-6.48020000	4.54460000	-1.53340000
H	-7.11650000	5.39580000	-1.76030000
C	-5.95240000	3.76710000	-2.56460000
H	-6.17410000	4.01040000	-3.60040000

C	-5.13050000	2.67720000	-2.26880000
H	-4.71460000	2.07950000	-3.07700000
C	-4.74770000	-0.00070000	-0.00210000
H	-5.41320000	0.40160000	0.77230000
H	-5.41020000	-0.40430000	-0.77830000
H	-1.17190000	0.27400000	-1.69290000
H	-1.17250000	-0.27510000	1.69370000
H	-1.98300000	3.35550000	4.32010000
H	-0.79770000	6.36380000	1.48270000
H	3.83730000	4.80140000	-1.61540000
H	0.89650000	3.21660000	-4.32910000
H	-1.98360000	-3.35870000	-4.31740000
H	-0.79820000	-6.36500000	-1.47790000
H	3.84120000	-4.79800000	1.61610000
H	0.89910000	-3.21600000	4.33010000

RuH₂[(*R*)-Tol-P-Phos][(*R,R*)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	1.21640000	-0.00020000	-0.00020000
P	-0.36310000	-1.60510000	-0.38680000
P	-0.36260000	1.60550000	0.38670000
C	-2.81560000	-0.48030000	0.58060000
C	-1.87670000	-1.50910000	0.71610000
C	-2.00310000	-2.42920000	1.79400000
C	-3.01340000	-2.33030000	2.71720000
C	-3.97040000	-1.29100000	2.63250000
C	-5.01900000	-1.17080000	3.58440000
C	-5.94890000	-0.16190000	3.49000000
C	-5.85710000	0.77550000	2.43410000
C	-4.85090000	0.68390000	1.49820000
C	-3.87400000	-0.35260000	1.55430000
C	-2.81550000	0.48170000	-0.58040000
C	-1.87610000	1.51010000	-0.71610000
C	-2.00220000	2.42990000	-1.79400000
C	-3.01240000	2.33140000	-2.71720000
C	-3.96990000	1.29250000	-2.63250000
C	-5.01850000	1.17250000	-3.58430000
C	-5.94900000	0.16400000	-3.48960000
C	-5.85770000	-0.77310000	-2.43330000
C	-4.85140000	-0.68170000	-1.49750000
C	-3.87390000	0.35420000	-1.55400000
C	-1.14240000	-1.87430000	-2.05440000
C	-0.61580000	-1.23820000	-3.18330000
C	-1.16400000	-1.46150000	-4.44830000
C	-2.25240000	-2.32250000	-4.62650000
C	-2.77400000	-2.96470000	-3.49390000
C	-2.23390000	-2.74190000	-2.22970000
C	0.33930000	-3.31130000	-0.05160000
C	1.07900000	-3.51450000	1.13150000
C	1.69800000	-4.73420000	1.39880000
C	1.61930000	-5.80330000	0.49350000
C	0.90410000	-5.59680000	-0.68980000
C	0.27380000	-4.37820000	-0.96000000
C	0.34100000	3.31100000	0.05130000

C	1.08050000	3.51400000	-1.13200000
C	1.70030000	4.73320000	-1.39910000
C	1.62300000	5.80200000	-0.49340000
C	0.90780000	5.59580000	0.69010000
C	0.27660000	4.37750000	0.96000000
C	-1.14140000	1.87510000	2.05440000
C	-2.23200000	2.74350000	2.23020000
C	-2.77120000	2.96690000	3.49460000
C	-2.24970000	2.32430000	4.62710000
C	-1.16220000	1.46200000	4.44830000
C	-0.61480000	1.23840000	3.18300000
H	1.27930000	-0.48440000	1.64220000
H	1.27890000	0.48420000	-1.64240000
H	-1.28740000	-3.23670000	1.88610000
H	-3.08960000	-3.05490000	3.52510000
H	-5.07060000	-1.89850000	4.39130000
H	-6.74970000	-0.08130000	4.22050000
H	-6.58650000	1.57820000	2.36200000
H	-4.79730000	1.41760000	0.70320000
H	-1.28640000	3.23720000	-1.88620000
H	-3.08840000	3.05590000	-3.52520000
H	-5.06990000	1.89980000	-4.39150000
H	-6.74990000	0.08360000	-4.22000000
H	-6.58750000	-1.57540000	-2.36080000
H	-4.79820000	-1.41510000	-0.70220000
H	0.21490000	-0.55020000	-3.04740000
H	-0.74220000	-0.94920000	-5.31100000
H	-3.62210000	-3.63780000	-3.60310000
H	-2.66540000	-3.24890000	-1.37040000
H	1.18190000	-2.68880000	1.82970000
H	2.26310000	-4.85160000	2.32140000
H	0.83630000	-6.40070000	-1.42020000
H	-0.26550000	-4.26760000	-1.89350000
H	1.18250000	2.68850000	-1.83050000
H	2.26510000	4.85050000	-2.32190000
H	0.84070000	6.39960000	1.42050000
H	-0.26270000	4.26740000	1.89350000
H	-2.66350000	3.25100000	1.37130000
H	-0.74040000	0.94930000	5.31090000
H	0.21530000	0.54970000	3.04670000
C	2.27760000	-7.12880000	0.79640000
H	2.36050000	-7.75020000	-0.10130000
H	3.28430000	-6.99240000	1.20840000
H	1.70170000	-7.69820000	1.53820000
C	-2.87690000	-2.52670000	-5.98680000
H	-3.77150000	-1.90030000	-6.10450000
H	-2.18300000	-2.26200000	-6.79160000
H	-3.18920000	-3.56680000	-6.13580000
C	2.28370000	7.12650000	-0.79560000
H	1.72090000	7.68750000	-1.55370000
H	2.34810000	7.75600000	0.09790000
H	3.29850000	6.98890000	-1.18700000
N	2.98050000	1.30120000	0.45800000
N	2.97990000	-1.30230000	-0.45830000
C	4.31330000	-0.78420000	-0.02010000
H	2.84530000	2.23990000	0.08380000
H	2.96400000	1.38060000	1.47180000
H	2.84380000	-2.24060000	-0.08340000
H	2.96340000	-1.38260000	-1.47200000
H	5.06220000	-1.06670000	-0.76950000

C	4.31360000	0.78240000	0.01970000
H	5.06270000	1.06470000	0.76900000
C	4.77190000	1.40340000	-1.29330000
C	6.03940000	2.00130000	-1.34940000
C	3.99250000	1.37010000	-2.46040000
C	6.52490000	2.54880000	-2.53820000
H	6.65420000	2.03950000	-0.45230000
C	4.47690000	1.92340000	-3.64760000
H	2.99390000	0.93700000	-2.42040000
C	5.74340000	2.51020000	-3.69390000
H	7.51010000	3.00760000	-2.55830000
H	3.85850000	1.89360000	-4.54140000
H	6.11720000	2.93600000	-4.62150000
C	4.77130000	-1.40540000	1.29280000
C	3.99220000	-1.37120000	2.45990000
C	6.03830000	-2.00420000	1.34870000
C	4.47620000	-1.92480000	3.64710000
H	2.99400000	-0.93730000	2.42010000
C	6.52360000	-2.55210000	2.53750000
H	6.65300000	-2.04300000	0.45160000
C	5.74230000	-2.51270000	3.69330000
H	3.85810000	-1.89420000	4.54120000
H	7.50840000	-3.01170000	2.55740000
H	6.11590000	-2.93870000	4.62090000
H	-3.61860000	3.64070000	3.60430000
C	-2.87340000	2.52900000	5.98780000
H	-2.17740000	2.26870000	6.79230000
H	-3.18950000	3.56820000	6.13490000
H	-3.76530000	1.89940000	6.10810000

RuH₂[(*R*)-Xyl-P-Phos][(*S,S*)-dppen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.11280000	0.00030000	-0.00140000
P	0.44720000	1.62900000	0.34030000
P	0.44830000	-1.62790000	-0.34090000
N	-2.79810000	1.48630000	0.15420000
H	-3.03910000	1.64300000	1.13200000
H	-2.42240000	2.37110000	-0.18110000
N	-2.79690000	-1.48740000	-0.15830000
H	-3.03730000	-1.64290000	-1.13640000
H	-2.42060000	-2.37230000	0.17600000
C	1.26060000	2.57240000	-1.04790000
C	0.74570000	2.46380000	-2.34110000
H	-0.08730000	1.78340000	-2.50910000
C	1.30940000	3.18410000	-3.40600000
C	2.39250000	4.02640000	-3.14460000
H	2.83540000	4.59260000	-3.96330000
C	2.93030000	4.15810000	-1.85480000
C	2.35950000	3.41820000	-0.81670000
H	2.77700000	3.50100000	0.18360000
C	0.76430000	3.02380000	-4.80760000
H	1.01230000	2.03600000	-5.21730000
H	1.17430000	3.77830000	-5.48770000

H	-0.32850000	3.11100000	-4.82460000
C	4.08560000	5.09960000	-1.59480000
H	4.58550000	4.86480000	-0.64950000
H	3.74730000	6.14330000	-1.53710000
H	4.83370000	5.05040000	-2.39490000
C	-0.26940000	3.02720000	1.35880000
C	-0.92210000	2.71130000	2.56770000
H	-0.95470000	1.67270000	2.88650000
C	-1.54020000	3.69640000	3.34180000
C	-1.53730000	5.01990000	2.87430000
H	-2.02850000	5.79400000	3.46210000
C	-0.92570000	5.36360000	1.66850000
C	-0.28900000	4.35670000	0.92260000
H	0.19300000	4.62810000	-0.01070000
C	-2.18640000	3.35020000	4.66510000
H	-3.13370000	3.88460000	4.80420000
H	-1.53670000	3.62390000	5.50710000
H	-2.38490000	2.27630000	4.74390000
C	-0.93920000	6.78860000	1.16180000
H	-1.45800000	7.45600000	1.85760000
H	-1.44190000	6.86270000	0.18930000
H	0.07910000	7.17350000	1.02530000
C	1.25810000	-2.57250000	1.04870000
C	2.35800000	-3.41820000	0.81980000
H	2.77870000	-3.49950000	-0.17940000
C	2.92590000	-4.15900000	1.85890000
C	2.38380000	-4.02890000	3.14730000
H	2.82470000	-4.59540000	3.96680000
C	1.29940000	-3.18790000	3.40600000
C	0.73940000	-2.46550000	2.34040000
H	-0.09360000	-1.78470000	2.50690000
C	4.08280000	-5.09920000	1.60190000
H	3.74670000	-6.14380000	1.54960000
H	4.83200000	-5.04460000	2.40050000
H	4.58090000	-4.86790000	0.65460000
C	0.74450000	-3.03460000	4.80450000
H	-0.34000000	-3.19650000	4.82490000
H	0.92360000	-2.02370000	5.19250000
H	1.20420000	-3.74530000	5.49980000
C	-0.26570000	-3.02610000	-1.36210000
C	-0.28500000	-4.35630000	-0.92730000
H	0.19480000	-4.62810000	0.00710000
C	-0.91930000	-5.36290000	-1.67580000
C	-1.52970000	-5.01810000	-2.88190000
H	-2.01990000	-5.79190000	-3.47100000
C	-1.53290000	-3.69420000	-3.34800000
C	-0.91680000	-2.70930000	-2.57190000
H	-0.95000000	-1.67010000	-2.88900000
C	-0.92740000	-6.78960000	-1.17390000
H	0.09070000	-7.19270000	-1.10130000
H	-1.49800000	-7.44510000	-1.83980000
H	-1.37090000	-6.85950000	-0.17300000
C	-2.17790000	-3.34670000	-4.67150000
H	-1.52580000	-3.61610000	-5.51310000
H	-2.37980000	-2.27320000	-4.74790000
H	-3.12320000	-3.88380000	-4.81370000
C	2.88960000	-0.21620000	-0.71130000
C	1.96070000	-1.10060000	-1.30210000
C	2.14350000	-1.49280000	-2.63080000
H	1.47230000	-2.17740000	-3.13070000

C	3.23550000	-0.98090000	-3.33370000
N	4.11680000	-0.13230000	-2.81290000
C	3.93900000	0.23170000	-1.54500000
O	3.39040000	-1.38680000	-4.61890000
C	4.50890000	-0.87000000	-5.33550000
H	4.44630000	-1.31570000	-6.33050000
H	5.45300000	-1.14990000	-4.85610000
H	4.46550000	0.22180000	-5.40730000
O	4.82440000	1.10060000	-1.00460000
C	5.88140000	1.56390000	-1.83960000
H	6.46250000	2.24600000	-1.21550000
H	5.49040000	2.09220000	-2.71480000
H	6.51100000	0.73560000	-2.18090000
C	2.88770000	0.21750000	0.71670000
C	3.93530000	-0.22990000	1.55290000
N	4.11040000	0.13510000	2.82100000
C	3.22790000	0.98420000	3.33910000
C	2.13740000	1.49530000	2.63340000
H	1.46540000	2.18030000	3.13130000
C	1.95750000	1.10210000	1.30490000
O	4.82200000	-1.09920000	1.01490000
C	5.87760000	-1.56150000	1.85230000
H	6.46000000	-2.24400000	1.22990000
H	5.48520000	-2.08910000	2.72730000
H	6.50640000	-0.73270000	2.19390000
O	3.38040000	1.39160000	4.62400000
C	4.49750000	0.87550000	5.34320000
H	4.43270000	1.32170000	6.33780000
H	5.44250000	1.15550000	4.86570000
H	4.45440000	-0.21620000	5.41550000
C	-3.98990000	1.13660000	-0.65840000
H	-3.57350000	0.77210000	-1.60200000
C	-3.98870000	-1.13830000	0.65420000
H	-3.57260000	-0.77290000	1.59750000
C	-4.88380000	-2.33280000	0.96490000
C	-5.41290000	-3.13850000	-0.05480000
H	-5.18010000	-2.92010000	-1.09490000
C	-6.23170000	-4.22660000	0.24570000
H	-6.62850000	-4.84140000	-0.55790000
C	-6.54210000	-4.52540000	1.57500000
H	-7.18080000	-5.37280000	1.80950000
C	-6.02380000	-3.73140000	2.59840000
H	-6.25540000	-3.95800000	3.63590000
C	-5.19900000	-2.64630000	2.29290000
H	-4.79070000	-2.03580000	3.09530000
C	-4.88620000	2.33040000	-0.96780000
C	-5.41620000	3.13420000	0.05280000
H	-5.18330000	2.91460000	1.09260000
C	-6.23610000	4.22180000	-0.24640000
H	-6.63370000	4.83520000	0.55790000
C	-6.54690000	4.52190000	-1.57530000
H	-7.18650000	5.36870000	-1.80890000
C	-6.02760000	3.72970000	-2.59970000
H	-6.25950000	3.95720000	-3.63690000
C	-5.20160000	2.64520000	-2.29540000
H	-4.79260000	2.03610000	-3.09860000
C	-4.80160000	-0.00170000	-0.00250000
H	-5.46670000	0.40950000	0.76760000
H	-5.46480000	-0.41410000	-0.77380000
H	-1.22670000	0.24730000	-1.69940000

H	-1.22830000	-0.24610000	1.69630000
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RuH₂[(S)-binap][(S)-daipen]

Coordinates (Angstroms)

X	Y	Z	
Ru	0.41960000	0.08150000	0.53620000
P	-1.49780000	1.03100000	1.32460000
P	-0.72370000	-1.19660000	-0.96870000
C	-1.43200000	-2.86740000	-0.54060000
C	-1.06210000	-3.48580000	0.66010000
C	-4.24540000	1.16270000	-3.04160000
C	-2.19410000	-0.36900000	-1.79040000
C	-6.67600000	-3.57740000	0.78110000
C	-5.02450000	-2.07670000	1.75200000
C	-2.36230000	-5.44710000	0.08580000
C	-1.25310000	1.64640000	3.08230000
C	0.59030000	-2.99150000	-2.83570000
C	-1.49240000	2.97150000	3.48110000
C	0.38050000	-1.66760000	-2.41560000
C	-0.70650000	2.49710000	5.72490000
C	-2.26670000	2.54000000	0.54480000
C	-0.70620000	0.76200000	4.03380000
C	-2.97990000	-0.11290000	1.45700000
C	-3.35700000	-0.07340000	-1.07070000
C	-2.08050000	0.07980000	-3.13610000
C	-6.56890000	1.83590000	-1.62280000
C	-4.39490000	0.71880000	-1.68800000
C	1.97900000	-0.94440000	-4.11480000
C	-5.58890000	1.09150000	-1.00450000
C	-4.05380000	4.18520000	0.39890000
C	1.47710000	-3.28710000	-3.87600000
C	-3.06860000	0.81170000	-3.74460000
C	-6.30300000	-3.13350000	-0.50950000
C	-6.04340000	-3.05820000	1.88630000
C	-2.28370000	-3.55620000	-1.42070000
C	-1.52500000	-4.76730000	0.97110000
C	-2.74300000	-4.83670000	-1.11240000
C	-3.38390000	-0.59000000	2.73590000
C	-4.37260000	-1.52990000	2.88270000
C	-4.64790000	-1.61140000	0.45080000
C	-3.33200000	4.89310000	-0.56610000
C	-1.21770000	3.39230000	4.78630000
C	-3.52610000	3.01600000	0.94690000
C	-5.27390000	1.92840000	-3.65420000
C	-3.62430000	-0.60180000	0.31500000
C	2.16680000	-2.26580000	-4.52820000
C	1.11080000	-0.64990000	-3.06110000
C	-1.55440000	3.25380000	-0.42630000
C	-6.41700000	2.25820000	-2.96460000
C	-5.32000000	-2.18200000	-0.66900000
C	-0.45130000	1.17750000	5.34220000
C	-2.08480000	4.42300000	-0.97870000
H	-0.42400000	-2.93480000	1.34760000
H	-7.45540000	-4.32640000	0.89420000
H	0.06060000	-3.80480000	-2.35400000

H	-1.89720000	3.68670000	2.77480000
H	-0.46960000	-0.25290000	3.72600000
H	-1.19520000	-0.17140000	-3.70580000
H	-7.46720000	2.10400000	-1.07270000
H	2.51320000	-0.13660000	-4.60960000
H	-5.72490000	0.78540000	0.02560000
H	-5.03080000	4.53920000	0.71830000
H	1.62050000	-4.32180000	-4.17780000
H	-2.95630000	1.12880000	-4.77920000
H	-6.79560000	-3.54870000	-1.38480000
H	-6.31220000	-3.39110000	2.88630000
H	-2.58740000	-3.08990000	-2.35440000
H	-1.23400000	-5.23130000	1.91050000
H	-3.40440000	-5.35440000	-1.80260000
H	-2.90930000	-0.19350000	3.62420000
H	-4.66650000	-1.86400000	3.87540000
H	-1.41080000	4.42510000	5.06610000
H	-4.09600000	2.47170000	1.69570000
H	-5.13590000	2.24910000	-4.68440000
H	1.00270000	0.37330000	-2.71050000
H	-0.59080000	2.86520000	-0.74780000
H	-7.19880000	2.84270000	-3.44240000
H	-5.04820000	-1.86120000	-1.66720000
H	-0.04470000	0.46970000	6.06030000
H	-1.52180000	4.96360000	-1.73580000
H	0.66860000	1.27940000	-0.65320000
H	0.36350000	-1.11780000	1.77130000
N	2.46420000	-0.69210000	0.03300000
N	1.81690000	1.25680000	1.82820000
C	3.15510000	0.60490000	1.97240000
C	3.58240000	0.16220000	0.53320000
H	2.50930000	-1.60860000	0.47240000
H	2.52300000	-0.83210000	-0.97300000
H	3.89520000	1.34030000	2.31360000
H	1.40080000	1.41350000	2.74390000
H	1.89570000	2.15880000	1.36670000
C	3.75590000	1.38860000	-0.40630000
C	3.89560000	1.17930000	-1.78330000
C	3.91560000	2.70790000	0.04840000
C	4.12250000	2.22310000	-2.67980000
H	3.84470000	0.17420000	-2.19030000
C	4.14550000	3.76420000	-0.82830000
H	3.87230000	2.94450000	1.10660000
C	4.24020000	3.53450000	-2.20470000
H	4.21810000	2.00030000	-3.73660000
H	4.25780000	4.77920000	-0.46030000
C	3.01670000	-0.44910000	3.11970000
H	2.00390000	-0.85670000	3.01240000
O	4.46330000	4.63190000	-2.98410000
C	4.55260000	4.44970000	-4.38740000
H	3.62810000	4.02310000	-4.79900000
H	4.70960000	5.44410000	-4.80960000
H	5.39890000	3.80440000	-4.65910000
C	4.95090000	-0.55640000	0.49920000
C	5.14060000	-1.79080000	-0.12430000
C	6.08920000	0.07120000	1.04020000
C	6.39750000	-2.40540000	-0.18860000
H	4.30300000	-2.31270000	-0.57740000
C	7.34040000	-0.52490000	0.99470000
H	6.00060000	1.05270000	1.49640000

C	7.50690000	-1.77670000	0.38090000
H	6.48860000	-3.36640000	-0.68200000
H	8.21120000	-0.03580000	1.42010000
O	8.77530000	-2.27940000	0.38740000
C	8.99740000	-3.54170000	-0.21910000
H	8.75410000	-3.52420000	-1.29000000
H	10.06140000	-3.75140000	-0.09510000
H	8.41260000	-4.33280000	0.26920000
C	3.98030000	-1.64610000	3.15090000
H	3.88800000	-2.29510000	2.27650000
H	5.02970000	-1.34420000	3.22930000
H	3.74250000	-2.25510000	4.03180000
C	3.11950000	0.28410000	4.47410000
H	2.44860000	1.14660000	4.55220000
H	2.86410000	-0.39500000	5.29550000
H	4.14400000	0.64080000	4.64690000
H	2.84720000	-2.49530000	-5.34430000
H	-2.72450000	-6.44290000	0.32870000
H	-3.74520000	5.80180000	-0.99680000
H	-0.50190000	2.82370000	6.74130000

RuH₂[(S)-binap][(S,S)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.19490000	0.00000000	0.00010000
P	0.38820000	-1.42790000	-0.82610000
P	0.38820000	1.42790000	0.82640000
C	1.15970000	1.21660000	2.50890000
C	0.59440000	0.31570000	3.41970000
C	3.99300000	1.98710000	-2.15840000
C	1.89950000	1.64800000	-0.25940000
C	5.97730000	-1.15600000	3.29600000
C	3.99310000	-1.98750000	2.15850000
C	2.20640000	0.96230000	5.10750000
C	-0.30990000	-3.16410000	-0.98630000
C	-0.21150000	3.94450000	2.14980000
C	-0.21320000	-3.94360000	-2.15030000
C	-0.30950000	3.16430000	0.98640000
C	-1.56710000	-5.69360000	-1.15760000
C	1.15990000	-1.21670000	-2.50850000
C	-1.06680000	-3.67710000	0.08660000
C	1.89940000	-1.64830000	0.25970000
C	2.84260000	0.62610000	-0.41940000
C	2.02130000	2.83490000	-1.03510000
C	5.88930000	-0.04260000	-2.54850000
C	3.90130000	0.78240000	-1.38860000
C	-1.68170000	4.92760000	-0.00510000
C	4.88250000	-0.22390000	-1.62640000
C	2.78230000	-1.86100000	-4.20470000
C	-0.83280000	5.19480000	2.23300000
C	3.03110000	3.00360000	-1.94840000
C	5.88950000	0.04210000	2.54860000
C	5.04250000	-2.14600000	3.10360000
C	2.26500000	1.98310000	2.91540000
C	1.11500000	0.18910000	4.71040000

C	2.78250000	1.86000000	4.20500000
C	2.02130000	-2.83520000	1.03530000
C	3.03120000	-3.00410000	1.94850000
C	3.90140000	-0.78280000	1.38880000
C	2.20720000	-0.96230000	-5.10680000
C	-0.83490000	-5.19370000	-2.23370000
C	2.26450000	-1.98410000	-2.91520000
C	5.04230000	2.14540000	-3.10360000
C	2.84260000	-0.62640000	0.41980000
C	-1.56590000	5.69410000	1.15720000
C	-1.06730000	3.67680000	-0.08610000
C	0.59560000	-0.31490000	-3.41900000
C	5.97710000	1.15540000	-3.29600000
C	4.88260000	0.22350000	1.62660000
C	-1.68160000	-4.92780000	0.00540000
C	1.11640000	-0.18820000	-4.70950000
H	-0.24210000	-0.29500000	3.08860000
H	6.77780000	-1.28790000	4.01920000
H	0.34710000	3.58210000	3.00450000
H	0.34470000	-3.58070000	-3.00530000
H	-1.18330000	-3.06650000	0.97760000
H	1.30290000	3.63340000	-0.89790000
H	6.62240000	-0.82970000	-2.70510000
H	-2.26110000	5.29470000	-0.84860000
H	4.83260000	-1.15210000	-1.07030000
H	3.63970000	-2.45930000	-4.50190000
H	-0.74170000	5.77570000	3.14760000
H	3.10360000	3.92640000	-2.51990000
H	6.62260000	0.82910000	2.70530000
H	5.09010000	-3.07150000	3.67290000
H	2.72350000	2.68180000	2.22040000
H	0.66880000	-0.51980000	5.40390000
H	3.64050000	2.45760000	4.50200000
H	1.30290000	-3.63380000	0.89800000
H	3.10370000	-3.92690000	2.51990000
H	-0.74490000	-5.77400000	-3.14880000
H	2.72220000	-2.68350000	-2.22050000
H	5.08990000	3.07100000	-3.67290000
H	-1.18460000	3.06560000	-0.97660000
H	-0.24040000	0.29650000	-3.08780000
H	6.77750000	1.28730000	-4.01920000
H	4.83270000	1.15170000	1.07050000
H	-2.26020000	-5.29530000	0.84920000
H	0.67100000	0.52140000	-5.40270000
H	-1.25700000	0.93040000	-1.43700000
H	-1.25720000	-0.93040000	1.43710000
H	-2.04910000	6.66550000	1.22510000
H	2.61310000	0.86220000	6.11070000
H	-2.05050000	-6.66480000	-1.22560000
H	2.61410000	-0.86210000	-6.11000000
N	-2.95680000	1.11930000	0.80880000
N	-2.95660000	-1.11940000	-0.80880000
C	-4.29170000	-0.74420000	-0.24550000
C	-4.29180000	0.74430000	0.24490000
H	-2.94030000	0.91450000	1.80480000
H	-2.82380000	2.12540000	0.70990000
H	-5.03620000	-0.79710000	-1.04860000
H	-2.82360000	-2.12550000	-0.70960000
H	-2.93980000	-0.91490000	-1.80500000
C	-4.75640000	-1.71750000	0.82970000

C	-6.01810000	-2.31580000	0.69890000
C	-3.98550000	-2.01510000	1.96440000
C	-6.50570000	-3.18680000	1.67490000
H	-6.62640000	-2.09890000	-0.17680000
C	-4.47190000	-2.89090000	2.93730000
H	-2.99130000	-1.58110000	2.05900000
C	-5.73250000	-3.47660000	2.79990000
H	-7.48590000	-3.64010000	1.55240000
H	-3.86020000	-3.11500000	3.80790000
H	-6.10780000	-4.15510000	3.56160000
C	-4.75600000	1.71780000	-0.83040000
C	-3.98480000	2.01510000	-1.96500000
C	-6.01750000	2.31640000	-0.69980000
C	-4.47080000	2.89110000	-2.93790000
H	-2.99070000	1.58070000	-2.05950000
C	-6.50470000	3.18760000	-1.67580000
H	-6.62600000	2.09970000	0.17590000
C	-5.73120000	3.47720000	-2.80070000
H	-3.85890000	3.11490000	-3.80850000
H	-7.48480000	3.64130000	-1.55350000
H	-6.10620000	4.15580000	-3.56240000
H	-5.03660000	0.79730000	1.04770000

RuH₂[(S)-SDP][(R,R)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.85170000	0.06240000	-0.05750000
P	0.64220000	-1.65070000	0.37050000
P	0.78350000	1.59130000	-0.50100000
C	1.31870000	-1.96380000	2.08180000
C	0.87470000	-1.19160000	3.16060000
C	1.31640000	-1.46200000	4.45950000
C	2.20110000	-2.51400000	4.69790000
C	2.65270000	-3.29330000	3.62800000
C	2.21850000	-3.01600000	2.33110000
C	-0.29600000	-3.26620000	0.10650000
C	-1.01160000	-3.43580000	-1.09700000
C	-1.80480000	-4.56250000	-1.31730000
C	-1.92010000	-5.54690000	-0.33190000
C	-1.23860000	-5.38490000	0.87270000
C	-0.43660000	-4.25880000	1.08970000
C	0.17540000	3.35160000	-0.79980000
C	0.64520000	4.52410000	-0.18780000
C	0.15560000	5.77970000	-0.56250000
C	-0.80500000	5.89640000	-1.56580000
C	-1.25810000	4.74370000	-2.21130000
C	-0.76840000	3.49310000	-1.83510000
C	1.79900000	1.56820000	-2.07410000
C	2.70680000	2.59710000	-2.37940000
C	3.35080000	2.63850000	-3.61590000
C	3.08560000	1.65630000	-4.57550000
C	2.17260000	0.64160000	-4.28870000
C	1.53010000	0.60040000	-3.04770000
H	-0.97200000	-0.44600000	-1.70040000
H	-0.85240000	0.60290000	1.55560000

H	0.18950000	-0.37160000	2.95900000
H	0.96880000	-0.84500000	5.28440000
H	3.34390000	-4.11420000	3.80330000
H	2.57720000	-3.62620000	1.50580000
H	-0.96340000	-2.65100000	-1.84520000
H	-2.34550000	-4.66010000	-2.25510000
H	-1.32820000	-6.13350000	1.65600000
H	0.07280000	-4.16250000	2.04050000
H	1.40920000	4.47240000	0.57890000
H	0.53750000	6.66910000	-0.06730000
H	-1.98320000	4.81790000	-3.01810000
H	-1.08700000	2.61060000	-2.38370000
H	2.89960000	3.38410000	-1.65480000
H	1.95500000	-0.12220000	-5.03090000
H	0.79990000	-0.17100000	-2.82310000
H	4.04880000	3.44280000	-3.83510000
C	4.30570000	-1.18380000	-1.71090000
C	3.34000000	-1.02590000	-0.69260000
C	2.19080000	-1.86530000	-0.69700000
C	2.12840000	-2.85710000	-1.69610000
C	3.10870000	-3.01630000	-2.67380000
C	4.20280000	-2.15970000	-2.69590000
C	3.09670000	0.94590000	1.20690000
C	3.73400000	1.04960000	2.46610000
C	3.25840000	1.87560000	3.47490000
C	2.08470000	2.59490000	3.25250000
C	1.44000000	2.49520000	2.02510000
C	1.94560000	1.72390000	0.95510000
C	3.91720000	-0.01480000	0.32770000
C	4.73670000	-0.81860000	1.39600000
C	4.94770000	0.15690000	2.56160000
C	5.44810000	-0.20260000	-1.58750000
C	4.94480000	0.79070000	-0.52980000
H	1.28520000	-3.53330000	-1.72150000
H	3.00290000	-3.80260000	-3.41710000
H	4.96890000	-2.24700000	-3.46300000
H	3.77430000	1.92890000	4.43090000
H	1.65730000	3.21360000	4.03770000
H	0.48970000	3.00110000	1.90470000
H	5.67110000	-1.20230000	0.97400000
H	4.15320000	-1.67330000	1.73830000
H	5.01750000	-0.35200000	3.52980000
H	5.87240000	0.73990000	2.44110000
H	5.67470000	0.28390000	-2.54340000
H	6.36770000	-0.71210000	-1.26550000
H	5.74590000	1.20070000	0.09410000
H	4.44610000	1.62810000	-1.01720000
H	-2.54350000	-6.42150000	-0.49870000
H	2.54050000	-2.72720000	5.70860000
H	-1.18420000	6.87320000	-1.85390000
H	3.58050000	1.69190000	-5.54310000
N	-2.61540000	1.39680000	-0.44050000
N	-2.65390000	-1.15000000	0.55360000
C	-3.99180000	-0.59900000	0.18630000
H	-2.42560000	2.35370000	-0.14760000
H	-2.67870000	1.41370000	-1.45430000
H	-2.59060000	-2.11440000	0.23020000
H	-2.56090000	-1.16650000	1.56630000
H	-4.70750000	-0.84320000	0.98070000
C	-3.93400000	0.96300000	0.11210000

H	-4.71990000	1.25840000	-0.59370000
C	-4.28040000	1.64140000	1.43080000
C	-5.58800000	2.11950000	1.60760000
C	-3.36430000	1.78240000	2.48350000
C	-5.97890000	2.71730000	2.80610000
H	-6.30760000	2.02650000	0.79640000
C	-3.75540000	2.38870000	3.67980000
H	-2.34560000	1.42010000	2.35110000
C	-5.06050000	2.85430000	3.84880000
H	-6.99610000	3.08280000	2.92060000
H	-3.03200000	2.49490000	4.48470000
H	-5.35930000	3.32370000	4.78250000
C	-4.53940000	-1.21790000	-1.09280000
C	-3.80220000	-1.25740000	-2.28680000
C	-5.84550000	-1.72820000	-1.09030000
C	-4.36730000	-1.79620000	-3.44480000
H	-2.77580000	-0.89090000	-2.29130000
C	-6.41060000	-2.26140000	-2.25010000
H	-6.42700000	-1.70900000	-0.17070000
C	-5.67160000	-2.29560000	-3.43360000
H	-3.78230000	-1.82380000	-4.36100000
H	-7.42430000	-2.65280000	-2.22600000
H	-6.10770000	-2.71070000	-4.33860000

RuH₂[(S)-tolbinap][(R)-1g]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.21290000	0.27010000	-0.43460000
P	0.64800000	1.63900000	-0.28380000
P	0.04230000	-1.59240000	-0.10260000
C	1.01460000	-2.41080000	-1.45840000
C	0.78630000	-2.02940000	-2.78500000
C	2.97370000	-0.94490000	3.53600000
C	1.30500000	-1.42910000	1.27560000
C	6.40110000	-1.93020000	-1.95950000
C	4.61990000	-0.27340000	-2.02630000
C	2.38350000	-3.68480000	-3.58910000
C	0.51370000	3.18620000	-1.33140000
C	-1.02140000	-4.29310000	-0.14720000
C	0.64000000	4.48620000	-0.82220000
C	-1.02530000	-3.03200000	0.46830000
C	0.16000000	5.47310000	-3.00050000
C	1.19820000	2.35700000	1.34490000
C	0.18160000	3.05580000	-2.69420000
C	2.27630000	0.90310000	-0.89570000
C	2.45680000	-0.65350000	1.11910000
C	1.01740000	-1.98520000	2.55420000
C	5.25070000	0.67410000	3.28360000
C	3.29790000	-0.38100000	2.26030000
C	-2.80970000	-3.84640000	1.92960000
C	4.45950000	0.44010000	2.18060000
C	2.75140000	3.64180000	2.70840000
C	-1.88770000	-5.30710000	0.27220000
C	1.82230000	-1.76160000	3.64230000
C	5.87790000	-2.42510000	-0.74140000

C	5.77890000	-0.87590000	-2.58620000
C	1.93630000	-3.44140000	-1.20970000
C	1.46170000	-2.66050000	-3.83220000
C	2.60500000	-4.06880000	-2.25810000
C	2.84320000	1.37120000	-2.11520000
C	3.97180000	0.81230000	-2.65970000
C	4.08780000	-0.75930000	-0.78940000
C	1.95400000	3.45770000	3.84790000
C	0.45760000	5.60570000	-1.64160000
C	2.38620000	3.09560000	1.48040000
C	3.80890000	-0.68760000	4.65630000
C	2.91110000	-0.14440000	-0.22050000
C	-2.78970000	-5.11070000	1.32230000
C	-1.95490000	-2.82780000	1.50970000
C	0.40060000	2.17350000	2.47930000
C	-0.00160000	6.68030000	-3.89430000
C	4.92850000	0.10290000	4.53730000
C	4.75750000	-1.85820000	-0.17530000
C	0.02490000	4.17240000	-3.51040000
C	0.77430000	2.71840000	3.71010000
C	3.14750000	-4.33750000	-4.71750000
C	-3.69770000	-6.22010000	1.79870000
C	2.38360000	4.00500000	5.18890000
H	0.08500000	-1.22040000	-2.97780000
H	7.28820000	-2.38360000	-2.39420000
H	-0.34160000	-4.49720000	-0.96590000
H	0.87250000	4.64370000	0.22450000
H	0.01310000	2.06250000	-3.09860000
H	0.14550000	-2.61410000	2.67580000
H	6.12920000	1.30720000	3.19000000
H	-3.50750000	-3.65380000	2.74280000
H	4.71910000	0.89440000	1.23230000
H	3.67630000	4.20960000	2.78890000
H	-1.85680000	-6.27050000	-0.23280000
H	1.58060000	-2.21190000	4.60280000
H	6.36380000	-3.26260000	-0.24750000
H	6.16380000	-0.48360000	-3.52490000
H	2.13490000	-3.75620000	-0.18830000
H	1.27370000	-2.34400000	-4.85650000
H	3.31990000	-4.85960000	-2.04050000
H	2.38360000	2.20300000	-2.63070000
H	4.37990000	1.20310000	-3.58930000
H	0.55380000	6.59960000	-1.20880000
H	3.03120000	3.24770000	0.61860000
H	3.54240000	-1.13080000	5.61330000
H	-2.01040000	-1.84410000	1.96940000
H	-0.49910000	1.57020000	2.38340000
H	-0.87860000	6.58460000	-4.54540000
H	0.87070000	6.81050000	-4.54880000
H	-0.11330000	7.59950000	-3.31000000
H	5.56310000	0.29120000	5.39950000
H	4.37410000	-2.25970000	0.75480000
H	-0.22360000	4.03260000	-4.56110000
H	0.14170000	2.55560000	4.58080000
H	3.23850000	-5.42000000	-4.57020000
H	4.16690000	-3.93470000	-4.78560000
H	2.66110000	-4.16640000	-5.68360000
H	-3.27600000	-6.72760000	2.67680000
H	-3.84510000	-6.97930000	1.02340000
H	-4.68220000	-5.83770000	2.09090000

H	3.10780000	3.33430000	5.67080000
H	1.53290000	4.11220000	5.87030000
H	2.86570000	4.98440000	5.09020000
H	-1.53070000	0.16250000	1.24700000
H	-1.09120000	0.37130000	-2.14880000
N	-3.03780000	-0.93060000	-0.81190000
N	-2.98380000	1.92770000	-0.45660000
C	-4.18530000	1.18390000	-0.90780000
C	-4.25320000	-0.23370000	-0.35430000
C	-2.82280000	3.08190000	-1.36340000
C	-3.19980000	2.45270000	0.91030000
H	-3.06380000	-1.07420000	-1.82040000
H	-2.97140000	-1.84750000	-0.37250000
H	-4.13690000	1.11840000	-2.00190000
H	-5.09820000	1.74330000	-0.65060000
H	-4.19520000	-0.20940000	0.73880000
H	-2.01000000	3.71430000	-1.01080000
H	-3.74840000	3.68270000	-1.40030000
H	-2.57660000	2.72580000	-2.36360000
H	-3.37950000	1.63230000	1.60290000
H	-4.05210000	3.15460000	0.93020000
H	-2.29790000	2.97210000	1.23740000
C	-5.55130000	-0.97050000	-0.76960000
H	-5.43710000	-2.02430000	-0.48090000
H	-5.63660000	-0.95400000	-1.86500000
C	-6.81390000	-0.41180000	-0.14510000
C	-7.73530000	0.32630000	-0.89980000
C	-7.08340000	-0.61850000	1.21630000
C	-8.89040000	0.84840000	-0.31330000
H	-7.54910000	0.48890000	-1.95920000
C	-8.23440000	-0.09710000	1.80710000
H	-6.38760000	-1.20090000	1.81700000
C	-9.14280000	0.63980000	1.04320000
H	-9.59330000	1.41520000	-0.91830000
H	-8.42510000	-0.27070000	2.86300000
H	-10.04150000	1.04360000	1.50130000

RuH₂[(S)-tolbinap][(R)-2g]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.51410000	0.87790000	-0.16920000
P	0.69400000	1.57020000	-0.21770000
P	-0.89000000	-1.29970000	0.02150000
C	-0.41570000	-2.33940000	-1.44470000
C	-0.65520000	-1.84410000	-2.73130000
C	2.53620000	-1.79920000	3.22610000
C	0.52190000	-1.60860000	1.21820000
C	4.69620000	-3.56260000	-2.72820000
C	3.56030000	-1.42050000	-2.52250000
C	0.18360000	-3.90040000	-3.73390000
C	0.96450000	3.14230000	-1.20170000
C	-2.76310000	-3.51600000	0.14760000
C	1.58950000	4.28710000	-0.68880000
C	-2.28470000	-2.33750000	0.74080000
C	1.22650000	5.51380000	-2.76580000

C	1.62370000	1.96910000	1.34650000
C	0.44770000	3.21940000	-2.51010000
C	1.90510000	0.38480000	-1.05280000
C	1.83550000	-1.25210000	0.90190000
C	0.23320000	-2.08540000	2.52830000
C	5.17550000	-1.04330000	2.65070000
C	2.86230000	-1.32770000	1.91400000
C	-4.02810000	-2.58620000	2.43810000
C	4.21400000	-0.94920000	1.66900000
C	3.65430000	2.58590000	2.53790000
C	-3.84420000	-4.21500000	0.69340000
C	1.20090000	-2.18390000	3.49550000
C	4.20940000	-3.92890000	-1.45100000
C	4.37240000	-2.33210000	-3.24990000
C	0.12840000	-3.62820000	-1.31640000
C	-0.35980000	-2.61670000	-3.85670000
C	0.41760000	-4.39540000	-2.44220000
C	2.42420000	0.71080000	-2.33830000
C	3.22310000	-0.15090000	-3.04610000
C	3.07090000	-1.77630000	-1.22520000
C	2.96490000	2.62580000	3.75900000
C	1.70920000	5.45120000	-1.45600000
C	2.99930000	2.25590000	1.35390000
C	3.54840000	-1.88410000	4.21970000
C	2.24840000	-0.84710000	-0.48580000
C	-4.48980000	-3.77450000	1.85280000
C	-2.95810000	-1.87830000	1.89230000
C	0.93320000	2.01190000	2.56250000
C	1.38140000	6.75970000	-3.60610000
C	4.84490000	-1.51780000	3.94200000
C	3.42150000	-3.06420000	-0.72400000
C	0.59100000	4.37150000	-3.27780000
C	1.59620000	2.33640000	3.74850000
C	0.54410000	-4.72000000	-4.95080000
C	-5.63180000	-4.55290000	2.46250000
C	3.69240000	2.92950000	5.04780000
H	-1.05770000	-0.83800000	-2.83140000
H	5.32010000	-4.25250000	-3.29040000
H	-2.29640000	-3.90130000	-0.75130000
H	1.98670000	4.28820000	0.31960000
H	-0.09920000	2.36830000	-2.90570000
H	-0.77580000	-2.38990000	2.77280000
H	6.19790000	-0.74640000	2.43170000
H	-4.51610000	-2.20550000	3.33370000
H	4.48850000	-0.57700000	0.68950000
H	4.72050000	2.80300000	2.51810000
H	-4.18830000	-5.12330000	0.20260000
H	0.94890000	-2.56160000	4.48420000
H	4.45750000	-4.90390000	-1.03960000
H	4.73360000	-2.03320000	-4.23150000
H	0.32730000	-4.03680000	-0.32880000
H	-0.54760000	-2.20950000	-4.84850000
H	0.84420000	-5.38870000	-2.31870000
H	2.19680000	1.67360000	-2.77380000
H	3.60720000	0.13810000	-4.02200000
H	2.19440000	6.32350000	-1.02230000
H	3.56400000	2.22560000	0.42560000
H	3.27460000	-2.24800000	5.20750000
H	-2.64000000	-0.93920000	2.33820000
H	-0.12380000	1.75520000	2.56450000

H	0.42480000	7.07180000	-4.04300000
H	2.07470000	6.59360000	-4.44110000
H	1.76980000	7.59550000	-3.01530000
H	5.61310000	-1.59060000	4.70740000
H	3.05530000	-3.37060000	0.24810000
H	0.18830000	4.39090000	-4.28920000
H	1.03970000	2.35510000	4.68380000
H	0.27770000	-5.77540000	-4.82010000
H	1.62460000	-4.68170000	-5.14360000
H	0.03680000	-4.35100000	-5.84840000
H	-5.28500000	-5.17660000	3.29750000
H	-6.09970000	-5.21930000	1.73030000
H	-6.40640000	-3.88690000	2.85930000
H	4.20010000	2.03390000	5.43060000
H	3.00370000	3.27400000	5.82650000
H	4.45920000	3.70010000	4.90700000
H	-1.66620000	0.81340000	1.53490000
H	-1.54530000	1.00890000	-1.88820000
N	-3.64790000	0.30850000	-0.37550000
N	-2.67430000	2.98200000	0.01390000
C	-4.06450000	2.67510000	-0.40360000
C	-4.58030000	1.33880000	0.12640000
C	-2.21000000	4.10210000	-0.82880000
C	-2.65910000	3.44510000	1.42010000
H	-3.78120000	0.16350000	-1.37530000
H	-3.82000000	-0.58020000	0.08890000
H	-4.07030000	2.63090000	-1.49920000
H	-4.72670000	3.50130000	-0.10310000
H	-4.49480000	1.31270000	1.21960000
H	-1.22340000	4.42520000	-0.49990000
H	-2.90400000	4.95800000	-0.75740000
H	-2.14080000	3.77420000	-1.86540000
H	-3.03540000	2.66370000	2.07780000
H	-3.26510000	4.36150000	1.53700000
H	-1.62940000	3.65600000	1.71280000
C	-6.06470000	1.07980000	-0.25410000
H	-6.15210000	1.20270000	-1.34600000
C	-6.50250000	-0.35230000	0.09680000
H	-7.56160000	-0.49630000	-0.14470000
H	-5.93740000	-1.11230000	-0.45230000
H	-6.37510000	-0.55170000	1.16860000
C	-7.01480000	2.08690000	0.41840000
H	-6.92960000	2.03290000	1.51170000
H	-6.81890000	3.12070000	0.11770000
H	-8.05550000	1.86230000	0.15840000

RuH₂[(S)-tolbinap][(R)-b]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.22380000	0.53400000	-0.19560000
P	0.86000000	1.54430000	-0.24850000
P	-0.29940000	-1.52510000	-0.02430000
C	0.35960000	-2.45580000	-1.49110000
C	0.05860000	-1.99720000	-2.77820000
C	3.06200000	-1.52610000	3.28470000

C	1.11070000	-1.63160000	1.20930000
C	5.68020000	-2.94620000	-2.54020000
C	4.23190000	-0.99520000	-2.40680000
C	1.24530000	-3.87560000	-3.77910000
C	0.88930000	3.11090000	-1.27370000
C	-1.82170000	-3.99350000	0.02010000
C	1.25970000	4.36440000	-0.76710000
C	-1.54240000	-2.76840000	0.64280000
C	0.75700000	5.45860000	-2.88810000
C	1.69770000	2.12730000	1.31030000
C	0.42420000	3.06210000	-2.60220000
C	2.26220000	0.54950000	-1.03140000
C	2.36070000	-1.06860000	0.94080000
C	0.86110000	-2.17180000	2.50290000
C	5.55160000	-0.32150000	2.81550000
C	3.34880000	-0.98530000	1.99020000
C	-3.27620000	-3.30220000	2.28230000
C	4.62310000	-0.37680000	1.79960000
C	3.59190000	3.09670000	2.49110000
C	-2.80220000	-4.85490000	0.52290000
C	1.80100000	-2.13190000	3.50120000
C	5.19970000	-3.37300000	-1.27960000
C	5.20000000	-1.78050000	-3.08930000
C	1.10910000	-3.63670000	-1.36140000
C	0.49560000	-2.70050000	-3.90310000
C	1.53990000	-4.33510000	-2.48680000
C	2.78360000	0.94370000	-2.29660000
C	3.73290000	0.20720000	-2.95900000
C	3.74620000	-1.41200000	-1.12630000
C	2.90130000	3.04090000	3.71130000
C	1.18550000	5.51550000	-1.55900000
C	3.00530000	2.64250000	1.31250000
C	4.04040000	-1.45800000	4.31270000
C	2.76230000	-0.61210000	-0.43400000
C	-3.54240000	-4.53350000	1.66360000
C	-2.30730000	-2.43560000	1.78110000
C	1.00610000	2.07340000	2.52510000
C	0.71610000	6.69430000	-3.75650000
C	5.26390000	-0.87100000	4.08710000
C	4.26270000	-2.63040000	-0.59570000
C	0.37550000	4.20590000	-3.39390000
C	1.60090000	2.52530000	3.70560000
C	1.75630000	-4.61280000	-4.99490000
C	-4.59450000	-5.46740000	2.21350000
C	3.56340000	3.48410000	4.99480000
H	-0.50740000	-1.07370000	-2.87940000
H	6.42230000	-3.53910000	-3.06840000
H	-1.27610000	-4.29060000	-0.86770000
H	1.60230000	4.45990000	0.25670000
H	0.06250000	2.11680000	-2.99510000
H	-0.09180000	-2.64160000	2.70740000
H	6.51390000	0.15170000	2.63860000
H	-3.84020000	-3.01420000	3.16780000
H	4.86050000	0.05750000	0.83610000
H	4.60630000	3.49010000	2.46810000
H	-2.99080000	-5.79650000	0.01130000
H	1.58320000	-2.56620000	4.47470000
H	5.57190000	-4.29790000	-0.84650000
H	5.55360000	-1.43730000	-4.05910000
H	1.35900000	-4.01460000	-0.37330000

H	0.25520000	-2.32340000	-4.89540000
H	2.12510000	-5.24390000	-2.36170000
H	2.43610000	1.86000000	-2.75290000
H	4.11230000	0.54550000	-3.92080000
H	1.47250000	6.47340000	-1.12940000
H	3.56950000	2.69080000	0.38450000
H	3.79920000	-1.88080000	5.28550000
H	-2.13930000	-1.47170000	2.25430000
H	0.00700000	1.64490000	2.53170000
H	-0.17770000	6.71100000	-4.39090000
H	1.58560000	6.73850000	-4.42630000
H	0.72110000	7.60870000	-3.15410000
H	6.00680000	-0.82590000	4.87920000
H	3.90700000	-2.98290000	0.36470000
H	0.01790000	4.12910000	-4.41920000
H	1.04640000	2.46590000	4.64030000
H	1.67660000	-5.69910000	-4.87110000
H	2.81560000	-4.38570000	-5.17490000
H	1.20220000	-4.33260000	-5.89690000
H	-4.33850000	-5.80460000	3.22610000
H	-4.70770000	-6.35660000	1.58530000
H	-5.57280000	-4.97500000	2.27750000
H	4.21100000	2.69200000	5.39420000
H	2.82410000	3.72290000	5.76670000
H	4.19190000	4.36880000	4.84090000
H	-1.31720000	0.41140000	1.50500000
H	-1.29590000	0.67270000	-1.91170000
N	-3.26500000	-0.29400000	-0.38670000
N	-2.74460000	2.52420000	-0.00920000
C	-5.69960000	0.03850000	0.17500000
C	-4.11300000	1.97030000	-0.15600000
C	-4.26350000	0.52440000	0.33310000
C	-2.48300000	3.46680000	-1.14310000
C	-2.56550000	3.28100000	1.26950000
C	-6.48030000	-0.22420000	1.30810000
C	-7.59880000	-0.57610000	-1.21730000
C	-8.36640000	-0.83210000	-0.07860000
C	-7.80310000	-0.65430000	1.18580000
C	-6.27880000	-0.14320000	-1.08990000
H	-3.45370000	-0.30490000	-1.38710000
H	-3.31610000	-1.25790000	-0.05960000
H	-4.35960000	1.97620000	-1.22360000
H	-4.86090000	2.60450000	0.34050000
H	-3.98640000	0.46150000	1.38660000
H	-1.50330000	3.90710000	-0.96370000
H	-2.39140000	2.84850000	-2.03800000
H	-3.10320000	4.23930000	1.19930000
H	-1.49860000	3.51050000	1.33550000
H	-6.04550000	-0.09150000	2.29650000
H	-8.02830000	-0.71310000	-2.20620000
H	-9.39450000	-1.16990000	-0.17730000
H	-8.39080000	-0.85380000	2.07810000
H	-5.69790000	0.05100000	-1.98930000
C	-3.49860000	4.59670000	-1.38820000
H	-3.15420000	5.17980000	-2.24990000
H	-4.50120000	4.22500000	-1.62610000
H	-3.58630000	5.28940000	-0.54500000
C	-3.00940000	2.59700000	2.55980000
H	-4.09500000	2.45030000	2.60200000
H	-2.50610000	1.63470000	2.68240000

H	-2.74160000	3.24640000	3.40190000
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RuH₂[(S)-tolbinap][(R)-d]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.06770000	-0.03370000	-0.26660000
P	0.64980000	1.52080000	-0.21240000
P	0.39720000	-1.75680000	-0.17230000
C	1.32060000	-2.37150000	-1.66280000
C	0.93900000	-1.92640000	-2.93300000
C	3.56290000	-0.99890000	3.24140000
C	1.75940000	-1.53490000	1.09950000
C	6.58840000	-1.30110000	-2.54560000
C	4.64600000	0.15410000	-2.37150000
C	2.62290000	-3.33720000	-3.98730000
C	0.25820000	3.08680000	-1.16150000
C	-0.38870000	-4.54150000	-0.33310000
C	0.24930000	4.36460000	-0.58630000
C	-0.45380000	-3.33700000	0.38210000
C	-0.42030000	5.39560000	-2.69280000
C	1.26850000	2.22960000	1.39690000
C	-0.12260000	2.98380000	-2.51450000
C	2.29170000	1.00490000	-0.99430000
C	2.80410000	-0.62950000	0.89980000
C	1.65050000	-2.19490000	2.35660000
C	5.61880000	0.88030000	2.91270000
C	3.70880000	-0.32930000	1.98420000
C	-1.98630000	-4.43990000	1.93610000
C	4.76280000	0.62190000	1.86490000
C	2.78680000	3.64040000	2.67340000
C	-1.10270000	-5.67030000	0.08230000
C	2.52190000	-1.94720000	3.38640000
C	6.22010000	-1.91670000	-1.32580000
C	5.81080000	-0.28780000	-3.05530000
C	2.36130000	-3.31020000	-1.56820000
C	1.58230000	-2.40580000	-4.07630000
C	2.99750000	-3.78630000	-2.71200000
C	2.71010000	1.60210000	-2.21760000
C	3.84180000	1.19980000	-2.88080000
C	4.26960000	-0.45410000	-1.13180000
C	2.14280000	3.30460000	3.87370000
C	-0.09210000	5.49450000	-1.33830000
C	2.36520000	3.10660000	1.45800000
C	4.46220000	-0.71450000	4.30390000
C	3.08630000	-0.00230000	-0.43670000
C	-1.90720000	-5.64700000	1.22450000
C	-1.28580000	-3.30920000	1.52170000
C	0.62380000	1.89510000	2.59220000
C	-0.74800000	6.61850000	-3.51770000
C	5.47400000	0.20420000	4.14710000
C	5.09680000	-1.50710000	-0.64210000
C	-0.43350000	4.11320000	-3.26550000
C	1.05660000	2.42540000	3.81030000
C	3.35000000	-3.82110000	-5.22010000
C	-2.67010000	-6.86840000	1.68010000

C	2.63960000	3.84330000	5.19470000
H	0.14250000	-1.18870000	-3.00440000
H	7.47940000	-1.63070000	-3.07360000
H	0.22020000	-4.61270000	-1.22660000
H	0.50820000	4.49570000	0.45790000
H	-0.19980000	1.99790000	-2.96310000
H	0.86720000	-2.92580000	2.50680000
H	6.41190000	1.61340000	2.79030000
H	-2.61290000	-4.38140000	2.82420000
H	4.88730000	1.15720000	0.93150000
H	3.63780000	4.31850000	2.69460000
H	-1.02860000	-6.58600000	-0.50060000
H	2.41890000	-2.47950000	4.32960000
H	6.82840000	-2.72320000	-0.92470000
H	6.07470000	0.19610000	-3.99310000
H	2.67770000	-3.67190000	-0.59310000
H	1.27410000	-2.04210000	-5.05470000
H	3.80640000	-4.50740000	-2.61430000
H	2.13140000	2.41190000	-2.63910000
H	4.13220000	1.68710000	-3.80910000
H	-0.09080000	6.47070000	-0.85760000
H	2.89310000	3.37900000	0.54750000
H	4.33230000	-1.24090000	5.24700000
H	-1.39040000	-2.37390000	2.06550000
H	-0.20320000	1.19080000	2.55170000
H	-1.69520000	6.49780000	-4.05750000
H	0.02730000	6.81010000	-4.27110000
H	-0.82910000	7.51320000	-2.89210000
H	6.15920000	0.41310000	4.96470000
H	4.83230000	-1.99990000	0.28530000
H	-0.70760000	3.99720000	-4.31250000
H	0.54550000	2.14150000	4.72840000
H	3.57250000	-4.89300000	-5.16320000
H	4.30860000	-3.29870000	-5.34040000
H	2.76320000	-3.64430000	-6.12770000
H	-2.30350000	-7.22910000	2.64990000
H	-2.57490000	-7.69000000	0.96300000
H	-3.73810000	-6.65040000	1.80200000
H	3.49430000	3.25760000	5.55930000
H	1.86150000	3.80090000	5.96420000
H	2.97430000	4.88330000	5.10670000
H	-1.15720000	-0.25900000	1.42490000
H	-1.14940000	0.15060000	-1.97830000
N	-2.80020000	-1.38360000	-0.50970000
N	-3.10410000	1.45260000	-0.06370000
C	-5.21710000	-1.77960000	0.08850000
C	-4.25930000	0.53180000	-0.20480000
C	-3.97760000	-0.90650000	0.24560000
C	-3.12760000	2.43100000	-1.19730000
C	-3.13700000	2.22400000	1.21810000
C	-5.89430000	-2.24770000	1.22210000
C	-6.86560000	-2.90710000	-1.30260000
C	-7.53150000	-3.36560000	-0.16350000
C	-7.04280000	-3.03250000	1.10050000
C	-5.72080000	-2.12000000	-1.17600000
H	-2.99090000	-1.40710000	-1.50960000
H	-2.57680000	-2.33520000	-0.22210000
H	-4.52270000	0.48730000	-1.26750000
H	-5.14640000	0.91360000	0.31910000
H	-3.67250000	-0.91080000	1.29340000

H	-2.30230000	3.12280000	-1.03080000
H	-2.88020000	1.86090000	-2.09630000
H	-3.93020000	2.98620000	1.16070000
H	-2.18140000	2.75450000	1.27350000
H	-5.51620000	-1.99500000	2.21030000
H	-7.23800000	-3.16210000	-2.29130000
H	-8.42300000	-3.97920000	-0.26170000
H	-7.55200000	-3.38630000	1.99320000
H	-5.21710000	-1.77320000	-2.07600000
C	-4.42110000	3.23980000	-1.42890000
H	-5.28570000	2.57260000	-1.54710000
H	-4.64430000	3.88350000	-0.56820000
C	-3.34760000	1.44180000	2.51520000
H	-4.34100000	0.97070000	2.52150000
H	-2.59930000	0.64460000	2.57730000
C	-4.30840000	4.12100000	-2.68250000
H	-4.09400000	3.48570000	-3.55360000
H	-3.44540000	4.79150000	-2.57740000
C	-5.57270000	4.94480000	-2.94990000
H	-5.46580000	5.56030000	-3.85080000
H	-6.44700000	4.29720000	-3.09150000
H	-5.79290000	5.61750000	-2.11170000
C	-3.23930000	2.36390000	3.73970000
H	-2.24030000	2.82020000	3.75860000
H	-3.95500000	3.19360000	3.64490000
C	-3.48770000	1.62680000	5.06020000
H	-4.49470000	1.19140000	5.08930000
H	-2.76970000	0.80880000	5.19640000
H	-3.39290000	2.30140000	5.91900000

RuH₂[(*S*)-tolbinap][(*R*)-dmapen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.27970000	0.77160000	-0.09990000
P	0.88180000	1.59270000	-0.21330000
P	-0.53060000	-1.36840000	0.05280000
C	-0.03020000	-2.36380000	-1.43490000
C	-0.33750000	-1.87830000	-2.71050000
C	2.99570000	-1.67910000	3.17190000
C	0.92730000	-1.59850000	1.21210000
C	5.11660000	-3.29240000	-2.83400000
C	3.86360000	-1.22040000	-2.59420000
C	0.60150000	-3.87100000	-3.75210000
C	1.02630000	3.17500000	-1.20540000
C	-2.25690000	-3.69590000	0.20180000
C	1.58470000	4.36080000	-0.70940000
C	-1.84180000	-2.49360000	0.79310000
C	1.08540000	5.55460000	-2.77750000
C	1.83230000	2.04920000	1.32270000
C	0.47380000	3.21260000	-2.50100000
C	2.13950000	0.48180000	-1.08140000
C	2.20910000	-1.16100000	0.86840000
C	0.69860000	-2.10070000	2.52460000
C	5.56880000	-0.75570000	2.54340000
C	3.26140000	-1.17890000	1.85680000

C	-3.53510000	-2.85640000	2.51980000
C	4.58080000	-0.71460000	1.58460000
C	3.85930000	2.78630000	2.44940000
C	-3.28280000	-4.46310000	0.76330000
C	1.69290000	-2.14710000	3.46850000
C	4.68180000	-3.68900000	-1.54710000
C	4.71000000	-2.08150000	-3.34340000
C	0.60030000	-3.61530000	-1.33200000
C	-0.02590000	-2.62420000	-3.84960000
C	0.90570000	-4.35580000	-2.47120000
C	2.61040000	0.84100000	-2.37650000
C	3.44190000	0.02890000	-3.10520000
C	3.42520000	-1.60700000	-1.28740000
C	3.20820000	2.78450000	3.69210000
C	1.60470000	5.52860000	-1.48060000
C	3.18770000	2.41860000	1.28610000
C	4.03410000	-1.70860000	4.14130000
C	2.56650000	-0.72910000	-0.52630000
C	-3.93490000	-4.06710000	1.93410000
C	-2.52000000	-2.08270000	1.96070000
C	1.17960000	2.05040000	2.56000000
C	1.12800000	6.80710000	-3.62130000
C	5.29860000	-1.26030000	3.83730000
C	3.86210000	-2.87320000	-0.79900000
C	0.51840000	4.36960000	-3.27300000
C	1.85960000	2.41410000	3.72490000
C	0.97510000	-4.66120000	-4.98450000
C	-5.02750000	-4.90630000	2.55360000
C	3.95730000	3.13170000	4.95720000
H	-0.80640000	-0.90010000	-2.79220000
H	5.76620000	-3.94360000	-3.41300000
H	-1.78490000	-4.04780000	-0.70770000
H	2.00600000	4.39150000	0.28870000
H	-0.02240000	2.32490000	-2.88210000
H	-0.28410000	-2.46810000	2.78900000
H	6.56520000	-0.39340000	2.30400000
H	-4.03040000	-2.51060000	3.42540000
H	4.80840000	-0.31750000	0.60290000
H	4.90940000	3.06710000	2.39600000
H	-3.57890000	-5.38880000	0.27390000
H	1.48790000	-2.54700000	4.45930000
H	4.99570000	-4.64880000	-1.14490000
H	5.03020000	-1.75990000	-4.33190000
H	0.85580000	-4.01540000	-0.35410000
H	-0.26860000	-2.22450000	-4.83250000
H	1.39940000	-5.31990000	-2.36670000
H	2.31850000	1.79030000	-2.80340000
H	3.78640000	0.34240000	-4.08840000
H	2.03980000	6.43320000	-1.06040000
H	3.72260000	2.42210000	0.33980000
H	3.80650000	-2.09610000	5.13180000
H	-2.24950000	-1.12990000	2.40900000
H	0.14050000	1.73140000	2.59480000
H	0.13210000	7.07250000	-3.99720000
H	1.77550000	6.67530000	-4.49800000
H	1.51040000	7.66070000	-3.05240000
H	6.08760000	-1.29100000	4.58430000
H	3.53790000	-3.20330000	0.18030000
H	0.09060000	4.35850000	-4.27410000
H	1.33330000	2.39910000	4.67750000

H	0.75920000	-5.72890000	-4.85990000
H	2.04870000	-4.57230000	-5.19780000
H	0.43350000	-4.30690000	-5.86780000
H	-4.69410000	-5.36050000	3.49600000
H	-5.33590000	-5.71800000	1.88700000
H	-5.91430000	-4.30390000	2.78420000
H	4.54180000	2.27280000	5.31370000
H	3.27360000	3.42000000	5.76260000
H	4.66070000	3.95700000	4.79680000
H	-1.37380000	0.69940000	1.60940000
H	-1.37930000	0.90000000	-1.81590000
N	-3.38740000	0.09710000	-0.21420000
N	-2.53510000	2.83560000	0.12760000
C	-5.78580000	0.76300000	0.18430000
C	-3.93590000	2.45100000	-0.16500000
C	-4.31060000	1.07840000	0.39470000
C	-2.19660000	3.95160000	-0.77890000
C	-2.42910000	3.33610000	1.51670000
C	-6.63850000	0.61650000	1.28550000
C	-7.67970000	0.33340000	-1.28130000
C	-8.51940000	0.19110000	-0.17390000
C	-7.99490000	0.33400000	1.11130000
C	-6.32600000	0.61810000	-1.10260000
H	-3.58290000	-0.01310000	-1.20730000
H	-3.51990000	-0.81410000	0.22260000
H	-4.04740000	2.42060000	-1.25460000
H	-4.63130000	3.21710000	0.21550000
H	-4.09820000	1.05620000	1.46800000
H	-1.21170000	4.34220000	-0.52860000
H	-2.93430000	4.76770000	-0.68550000
H	-2.17680000	3.59100000	-1.80680000
H	-2.71900000	2.55750000	2.22040000
H	-3.06250000	4.22950000	1.66020000
H	-1.38960000	3.59650000	1.72220000
H	-6.23490000	0.72420000	2.29000000
H	-8.07950000	0.22350000	-2.28590000
H	-9.57390000	-0.03110000	-0.31310000
H	-8.63910000	0.22280000	1.97960000
H	-5.68870000	0.72730000	-1.97780000

RuH₂[(*S*)-tolbinap][(*R,R*)-dmpen]

Coordinates (Angstroms)

X	Y	Z
Ru	-0.92520000	0.16170000
P	0.46210000	-1.61790000
P	0.86940000	1.62840000
C	1.55890000	2.40750000
C	0.90540000	2.21250000
C	4.71430000	-0.12000000
C	2.45620000	0.96330000
C	5.75250000	0.42310000
C	3.74770000	-0.73400000
C	2.53490000	3.60450000
C	-0.45270000	-3.09540000
C	0.65690000	4.46110000

C	-0.44380000	-4.37010000	0.16990000
C	0.54050000	3.14530000	-1.32430000
C	-1.99280000	-5.24180000	1.84140000
C	1.32100000	-2.42190000	-1.40300000
C	-1.27080000	-2.91410000	1.89070000
C	1.86160000	-1.35260000	1.25740000
C	3.22080000	-0.03110000	-0.43720000
C	2.85280000	1.42800000	-2.34180000
C	6.22910000	-2.16640000	-1.25250000
C	4.35560000	-0.59950000	-1.12710000
C	-0.24270000	4.05480000	-3.45040000
C	5.15050000	-1.64510000	-0.57290000
C	2.90060000	-4.01880000	-2.33670000
C	0.32530000	5.55070000	-1.66860000
C	3.93920000	0.91340000	-3.00310000
C	5.90480000	0.97430000	2.75920000
C	4.69090000	-0.41160000	4.31560000
C	2.71510000	3.20630000	1.25590000
C	1.38780000	2.80400000	3.66110000
C	3.18760000	3.80010000	2.42360000
C	1.74570000	-1.88690000	2.57200000
C	2.65570000	-1.59840000	3.55700000
C	3.89920000	-0.18990000	1.98740000
C	2.51280000	-3.68560000	-3.64320000
C	-1.19900000	-5.41850000	0.70520000
C	2.31940000	-3.39560000	-1.23520000
C	5.83300000	-0.67560000	-3.10540000
C	2.94890000	-0.52870000	0.95510000
C	-0.11800000	5.37230000	-2.98150000
C	0.06180000	2.96700000	-2.63780000
C	0.92700000	-2.09130000	-2.70410000
C	6.58150000	-1.67720000	-2.53280000
C	5.00540000	0.67850000	1.75880000
C	-2.01400000	-3.96520000	2.42400000
C	1.51650000	-2.71640000	-3.80530000
H	0.03240000	1.56440000	2.51190000
H	6.47120000	0.66100000	4.83330000
H	0.99910000	4.65450000	0.15450000
H	0.15440000	-4.56000000	-0.71330000
H	-1.32860000	-1.92350000	2.33510000
H	2.29280000	2.22270000	-2.81500000
H	6.81400000	-2.96380000	-0.80130000
H	-0.60080000	3.87870000	-4.46330000
H	4.89700000	-2.04180000	0.40230000
H	3.67660000	-4.76570000	-2.18210000
H	0.41920000	6.55810000	-1.26780000
H	4.21580000	1.30010000	-3.98170000
H	6.73800000	1.64120000	2.55290000
H	4.55470000	-0.84130000	5.30560000
H	3.25050000	3.36890000	0.32390000
H	0.86690000	2.63070000	4.60090000
H	4.08530000	4.41430000	2.38730000
H	0.92390000	-2.55080000	2.80540000
H	2.54490000	-2.03320000	4.54810000
H	-1.16660000	-6.39310000	0.22260000
H	2.64470000	-3.67000000	-0.23490000
H	6.08500000	-0.28860000	-4.09030000
H	-0.10300000	1.95700000	-3.00070000
H	0.16490000	-1.32630000	-2.83630000
H	7.43730000	-2.09390000	-3.05750000

H	5.13710000	1.11800000	0.77780000
H	-2.62600000	-3.78960000	3.30710000
H	1.19960000	-2.44000000	-4.80910000
H	-1.00520000	0.21990000	-1.91790000
H	-1.04740000	0.08770000	1.51040000
C	3.08480000	4.20600000	4.92210000
H	3.90740000	3.59590000	5.31900000
H	3.48200000	5.21380000	4.75370000
H	2.31790000	4.26910000	5.70130000
C	-0.45240000	6.54810000	-3.86910000
H	-0.43020000	7.48990000	-3.31140000
H	0.26100000	6.63730000	-4.69900000
H	-1.44920000	6.44420000	-4.31500000
C	-2.81530000	-6.37100000	2.41580000
H	-3.89010000	-6.16830000	2.32300000
H	-2.61070000	-7.31620000	1.90290000
H	-2.60700000	-6.51560000	3.48300000
C	3.17880000	-4.33330000	-4.83470000
H	4.16300000	-3.88540000	-5.02670000
H	3.33950000	-5.40580000	-4.67350000
H	2.58010000	-4.21320000	-5.74370000
N	-2.82750000	1.71200000	-0.04630000
N	-2.69350000	-1.13230000	-0.33840000
H	-2.52660000	-2.03560000	0.10350000
H	-2.83690000	-1.31170000	-1.33090000
C	-4.05490000	0.88510000	-0.34840000
H	-4.02220000	0.76150000	-1.43730000
C	-3.91200000	-0.53050000	0.24970000
H	-3.71130000	-0.45210000	1.32240000
C	-5.13100000	-1.42200000	0.04300000
C	-5.72270000	-2.06900000	1.13460000
C	-5.64980000	-1.66640000	-1.23760000
C	-6.80690000	-2.93130000	0.95870000
H	-5.32870000	-1.89690000	2.13380000
C	-6.73210000	-2.52700000	-1.41840000
H	-5.21150000	-1.17940000	-2.10620000
C	-7.31590000	-3.16220000	-0.31950000
H	-7.25220000	-3.42130000	1.82070000
H	-7.12140000	-2.70050000	-2.41810000
H	-8.15970000	-3.83210000	-0.46030000
C	-5.38740000	1.55510000	-0.01590000
C	-6.12060000	2.17670000	-1.03670000
C	-5.92240000	1.57220000	1.28180000
C	-7.34060000	2.80370000	-0.77560000
H	-5.73390000	2.16360000	-2.05310000
C	-7.14090000	2.19650000	1.54870000
H	-5.38920000	1.08980000	2.09540000
C	-7.85440000	2.81700000	0.52110000
H	-7.88860000	3.27640000	-1.58640000
H	-7.53510000	2.19460000	2.56160000
H	-8.80460000	3.30140000	0.72960000
C	-2.78790000	2.84380000	-0.99640000
H	-3.69350000	3.46460000	-0.92180000
H	-1.92300000	3.46420000	-0.77200000
H	-2.68320000	2.46370000	-2.01320000
C	-2.82820000	2.27880000	1.32290000
H	-1.87030000	2.77550000	1.48310000
H	-3.64000000	3.00750000	1.46390000
H	-2.90790000	1.48260000	2.06200000

RuH₂[(S)-tolbinap][(S)-daipen]

Coordinates (Angstroms)

X	Y	Z	
Ru	0.46530000	-0.29010000	-0.47070000
P	-1.49850000	-1.40130000	-0.80470000
P	-0.59600000	1.49930000	0.46770000
C	-1.30060000	2.89580000	-0.54300000
C	-1.01140000	2.98060000	-1.90950000
C	-4.07390000	0.18120000	3.37380000
C	-2.04910000	1.08200000	1.58220000
C	-6.53330000	3.27430000	-1.88170000
C	-4.95850000	1.45870000	-2.26570000
C	-2.29090000	5.04510000	-2.10760000
C	-1.33560000	-2.62670000	-2.21550000
C	0.82160000	3.82390000	1.47250000
C	-1.63740000	-3.99190000	-2.10200000
C	0.56320000	2.45050000	1.59660000
C	-0.91020000	-4.42660000	-4.38970000
C	-2.27100000	-2.48200000	0.49820000
C	-0.78630000	-2.18560000	-3.43660000
C	-2.95940000	-0.33440000	-1.31110000
C	-3.24460000	0.57650000	1.05940000
C	-1.89070000	1.15980000	2.99480000
C	-6.46520000	-0.89220000	2.37620000
C	-4.27080000	0.10130000	1.95730000
C	2.21230000	2.38740000	3.39760000
C	-5.49860000	-0.45690000	1.49710000
C	-4.09680000	-3.87100000	1.31020000
C	1.75370000	4.46310000	2.29610000
C	-2.86490000	0.73210000	3.86090000
C	-6.13680000	3.31480000	-0.52400000
C	-5.95000000	2.36390000	-2.73170000
C	-2.09070000	3.90540000	0.03320000
C	-1.50070000	4.04050000	-2.67650000
C	-2.57100000	4.96290000	-0.73560000
C	-3.39290000	-0.34580000	-2.66690000
C	-4.35860000	0.51210000	-3.12960000
C	-4.55580000	1.48600000	-0.89160000
C	-3.37530000	-4.19860000	2.46800000
C	-1.42270000	-4.87140000	-3.16770000
C	-3.55840000	-3.02400000	0.34480000
C	-5.08870000	-0.27610000	4.25730000
C	-3.55330000	0.56190000	-0.41570000
C	2.45650000	3.76440000	3.28200000
C	1.29930000	1.73950000	2.56610000
C	-1.54600000	-2.81300000	1.64780000
C	-6.26470000	-0.80030000	3.77380000
C	-5.17790000	2.44980000	-0.04550000
C	-0.59250000	-3.06420000	-4.50170000
C	-2.09310000	-3.65880000	2.61550000
H	-0.41410000	2.19070000	-2.35990000
H	-7.29340000	3.96000000	-2.24700000
H	0.29640000	4.41120000	0.72820000
H	-2.04250000	-4.38470000	-1.17680000
H	-0.49690000	-1.14220000	-3.53110000

H	-0.98010000	1.57900000	3.40340000
H	-7.39050000	-1.31350000	1.99180000
H	2.74930000	1.80980000	4.14830000
H	-5.67160000	-0.54370000	0.43150000
H	-5.09750000	-4.27520000	1.17030000
H	1.92980000	5.52930000	2.16800000
H	-2.71650000	0.81470000	4.93550000
H	-6.59090000	4.03850000	0.14800000
H	-6.23890000	2.31960000	-3.77950000
H	-2.33270000	3.86570000	1.09250000
H	-1.26920000	4.08100000	-3.73930000
H	-3.18460000	5.73000000	-0.26740000
H	-2.95770000	-1.05850000	-3.35560000
H	-4.67420000	0.47090000	-4.17000000
H	-1.66480000	-5.92480000	-3.04130000
H	-4.14540000	-2.78410000	-0.53840000
H	-4.91400000	-0.20090000	5.32830000
H	1.15890000	0.66420000	2.64280000
H	-0.55600000	-2.38170000	1.77630000
H	-7.03640000	-1.14410000	4.45770000
H	-4.88490000	2.50500000	0.99580000
H	-0.17820000	-2.68580000	-5.43440000
H	-1.51230000	-3.89700000	3.50460000
H	0.71750000	-0.96490000	1.07590000
H	0.39960000	0.36270000	-2.06410000
C	-0.71330000	-5.36990000	-5.55310000
H	0.25680000	-5.21290000	-6.03930000
H	-0.76610000	-6.41590000	-5.23410000
H	-1.48430000	-5.22100000	-6.32080000
C	-3.98500000	-5.07710000	3.53530000
H	-4.67750000	-4.50440000	4.16680000
H	-4.55640000	-5.90500000	3.09940000
H	-3.21830000	-5.50260000	4.19130000
C	-2.86050000	6.16500000	-2.94650000
H	-3.90610000	5.96140000	-3.21380000
H	-2.84530000	7.12040000	-2.40910000
H	-2.30210000	6.29170000	-3.88010000
C	3.43510000	4.46170000	4.19780000
H	3.67740000	5.46580000	3.83470000
H	3.02530000	4.56830000	5.21100000
H	4.37250000	3.90020000	4.28920000
N	2.54240000	0.54360000	-0.32730000
N	1.79480000	-1.90510000	-1.27060000
C	3.14210000	-1.39290000	-1.67020000
C	3.62230000	-0.47260000	-0.49710000
H	2.59300000	1.22670000	-1.07960000
H	2.63810000	1.04920000	0.55060000
H	3.85510000	-2.22520000	-1.73690000
H	1.34460000	-2.37130000	-2.05590000
H	1.86910000	-2.57810000	-0.51270000
C	3.78690000	-1.28250000	0.81950000
C	3.94810000	-0.59830000	2.02980000
C	3.91930000	-2.68040000	0.86560000
C	4.17150000	-1.25720000	3.23830000
H	3.91540000	0.48640000	2.05220000
C	4.14600000	-3.35810000	2.06010000
H	3.85580000	-3.27860000	-0.03770000
C	4.26350000	-2.65360000	3.26260000
H	4.28210000	-0.67330000	4.14520000
H	4.23700000	-4.43960000	2.07840000

C	2.99550000	-0.81860000	-3.11760000
H	1.99580000	-0.36730000	-3.14570000
O	4.48170000	-3.40400000	4.38120000
C	4.59080000	-2.73360000	5.62560000
H	3.67610000	-2.17460000	5.86480000
H	4.74280000	-3.51320000	6.37440000
H	5.44710000	-2.04580000	5.64150000
C	5.01110000	0.16080000	-0.74570000
C	5.24860000	1.53030000	-0.61340000
C	6.11840000	-0.65690000	-1.04120000
C	6.52170000	2.08480000	-0.79600000
H	4.43640000	2.20790000	-0.36740000
C	7.38500000	-0.12590000	-1.23460000
H	5.99340000	-1.73340000	-1.11090000
C	7.59930000	1.25670000	-1.11730000
H	6.64990000	3.15560000	-0.68550000
H	8.23140000	-0.76420000	-1.46860000
O	8.87940000	1.68130000	-1.32530000
C	9.14980000	3.06870000	-1.21370000
H	8.93280000	3.44290000	-0.20420000
H	10.21560000	3.18460000	-1.41920000
H	8.57420000	3.65250000	-1.94450000
C	3.98820000	0.25490000	-3.59040000
H	3.94030000	1.17340000	-3.00070000
H	5.02630000	-0.09290000	-3.57590000
H	3.74050000	0.52120000	-4.62530000
C	3.04300000	-1.99120000	-4.11960000
H	2.34490000	-2.79840000	-3.87310000
H	2.78690000	-1.64240000	-5.12660000
H	4.05200000	-2.42310000	-4.16600000

RuH₂[(S)-tolbinap][(S,S)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.21600000	0.00000000	-0.00040000
P	0.36310000	-1.60550000	-0.38640000
P	0.36290000	1.60560000	0.38590000
C	1.14190000	1.87590000	2.05350000
C	0.61550000	1.23990000	3.18270000
C	3.97130000	1.29140000	-2.63230000
C	1.87680000	1.50970000	-0.71670000
C	5.94890000	-0.16120000	3.49020000
C	3.97050000	-1.29080000	2.63300000
C	2.25070000	2.32690000	4.62560000
C	-0.34040000	-3.31100000	-0.05050000
C	-0.27770000	4.37760000	0.95870000
C	-0.27760000	-4.37750000	-0.95930000
C	-0.34070000	3.31100000	0.04990000
C	-1.62240000	-5.80170000	0.49580000
C	1.14260000	-1.87570000	-2.05370000
C	-1.07850000	-3.51380000	1.13380000
C	1.87670000	-1.50950000	0.71660000
C	2.81590000	0.48090000	-0.58070000
C	2.00370000	2.42960000	-1.79470000
C	5.85780000	-0.77540000	-2.43320000

C	3.87450000	0.35290000	-1.55410000
C	-1.69930000	4.73260000	-1.40180000
C	4.85120000	-0.68370000	-1.49770000
C	2.77270000	-2.96900000	-3.49270000
C	-0.90930000	5.59550000	0.68820000
C	3.01430000	2.33080000	-2.71740000
C	5.85700000	0.77600000	2.43420000
C	5.01910000	-1.17030000	3.58480000
C	2.23250000	2.74460000	2.22850000
C	1.16320000	1.46460000	4.44770000
C	2.77210000	2.96880000	3.49270000
C	2.00330000	-2.42930000	1.79470000
C	3.01360000	-2.33020000	2.71780000
C	3.87410000	-0.35250000	1.55450000
C	2.25220000	-2.32630000	-4.62560000
C	-0.90880000	-5.59560000	-0.68850000
C	2.23280000	-2.74500000	-2.22860000
C	5.02030000	1.17110000	-3.58380000
C	2.81580000	-0.48070000	0.58080000
C	-1.62330000	5.80140000	-0.49590000
C	-1.07920000	3.51370000	-1.13410000
C	0.61710000	-1.23890000	-3.18290000
C	5.95010000	0.16210000	-3.48900000
C	4.85080000	0.68410000	1.49830000
C	-1.69820000	-4.73280000	1.40180000
C	1.16510000	-1.46340000	-4.44780000
H	-0.21460000	0.55100000	3.04700000
H	6.74970000	-0.08040000	4.22070000
H	0.26080000	4.26750000	1.89280000
H	0.26060000	-4.26740000	-1.89360000
H	-1.17920000	-2.68820000	1.83250000
H	1.28810000	3.23720000	-1.88700000
H	6.58700000	-1.57820000	-2.36090000
H	-2.26310000	4.84970000	-2.32520000
H	4.79720000	-1.41730000	-0.70270000
H	3.61950000	-3.64360000	-3.60180000
H	-0.84340000	6.39930000	1.41880000
H	3.09100000	3.05540000	-3.52520000
H	6.58610000	1.57880000	2.36200000
H	5.07090000	-1.89780000	4.39180000
H	2.66370000	3.25170000	1.36900000
H	0.74150000	0.95260000	5.31070000
H	3.61930000	3.64280000	3.60180000
H	1.28770000	-3.23690000	1.88700000
H	3.08990000	-3.05470000	3.52580000
H	-0.84290000	-6.39940000	-1.41920000
H	2.66330000	-3.25260000	-1.36920000
H	5.07240000	1.89880000	-4.39060000
H	-1.18020000	2.68800000	-1.83260000
H	-0.21260000	-0.54960000	-3.04730000
H	6.75120000	0.08150000	-4.21920000
H	4.79710000	1.41760000	0.70310000
H	-2.26160000	-4.85010000	2.32540000
H	0.74420000	-0.95070000	-5.31070000
H	-1.27880000	0.48320000	-1.64300000
H	-1.27880000	-0.48330000	1.64230000
C	2.87470000	2.53230000	5.98590000
H	3.76430000	1.89990000	6.10770000
H	3.19440000	3.57070000	6.13100000
H	2.17770000	2.27610000	6.79090000

C	-2.28490000	7.12540000	-0.79860000
H	-2.34420000	7.75770000	0.09330000
H	-1.72600000	7.68380000	-1.56140000
H	-3.30190000	6.98720000	-1.18410000
C	-2.28380000	-7.12560000	0.79880000
H	-3.30240000	-6.98760000	1.18010000
H	-2.33930000	-7.75970000	-0.09220000
H	-1.72730000	-7.68200000	1.56480000
C	2.87660000	-2.53170000	-5.98580000
H	3.76690000	-1.90010000	-6.10680000
H	3.19520000	-3.57030000	-6.13120000
H	2.18020000	-2.27430000	-6.79090000
N	-2.97980000	1.30180000	0.45720000
N	-2.97970000	-1.30210000	-0.45780000
C	-4.31300000	-0.78360000	-0.01980000
C	-4.31320000	0.78300000	0.01960000
H	-2.96290000	1.38230000	1.47080000
H	-2.84400000	2.23990000	0.08180000
H	-5.06200000	-1.06630000	-0.76910000
H	-2.84360000	-2.24030000	-0.08260000
H	-2.96290000	-1.38250000	-1.47150000
C	-4.77100000	-1.40460000	1.29330000
C	-6.03800000	-2.00370000	1.34940000
C	-3.99170000	-1.37030000	2.46030000
C	-6.52300000	-2.55150000	2.53840000
H	-6.65270000	-2.04260000	0.45230000
C	-4.47550000	-1.92380000	3.64760000
H	-2.99360000	-0.93620000	2.42020000
C	-5.74150000	-2.51190000	3.69400000
H	-7.50770000	-3.01130000	2.55850000
H	-3.85720000	-1.89320000	4.54150000
H	-6.11480000	-2.93800000	4.62170000
C	-4.77190000	1.40380000	-1.29330000
C	-3.99330000	1.36940000	-2.46080000
C	-6.03880000	2.00290000	-1.34870000
C	-4.47790000	1.92270000	-3.64790000
H	-2.99510000	0.93540000	-2.42130000
C	-6.52460000	2.55050000	-2.53750000
H	-6.65300000	2.04200000	-0.45130000
C	-5.74390000	2.51070000	-3.69360000
H	-3.86010000	1.89190000	-4.54220000
H	-7.50940000	3.01030000	-2.55700000
H	-6.11780000	2.93660000	-4.62120000
H	-5.06190000	1.06550000	0.76920000

RuH₂[(S)-tolbinap][(S,S)-dmpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.14350000	0.13920000	-0.00230000
P	0.27590000	-1.57560000	-0.46440000
P	0.63180000	1.60720000	0.26730000
C	1.36100000	1.92810000	1.95160000
C	0.74800000	1.39010000	3.08810000
C	4.45710000	0.72030000	-2.38590000
C	2.20590000	1.25530000	-0.71320000

C	5.64110000	-0.84640000	3.88560000
C	3.66370000	-1.77310000	2.81320000
C	2.39620000	2.43730000	4.54530000
C	-0.58900000	-3.23350000	-0.32980000
C	0.35210000	4.47960000	0.52760000
C	-0.71720000	-4.11700000	-1.41240000
C	0.23070000	3.34850000	-0.29060000
C	-2.11190000	-5.64130000	-0.11290000
C	1.10120000	-1.78730000	-2.11730000
C	-1.26610000	-3.57400000	0.85800000
C	1.72190000	-1.72290000	0.72430000
C	3.00040000	0.13540000	-0.45210000
C	2.56820000	2.11460000	-1.78980000
C	6.02710000	-1.56140000	-1.95040000
C	4.13250000	-0.15690000	-1.30220000
C	-0.63620000	4.80610000	-2.04620000
C	4.95520000	-1.30760000	-1.12360000
C	2.66470000	-2.94540000	-3.57700000
C	-0.01960000	5.74770000	0.06780000
C	3.65210000	1.86450000	-2.59270000
C	5.72090000	0.13250000	2.86700000
C	4.62900000	-1.77730000	3.85580000
C	2.50740000	2.72210000	2.13040000
C	1.25890000	1.64360000	4.36340000
C	3.00930000	2.97640000	3.40440000
C	1.69040000	-2.70210000	1.75750000
C	2.62720000	-2.73530000	2.75920000
C	3.74160000	-0.79300000	1.77230000
C	2.26150000	-2.17070000	-4.67520000
C	-1.46310000	-5.29430000	-1.30190000
C	2.09880000	-2.75570000	-2.31930000
C	5.57010000	0.43500000	-3.22220000
C	2.76980000	-0.79790000	0.70480000
C	-0.50900000	5.93890000	-1.22690000
C	-0.29140000	3.53900000	-1.58490000
C	0.68780000	-1.02130000	-3.21170000
C	6.34530000	-0.68140000	-3.01170000
C	4.80040000	0.15790000	1.84270000
C	-2.00310000	-4.75220000	0.96640000
C	1.26260000	-1.21260000	-4.47060000
H	-0.11800000	0.74690000	2.95070000
H	6.37640000	-0.85860000	4.68590000
H	0.72930000	4.38540000	1.53920000
H	-0.23680000	-3.89370000	-2.35760000
H	-1.22640000	-2.88970000	1.69870000
H	1.98130000	3.00250000	-1.97980000
H	6.63330000	-2.44860000	-1.78660000
H	-1.02920000	4.91630000	-3.05530000
H	4.72880000	-2.00040000	-0.32290000
H	3.44000000	-3.69740000	-3.70760000
H	0.07910000	6.60230000	0.73420000
H	3.90210000	2.54860000	-3.40080000
H	6.51500000	0.87410000	2.89410000
H	4.54960000	-2.53530000	4.63190000
H	3.01250000	3.14920000	1.26780000
H	0.76700000	1.20830000	5.23130000
H	3.89810000	3.59440000	3.51620000
H	0.92020000	-3.46120000	1.74970000
H	2.58180000	-3.50720000	3.52450000
H	-1.54060000	-5.95300000	-2.16450000

H	2.43410000	-3.36900000	-1.48690000
H	5.79530000	1.12170000	-4.03520000
H	-0.45190000	2.67180000	-2.21820000
H	-0.08220000	-0.26970000	-3.05580000
H	7.19610000	-0.89040000	-3.65490000
H	4.87510000	0.92040000	1.07700000
H	-2.51480000	-4.97340000	1.90070000
H	0.93090000	-0.60090000	-5.30750000
H	-1.28640000	0.65410000	-1.63320000
H	-1.12120000	-0.40360000	1.61920000
C	2.97510000	2.67610000	5.92000000
H	3.80780000	1.98830000	6.11970000
H	3.36620000	3.69500000	6.02190000
H	2.22650000	2.51990000	6.70400000
C	-0.88530000	7.31110000	-1.73450000
H	-0.88450000	8.05070000	-0.92730000
H	-0.18210000	7.65860000	-2.50280000
H	-1.88270000	7.31080000	-2.19060000
C	-2.89500000	-6.92670000	0.01350000
H	-3.83370000	-6.77250000	0.55790000
H	-3.13720000	-7.34660000	-0.96820000
H	-2.32460000	-7.68660000	0.56420000
C	2.91460000	-2.34800000	-6.02590000
H	3.89390000	-1.85180000	-6.05560000
H	3.08280000	-3.40630000	-6.25720000
H	2.30380000	-1.91860000	-6.82700000
N	-3.05620000	1.59330000	0.61440000
N	-2.96940000	-1.10290000	-0.33840000
C	-4.27400000	-0.63060000	0.20200000
C	-4.33710000	0.93390000	0.16350000
H	-5.06110000	-0.94880000	-0.49230000
H	-2.81130000	-2.06100000	-0.02850000
H	-3.03230000	-1.13770000	-1.35320000
C	-4.65810000	-1.27690000	1.53090000
C	-6.01890000	-1.53360000	1.75900000
C	-3.73720000	-1.64210000	2.52270000
C	-6.45390000	-2.12310000	2.94650000
H	-6.74800000	-1.27450000	0.99350000
C	-4.17040000	-2.24210000	3.70770000
H	-2.68270000	-1.42390000	2.36990000
C	-5.52780000	-2.48330000	3.92690000
H	-7.51360000	-2.31050000	3.09890000
H	-3.43980000	-2.51470000	4.46540000
H	-5.86100000	-2.94830000	4.85110000
C	-4.85430000	1.36930000	-1.21040000
C	-4.11560000	1.22150000	-2.39570000
C	-6.16590000	1.85670000	-1.30070000
C	-4.68150000	1.55230000	-3.62820000
H	-3.07760000	0.89500000	-2.33920000
C	-6.73360000	2.18320000	-2.53440000
H	-6.75390000	1.98290000	-0.39400000
C	-5.99210000	2.02930000	-3.70580000
H	-4.08980000	1.43910000	-4.53360000
H	-7.75230000	2.56020000	-2.57610000
H	-6.42850000	2.28300000	-4.66840000
H	-5.11920000	1.22930000	0.87930000
C	-3.03360000	2.99300000	0.13020000
H	-2.89690000	3.03000000	-0.94640000
H	-3.96770000	3.51560000	0.39490000
H	-2.20140000	3.51060000	0.60360000

C	-3.05950000	1.68550000	2.09690000
H	-3.89240000	2.32270000	2.44410000
H	-3.15190000	0.70320000	2.54640000
H	-2.11430000	2.12230000	2.42170000

RuH₂[(*S*)-xylbinap][(*S*)-daipen]

Coordinates (Angstroms)

X	Y	Z	
Ru	0.50670000	-0.27910000	-0.45920000
P	-1.46560000	-1.37780000	-0.77670000
P	-0.52470000	1.52810000	0.47100000
C	-1.25870000	2.91350000	-0.54060000
C	-1.01960000	2.96680000	-1.91460000
C	-3.95000000	0.25590000	3.46050000
C	-1.95550000	1.13420000	1.62230000
C	-6.56150000	3.26400000	-1.70860000
C	-4.98740000	1.45850000	-2.14010000
C	-2.24320000	5.03560000	-2.06490000
C	-1.31020000	-2.59230000	-2.19980000
C	0.99830000	3.83980000	1.28120000
C	-1.51450000	-3.96940000	-2.05080000
C	0.67290000	2.50320000	1.54040000
C	-0.89640000	-4.35370000	-4.34850000
C	-2.22690000	-2.47390000	0.52500000
C	-0.86050000	-2.11900000	-3.44930000
C	-2.94100000	-0.31580000	-1.24940000
C	-3.15520000	0.61130000	1.12690000
C	-1.78320000	1.24960000	3.03010000
C	-6.34660000	-0.85450000	2.51800000
C	-4.16290000	0.14180000	2.04870000
C	2.28580000	2.51540000	3.38480000
C	-5.39180000	-0.43720000	1.61670000
C	-4.04850000	-3.90170000	1.30100000
C	1.95800000	4.52660000	2.04460000
C	-2.74240000	0.83370000	3.91870000
C	-6.10410000	3.32600000	-0.37070000
C	-6.00710000	2.34940000	-2.57280000
C	-2.00430000	3.94050000	0.06280000
C	-1.51400000	4.02420000	-2.69400000
C	-2.50230000	5.00900000	-0.68650000
C	-3.43290000	-0.34540000	-2.58480000
C	-4.42180000	0.50250000	-3.01660000
C	-4.52490000	1.50490000	-0.78560000
C	-3.28750000	-4.20860000	2.43850000
C	-1.30380000	-4.86260000	-3.11490000
C	-3.50480000	-3.03160000	0.35270000
C	-4.95110000	-0.18680000	4.36710000
C	-3.50300000	0.58680000	-0.33990000
C	2.58060000	3.85750000	3.09780000
C	1.35970000	1.84320000	2.58100000
C	-1.49590000	-2.79440000	1.67030000
C	-6.13000000	-0.72800000	3.91090000
C	-5.11430000	2.47710000	0.07440000
C	-0.67710000	-2.98010000	-4.53540000
C	-2.01920000	-3.66000000	2.64280000

H	-0.44820000	2.15890000	-2.36780000
H	-7.34400000	3.93800000	-2.04750000
H	0.50070000	4.37060000	0.47700000
H	-1.84390000	-4.36740000	-1.09700000
H	-0.64180000	-1.06000000	-3.55750000
H	-0.87570000	1.69370000	3.41780000
H	-7.27670000	-1.28400000	2.15460000
H	-5.57720000	-0.55040000	0.55570000
H	-2.58420000	0.94960000	4.98900000
H	-6.53870000	4.04980000	0.31410000
H	-6.34160000	2.28960000	-3.60610000
H	-2.19360000	3.91210000	1.13360000
H	-3.02760000	-1.06750000	-3.28140000
H	-4.78470000	0.44360000	-4.04060000
H	-4.08240000	-2.79230000	-0.53750000
H	-4.76420000	-0.08500000	5.43390000
H	1.16370000	0.78750000	2.75150000
H	-0.51270000	-2.34480000	1.79560000
H	-6.89170000	-1.05910000	4.61190000
H	-4.77580000	2.54850000	1.10060000
H	0.76280000	-0.95640000	1.08550000
H	0.43990000	0.38000000	-2.04860000
N	2.59980000	0.50890000	-0.29610000
N	1.80220000	-1.90240000	-1.29610000
C	3.15400000	-1.40280000	-1.69510000
C	3.65840000	-0.52300000	-0.50240000
H	2.66990000	1.21990000	-1.02010000
H	2.69940000	0.97630000	0.60220000
H	3.85180000	-2.24470000	-1.78910000
H	1.33640000	-2.33950000	-2.08910000
H	1.87170000	-2.59650000	-0.55680000
C	3.82340000	-1.37800000	0.78600000
C	4.00710000	-0.74150000	2.01890000
C	3.94800000	-2.77750000	0.77840000
C	4.25890000	-1.44770000	3.19500000
H	3.97560000	0.34190000	2.08380000
C	4.19610000	-3.50200000	1.94060000
H	3.86350000	-3.34190000	-0.14440000
C	4.34770000	-2.84400000	3.16480000
H	4.39660000	-0.89910000	4.11910000
H	4.28170000	-4.58390000	1.91470000
C	3.00720000	-0.79310000	-3.12740000
H	2.01160000	-0.33280000	-3.14110000
O	4.59180000	-3.63580000	4.24920000
C	4.74390000	-3.01170000	5.51310000
H	3.84090000	-2.45680000	5.80120000
H	4.91380000	-3.81910000	6.22800000
H	5.60470000	-2.32970000	5.52710000
C	5.05670000	0.09290000	-0.74410000
C	5.32130000	1.45180000	-0.56320000
C	6.14520000	-0.73310000	-1.08320000
C	6.60230000	1.98940000	-0.74020000
H	4.52520000	2.13380000	-0.28010000
C	7.41930000	-0.21850000	-1.27140000
H	5.99980000	-1.80370000	-1.19210000
C	7.66060000	1.15460000	-1.10530000
H	6.75220000	3.05260000	-0.59040000
H	8.25090000	-0.86280000	-1.53940000
O	8.94600000	1.56330000	-1.31270000
C	9.24310000	2.94070000	-1.15530000

H	9.04570000	3.28220000	-0.13030000
H	10.30810000	3.04490000	-1.37080000
H	8.66890000	3.56040000	-1.85710000
C	4.00830000	0.28150000	-3.57890000
H	3.97540000	1.18450000	-2.96460000
H	5.04250000	-0.07760000	-3.58210000
H	3.75600000	0.57840000	-4.60450000
C	3.04020000	-1.94450000	-4.15400000
H	2.33010000	-2.74660000	-3.92350000
H	2.79100000	-1.57250000	-5.15390000
H	4.04270000	-2.39060000	-4.20750000
H	-3.70010000	-4.88770000	3.18360000
C	-1.22910000	-3.96920000	3.89470000
H	-1.59550000	-4.87600000	4.38830000
H	-0.16490000	-4.10710000	3.67280000
H	-1.30200000	-3.14710000	4.61920000
C	-5.43700000	-4.47270000	1.12610000
H	-5.50870000	-5.49020000	1.52700000
H	-6.18000000	-3.86030000	1.65430000
H	-5.72940000	-4.50280000	0.07090000
H	-0.74060000	-5.03680000	-5.18230000
C	-1.53810000	-6.34430000	-2.91960000
H	-1.01650000	-6.71920000	-2.03090000
H	-2.60450000	-6.56400000	-2.77990000
H	-1.19170000	-6.92190000	-3.78280000
C	-0.27220000	-2.44620000	-5.89140000
H	-1.12470000	-2.43980000	-6.58370000
H	0.10050000	-1.41970000	-5.82130000
H	0.50980000	-3.06150000	-6.35160000
H	3.31050000	4.38550000	3.70990000
C	2.28370000	5.97040000	1.73220000
H	2.61300000	6.09150000	0.69280000
H	1.40550000	6.61480000	1.86430000
H	3.07750000	6.35190000	2.38260000
C	2.94290000	1.82700000	4.56050000
H	2.59890000	2.25630000	5.51060000
H	2.70770000	0.75900000	4.57620000
H	4.03460000	1.93850000	4.53850000
H	-2.62620000	5.86440000	-2.65890000
C	-1.27440000	4.04850000	-4.18700000
H	-1.50470000	5.02980000	-4.61590000
H	-0.23320000	3.80700000	-4.43030000
H	-1.90300000	3.30770000	-4.69840000
C	-3.33290000	6.09270000	-0.03850000
H	-3.15930000	7.06880000	-0.50580000
H	-4.40420000	5.87040000	-0.13280000
H	-3.11140000	6.18420000	1.03040000

RuH₂[(S)-xylbinap][(S,S)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	1.23220000	-0.00030000	0.00000000
P	-0.34180000	1.65060000	-0.10480000
P	-0.34230000	-1.65060000	0.10470000
C	-1.12370000	-2.20590000	1.70310000

C	-0.60970000	-1.75410000	2.91940000
C	-3.96650000	-0.83630000	-2.80050000
C	-1.85900000	-1.37270000	-0.96090000
C	-5.94680000	-0.42070000	3.44630000
C	-3.96590000	0.83740000	2.80070000
C	-2.19430000	-3.11520000	4.11730000
C	0.37010000	3.27370000	0.51760000
C	0.36340000	-4.45300000	0.24210000
C	0.36610000	4.45240000	-0.24310000
C	0.36880000	-3.27390000	-0.51800000
C	1.62780000	5.60280000	1.45740000
C	-1.12310000	2.20610000	-1.70310000
C	1.04390000	3.28490000	1.75340000
C	-1.85850000	1.37330000	0.96090000
C	-2.79210000	-0.37620000	-0.65320000
C	-2.00180000	-2.10640000	-2.17170000
C	-5.83990000	1.17830000	-2.25410000
C	-3.85460000	-0.08410000	-1.58640000
C	1.65940000	-4.44470000	-2.24310000
C	-4.82320000	0.93610000	-1.35640000
C	-2.73580000	3.58550000	-2.91140000
C	0.98750000	-5.62240000	-0.21440000
C	-3.01870000	-1.85530000	-3.05800000
C	-5.84000000	-1.17650000	2.25460000
C	-5.02270000	0.56260000	3.71050000
C	-2.19170000	-3.12010000	1.71250000
C	-1.14170000	-2.19840000	4.13990000
C	-2.73660000	-3.58480000	2.91160000
C	-2.00110000	2.10700000	2.17170000
C	-3.01790000	1.85620000	3.05810000
C	-3.85450000	0.08530000	1.58660000
C	-2.19350000	3.11620000	-4.11720000
C	0.99080000	5.62160000	0.21310000
C	-2.19100000	3.12040000	-1.71240000
C	-5.02330000	-0.56120000	-3.71010000
C	-2.79200000	0.37710000	0.65330000
C	1.62560000	-5.60340000	-1.45810000
C	1.04360000	-3.28490000	-1.75320000
C	-0.60910000	1.75460000	-2.91950000
C	-5.94710000	0.42240000	-3.44580000
C	-4.82340000	-0.93470000	1.35670000
C	1.66010000	4.44450000	2.24310000
C	-1.14090000	2.19920000	-4.13990000
H	0.20610000	-1.03450000	2.89870000
H	-6.75420000	-0.62000000	4.14600000
H	-0.12700000	-4.47280000	1.20860000
H	-0.12360000	4.47200000	-1.21000000
H	1.09870000	2.36200000	2.32570000
H	-1.29560000	-2.89540000	-2.39770000
H	-6.56760000	1.95790000	-2.04350000
H	-4.75740000	1.53230000	-0.45460000
H	-3.10920000	-2.44340000	-3.96880000
H	-6.56790000	-1.95590000	2.04410000
H	-5.08530000	1.15130000	4.62300000
H	-2.60100000	-3.48270000	0.77230000
H	-1.29470000	2.89580000	2.39770000
H	-3.10810000	2.44420000	3.96900000
H	-2.60020000	3.48300000	-0.77210000
H	-5.08620000	-1.14990000	-4.62250000
H	1.09950000	-2.36170000	-2.32490000

H	0.20670000	1.03490000	-2.89900000
H	-6.75460000	0.62180000	-4.14540000
H	-4.75780000	-1.53080000	0.45490000
H	1.28990000	-0.18430000	-1.70100000
H	1.28950000	0.18360000	1.70100000
H	2.11480000	-6.50610000	-1.82070000
H	-2.61050000	-3.47150000	5.05870000
H	2.11740000	6.50540000	1.81990000
H	-2.60950000	3.47290000	-5.05850000
C	0.95140000	6.88520000	-0.61720000
H	0.05970000	7.48450000	-0.38770000
H	1.82490000	7.51830000	-0.42660000
H	0.92160000	6.66000000	-1.68860000
C	2.33510000	4.44300000	3.59650000
H	2.99740000	5.30730000	3.71340000
H	1.59560000	4.48410000	4.40740000
H	2.93020000	3.53580000	3.74650000
C	-3.90400000	4.54440000	-2.91490000
H	-3.83450000	5.26280000	-3.73990000
H	-4.85220000	4.00300000	-3.03170000
H	-3.96310000	5.10890000	-1.97810000
C	-0.59120000	1.67500000	-5.44750000
H	-0.95140000	2.26160000	-6.29950000
H	0.50490000	1.69720000	-5.46020000
H	-0.89270000	0.63220000	-5.61200000
C	-3.90490000	-4.54350000	2.91530000
H	-3.83390000	-5.26370000	3.73870000
H	-4.85290000	-4.00240000	3.03510000
H	-3.96590000	-5.10600000	1.97740000
C	-0.59150000	-1.67430000	5.44730000
H	-0.88430000	-0.62840000	5.60720000
H	-0.95900000	-2.25490000	6.30020000
H	0.50450000	-1.70590000	5.46340000
C	0.94650000	-6.88650000	0.61530000
H	0.05330000	-7.48370000	0.38660000
H	1.81840000	-7.52120000	0.42320000
H	0.91850000	-6.66180000	1.68690000
C	2.33540000	-4.44290000	-3.59600000
H	1.59660000	-4.48580000	-4.40740000
H	2.92910000	-3.53490000	-3.74610000
H	2.99920000	-5.30620000	-3.71180000
N	2.99980000	-1.37130000	0.16540000
N	3.00030000	1.37020000	-0.16490000
C	4.33050000	0.76670000	0.15770000
C	4.33020000	-0.76830000	-0.15730000
H	2.99710000	-1.68300000	1.13360000
H	2.85360000	-2.19820000	-0.41300000
H	5.08440000	1.21030000	-0.50340000
H	2.85430000	2.19710000	0.41350000
H	2.99780000	1.68200000	-1.13310000
C	4.78900000	1.06270000	1.57950000
C	6.07410000	1.59060000	1.77330000
C	4.00360000	0.77530000	2.70680000
C	6.57170000	1.82240000	3.05690000
H	6.69450000	1.82130000	0.90960000
C	4.50120000	1.01160000	3.99080000
H	2.99270000	0.39510000	2.56500000
C	5.78550000	1.53050000	4.17230000
H	7.57020000	2.23290000	3.18280000
H	3.87970000	0.78490000	4.85390000

H	6.16870000	1.70840000	5.17380000
C	4.78820000	-1.06420000	-1.57920000
C	4.00290000	-0.77570000	-2.70630000
C	6.07290000	-1.59320000	-1.77340000
C	4.50020000	-1.01170000	-3.99050000
H	2.99240000	-0.39460000	-2.56420000
C	6.57010000	-1.82480000	-3.05710000
H	6.69310000	-1.82490000	-0.90980000
C	5.78410000	-1.53170000	-4.17240000
H	3.87880000	-0.78400000	-4.85340000
H	7.56820000	-2.23620000	-3.18330000
H	6.16700000	-1.70940000	-5.17400000
H	5.08400000	-1.21220000	0.50370000

RuH₂[(*S*)-Xyl-P-Phos][(*S,S*)-dppen]

Coordinates (Angstroms)

X	Y	Z	
Ru	1.33340000	0.25760000	0.35920000
P	-1.00050000	0.40710000	0.82160000
P	1.53520000	-1.91670000	0.25540000
N	1.34220000	2.48290000	0.03440000
H	1.01380000	2.65750000	-0.91490000
H	0.61170000	2.86150000	0.63590000
N	3.52180000	0.49150000	-0.12460000
H	4.02760000	0.76260000	0.71760000
H	3.88970000	-0.42420000	-0.37940000
C	-1.51880000	0.92400000	2.53940000
C	-0.59660000	1.35510000	3.49680000
H	0.46080000	1.35450000	3.24680000
C	-1.01440000	1.75740000	4.77370000
C	-2.37960000	1.72810000	5.07090000
H	-2.71550000	2.04150000	6.05830000
C	-3.32790000	1.30010000	4.13230000
C	-2.88540000	0.89810000	2.86800000
H	-3.61380000	0.56960000	2.13010000
C	-1.64920000	1.82210000	-0.20290000
C	-1.42760000	1.83560000	-1.59280000
H	-1.05730000	0.94350000	-2.08390000
C	-1.71800000	2.96670000	-2.36190000
C	-2.21150000	4.11200000	-1.71640000
H	-2.43270000	4.99960000	-2.30750000
C	-2.43500000	4.13530000	-0.33980000
C	-2.15210000	2.98020000	0.40780000
H	-2.32810000	3.00130000	1.47700000
C	0.62830000	-3.26940000	-0.52470000
C	0.74840000	-4.57610000	0.00480000
H	1.35760000	-4.74940000	0.88700000
C	0.08300000	-5.64830000	-0.58040000
C	-0.69500000	-5.40550000	-1.72540000
H	-1.20570000	-6.24100000	-2.20240000
C	-0.83250000	-4.13050000	-2.27830000
C	-0.18360000	-3.05010000	-1.65360000
H	-0.31460000	-2.05290000	-2.06190000
C	3.17540000	-2.64490000	0.61380000
C	3.80600000	-3.56570000	-0.24580000

H	3.29140000	-3.90210000	-1.14090000
C	5.08680000	-4.05190000	0.03170000
C	5.73450000	-3.60980000	1.19410000
H	6.73130000	-3.98660000	1.41890000
C	5.13640000	-2.69970000	2.07470000
C	3.85920000	-2.21680000	1.76830000
H	3.37250000	-1.50920000	2.43560000
C	-3.05040000	-1.45870000	-0.17790000
C	-2.03330000	-1.14330000	0.73030000
C	-1.69510000	-2.04920000	1.75370000
H	-0.92480000	-1.83650000	2.48540000
C	-2.39390000	-3.24700000	1.83310000
N	-3.38000000	-3.57730000	1.00130000
C	-3.68860000	-2.70900000	0.04210000
O	-2.04460000	-4.11220000	2.82270000
C	-2.78350000	-5.32600000	2.91230000
H	-2.35370000	-5.86550000	3.75930000
H	-2.68730000	-5.92140000	1.99790000
H	-3.84740000	-5.13480000	3.08970000
O	-4.69240000	-3.02770000	-0.80440000
C	-5.33460000	-4.28350000	-0.61880000
H	-6.09300000	-4.33670000	-1.40260000
H	-5.80560000	-4.35010000	0.36810000
H	-4.62540000	-5.11160000	-0.72230000
C	-3.47940000	-0.64690000	-1.35610000
C	-4.53970000	0.26310000	-1.22490000
N	-5.02430000	0.99710000	-2.22540000
C	-4.46040000	0.81740000	-3.42090000
C	-3.41830000	-0.08220000	-3.66640000
H	-3.04560000	-0.15510000	-4.68890000
C	-2.88760000	-0.84820000	-2.61990000
O	-5.10530000	0.42660000	0.01820000
C	-6.18170000	1.35040000	0.11880000
H	-6.49660000	1.32170000	1.16580000
H	-7.01660000	1.06470000	-0.53000000
H	-5.86740000	2.36440000	-0.15210000
O	-4.91530000	1.57600000	-4.47080000
C	-6.01250000	2.44300000	-4.21530000
H	-6.22200000	2.94100000	-5.16590000
H	-5.77010000	3.18610000	-3.44740000
H	-6.89620000	1.88550000	-3.88400000
C	2.61090000	3.19410000	0.32280000
H	2.95780000	2.77460000	1.27250000
C	3.78480000	1.44510000	-1.24270000
H	2.98420000	1.24860000	-1.96050000
C	5.11410000	1.18850000	-1.94060000
C	6.33230000	1.25080000	-1.24640000
H	6.34260000	1.49180000	-0.18510000
C	7.53940000	1.00650000	-1.90010000
H	8.47320000	1.05700000	-1.34640000
C	7.54910000	0.70210000	-3.26400000
H	8.48980000	0.51460000	-3.77420000
C	6.34490000	0.63890000	-3.96570000
H	6.34200000	0.40030000	-5.02570000
C	5.13720000	0.87750000	-3.30580000
H	4.20090000	0.82060000	-3.85640000
C	2.43240000	4.69540000	0.52050000
C	1.65550000	5.46790000	-0.35540000
H	1.13190000	4.99810000	-1.18470000
C	1.52560000	6.84420000	-0.16430000

H	0.91490000	7.42640000	-0.84900000
C	2.17650000	7.47130000	0.90070000
H	2.07440000	8.54290000	1.04820000
C	2.95260000	6.71240000	1.77770000
H	3.45670000	7.18940000	2.61390000
C	3.07470000	5.33470000	1.58860000
H	3.67280000	4.74660000	2.28180000
C	3.67170000	2.90900000	-0.76110000
H	3.47810000	3.53430000	-1.64150000
H	4.63580000	3.24880000	-0.36390000
H	1.72620000	0.79520000	1.91280000
H	0.95860000	0.26630000	-1.26840000
C	-1.63560000	-3.89980000	-3.53310000
H	-0.97460000	-3.79360000	-4.40450000
H	-2.31610000	-4.73480000	-3.73430000
H	-2.20220000	-2.96050000	-3.42880000
C	0.18490000	-7.04160000	-0.00220000
H	-0.77870000	-7.37670000	0.40310000
H	0.48260000	-7.77210000	-0.76460000
H	0.91790000	-7.08530000	0.80990000
C	5.84410000	-2.27460000	3.34180000
H	5.78540000	-3.05700000	4.10960000
H	6.90760000	-2.07920000	3.16230000
H	5.39790000	-1.36890000	3.76540000
C	5.76130000	-5.03930000	-0.89360000
H	6.77130000	-4.70910000	-1.16430000
H	5.86050000	-6.02390000	-0.41890000
H	5.19170000	-5.17340000	-1.81810000
C	-1.54150000	2.95330000	-3.86340000
H	-2.49790000	2.75090000	-4.36030000
H	-1.17000000	3.91790000	-4.23100000
H	-0.84480000	2.17020000	-4.17760000
C	-2.93510000	5.38550000	0.34930000
H	-3.46710000	6.04060000	-0.34880000
H	-3.61660000	5.14380000	1.17230000
H	-2.10540000	5.96560000	0.77620000
C	-4.80080000	1.26040000	4.47390000
H	-5.18120000	0.23130000	4.47060000
H	-4.99410000	1.68430000	5.46480000
H	-5.39620000	1.82330000	3.74480000
C	-0.00090000	2.18320000	5.81250000
H	-0.46600000	2.77610000	6.60740000
H	0.47210000	1.31290000	6.28700000
H	0.80190000	2.78300000	5.36850000

RuH₂[(S)-Xyl-SDP][(R,R)-dpen]

Coordinates (Angstroms)

X	Y	Z
Ru	-0.89910000	0.20680000
P	0.31200000	-1.75100000
P	0.93600000	1.55940000
C	0.86300000	-2.73050000
C	0.50780000	-2.31640000
C	0.86450000	-3.06990000
C	1.57520000	-4.25650000

C	1.94630000	-4.70460000	2.27750000
C	1.58870000	-3.92840000	1.17360000
C	-0.83740000	-3.02010000	-0.96090000
C	-1.46980000	-2.69500000	-2.17530000
C	-2.38650000	-3.56330000	-2.78430000
C	-2.70530000	-4.76270000	-2.13730000
C	-2.12620000	-5.10330000	-0.91130000
C	-1.19530000	-4.22620000	-0.33760000
C	0.56030000	3.39150000	0.30580000
C	1.15520000	4.26040000	1.22770000
C	0.84770000	5.63110000	1.25000000
C	-0.05880000	6.13470000	0.31640000
C	-0.65080000	5.30250000	-0.64420000
C	-0.32930000	3.94340000	-0.63640000
C	1.99880000	1.87580000	-1.44440000
C	3.06500000	2.79230000	-1.40580000
C	3.76020000	3.14460000	-2.56350000
C	3.35830000	2.57380000	-3.78260000
C	2.29250000	1.67630000	-3.85500000
C	1.61640000	1.33590000	-2.67120000
H	-1.08000000	0.33530000	-1.66950000
H	-0.82780000	0.13510000	1.73460000
H	-0.04060000	-1.38220000	2.71050000
H	1.87430000	-4.26230000	0.17870000
H	-1.25410000	-1.73420000	-2.63450000
H	-0.75250000	-4.50010000	0.61240000
H	1.88730000	3.88840000	1.93620000
H	-0.73690000	3.30090000	-1.41400000
H	3.34360000	3.25810000	-0.46340000
H	0.76630000	0.65950000	-2.69500000
C	4.11660000	-1.18200000	-1.95060000
C	3.11980000	-1.20640000	-0.94990000
C	1.87320000	-1.83140000	-1.23790000
C	1.74270000	-2.44790000	-2.49780000
C	2.75230000	-2.43950000	-3.45940000
C	3.94780000	-1.78270000	-3.19340000
C	3.05300000	0.09600000	1.48250000
C	3.63920000	-0.29060000	2.71090000
C	3.25250000	0.25920000	3.92590000
C	2.21820000	1.19470000	3.93740000
C	1.62180000	1.57350000	2.74010000
C	2.04780000	1.08740000	1.48440000
C	3.76920000	-0.66140000	0.34820000
C	4.40170000	-1.87430000	1.11460000
C	4.69770000	-1.35120000	2.52650000
C	5.37310000	-0.47050000	-1.50590000
C	4.94580000	0.20870000	-0.19770000
H	0.82100000	-2.95620000	-2.74490000
H	2.59250000	-2.94050000	-4.41120000
H	4.74320000	-1.74180000	-3.93430000
H	3.72940000	-0.05960000	4.85010000
H	1.86040000	1.61340000	4.87490000
H	0.76840000	2.23910000	2.78380000
H	5.28740000	-2.25560000	0.59610000
H	3.67660000	-2.68630000	1.17310000
H	4.63920000	-2.13700000	3.28840000
H	5.70480000	-0.91470000	2.59670000
H	5.72470000	0.24770000	-2.25620000
H	6.19180000	-1.18680000	-1.34690000
H	5.75520000	0.28440000	0.53570000

H	4.59080000	1.21810000	-0.40470000
H	-3.42620000	-5.43900000	-2.59430000
H	1.85250000	-4.85010000	4.42710000
H	-0.29650000	7.19730000	0.32210000
H	3.88360000	2.85130000	-4.69580000
C	1.48700000	6.53570000	2.27980000
H	1.41780000	7.58850000	1.98660000
H	0.99800000	6.43460000	3.25800000
H	2.54600000	6.29310000	2.42430000
C	-1.61480000	5.86830000	-1.66300000
H	-1.79640000	5.15990000	-2.47800000
H	-2.58570000	6.10740000	-1.20820000
H	-1.23190000	6.79600000	-2.10420000
C	4.91530000	4.12010000	-2.51580000
H	5.87460000	3.61780000	-2.69860000
H	4.81290000	4.90160000	-3.27860000
H	4.98210000	4.61160000	-1.53960000
C	1.85890000	1.08080000	-5.17530000
H	2.43860000	1.48910000	-6.01010000
H	1.98660000	-0.00830000	-5.17430000
H	0.79820000	1.28020000	-5.37310000
C	0.48960000	-2.58380000	5.12010000
H	0.80380000	-3.29080000	5.89520000
H	0.95920000	-1.61560000	5.33300000
H	-0.59430000	-2.44180000	5.21430000
C	2.71600000	-5.99580000	2.10990000
H	3.66760000	-5.97040000	2.65590000
H	2.14980000	-6.85390000	2.49460000
H	2.94170000	-6.19110000	1.05670000
C	-2.47200000	-6.40830000	-0.22900000
H	-1.83940000	-7.22860000	-0.59480000
H	-2.32550000	-6.34490000	0.85440000
H	-3.51280000	-6.69610000	-0.41510000
C	-3.01730000	-3.20380000	-4.11090000
H	-3.53290000	-2.23820000	-4.05860000
H	-2.26080000	-3.12440000	-4.90200000
H	-3.74610000	-3.95910000	-4.42270000
N	-2.43530000	1.82750000	0.27350000
N	-2.86980000	-0.87760000	0.22960000
C	-4.10190000	-0.03700000	0.17360000
H	-2.09620000	2.55880000	0.89540000
H	-2.49580000	2.24600000	-0.65010000
H	-2.93750000	-1.62500000	-0.46010000
H	-2.80370000	-1.31900000	1.14350000
H	-4.85500000	-0.46150000	0.84860000
C	-3.80260000	1.40700000	0.70120000
H	-4.53480000	2.06020000	0.21110000
C	-4.04570000	1.56300000	2.19690000
C	-5.28870000	2.06490000	2.61380000
C	-3.10450000	1.20520000	3.17260000
C	-5.59270000	2.19920000	3.96860000
H	-6.02600000	2.35890000	1.86900000
C	-3.40730000	1.34900000	4.52910000
H	-2.13780000	0.81470000	2.85660000
C	-4.64930000	1.84060000	4.93360000
H	-6.56090000	2.59200000	4.26850000
H	-2.66430000	1.07100000	5.27270000
H	-4.88000000	1.94820000	5.99040000
C	-4.73000000	-0.01020000	-1.21290000
C	-3.99870000	0.31360000	-2.36650000

C	-6.10500000	-0.25760000	-1.33450000
C	-4.63980000	0.39320000	-3.60570000
H	-2.92280000	0.47270000	-2.28860000
C	-6.74390000	-0.17630000	-2.57290000
H	-6.68330000	-0.51620000	-0.44970000
C	-6.01200000	0.15390000	-3.71450000
H	-4.06030000	0.64580000	-4.49050000
H	-7.81020000	-0.37410000	-2.64440000
H	-6.50550000	0.22020000	-4.68060000

RuH₂[(*R*)-Tol-P-Pphos][(*R,R*)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	1.02100000	0.00160000	-0.00290000
P	-0.53590000	1.65660000	0.19630000
P	-0.53610000	-1.65370000	-0.19780000
O	-3.46680000	2.78370000	-3.94230000
O	-4.90120000	-0.72840000	-1.31210000
O	-4.90180000	0.72990000	1.31110000
O	-3.46490000	-2.77980000	3.94310000
N	2.74590000	1.36320000	0.27710000
H	2.82530000	1.96860000	-0.53890000
H	2.58950000	1.97760000	1.07370000
N	2.74480000	-1.36100000	-0.28570000
H	2.82290000	-1.96840000	0.52900000
H	2.58790000	-1.97330000	-1.08380000
N	-4.19230000	1.01630000	-2.63410000
N	-4.19160000	-1.01360000	2.63420000
C	-2.04850000	1.46510000	-0.88090000
C	-2.22930000	2.25950000	-2.01610000
H	-1.56050000	3.06990000	-2.27150000
C	-3.31470000	1.99120000	-2.85230000
C	-4.01790000	0.27010000	-1.54580000
C	-2.97410000	0.43410000	-0.60800000
C	-2.97390000	-0.43150000	0.60770000
C	-2.04760000	-1.46190000	0.88090000
C	-2.22790000	-2.25590000	2.01650000
H	-1.55860000	-3.06580000	2.27220000
C	-3.31340000	-1.98780000	2.85260000
C	-4.01780000	-0.26790000	1.54540000
C	-4.57390000	2.51110000	-4.79740000
H	-4.50850000	3.24890000	-5.59970000
H	-5.52470000	2.61750000	-4.26440000
H	-4.51780000	1.49840000	-5.21000000
C	-5.93460000	-0.92840000	-2.27150000
H	-6.52510000	-1.76320000	-1.88760000
H	-5.51740000	-1.18060000	-3.25160000
H	-6.56200000	-0.03710000	-2.37330000
C	-4.57220000	-2.50780000	4.79790000
H	-4.50670000	-3.24560000	5.60030000
H	-5.52290000	-2.61460000	4.26480000
H	-4.51670000	-1.49510000	5.21070000
C	-5.93640000	0.92890000	2.26950000

H	-6.52790000	1.76240000	1.88460000
H	-5.52050000	1.18250000	3.24980000
H	-6.56240000	0.03670000	2.37140000
C	-1.32910000	2.11000000	1.81880000
C	-2.45290000	2.94690000	1.89550000
H	-2.91840000	3.31780000	0.98670000
C	-2.98810000	3.30920000	3.13280000
H	-3.85860000	3.96140000	3.16860000
C	-2.42430000	2.84680000	4.32930000
C	-1.30650000	2.00510000	4.24630000
H	-0.85500000	1.62400000	5.16080000
C	-0.76710000	1.63940000	3.01350000
H	0.08330000	0.96360000	2.95320000
C	-3.00530000	3.23170000	5.67070000
H	-3.83730000	3.93500000	5.56100000
H	-2.25140000	3.70280000	6.31390000
H	-3.38070000	2.35290000	6.21060000
C	0.17720000	3.30170000	-0.33190000
C	0.15670000	4.45160000	0.46940000
H	-0.35270000	4.43950000	1.42650000
C	0.78460000	5.63070000	0.05540000
H	0.75010000	6.50460000	0.70310000
C	1.44840000	5.71170000	-1.17190000
C	1.47050000	4.56110000	-1.97570000
H	1.97420000	4.59170000	-2.94050000
C	0.86020000	3.37850000	-1.56290000
H	0.91290000	2.48950000	-2.18610000
C	2.13630000	6.98190000	-1.61440000
H	1.90220000	7.22150000	-2.65840000
H	3.22850000	6.89090000	-1.54280000
H	1.83670000	7.83520000	-0.99720000
C	-1.33180000	-2.11100000	-1.81820000
C	-2.45000000	-2.95680000	-1.89100000
H	-2.91010000	-3.32990000	-0.98020000
C	-2.98800000	-3.32160000	-3.12550000
H	-3.85490000	-3.97880000	-3.15780000
C	-1.32540000	-1.99860000	-4.24540000
H	-0.88590000	-1.60690000	-5.16110000
C	-0.78160000	-1.63160000	-3.01400000
H	0.06140000	-0.94630000	-2.95680000
C	-2.43250000	-2.85360000	-4.32460000
C	-2.99740000	-3.27150000	-5.66290000
H	-3.00970000	-2.43560000	-6.37180000
H	-4.02080000	-3.64960000	-5.56750000
H	-2.39540000	-4.06980000	-6.11790000
C	0.17890000	-3.29760000	0.33220000
C	0.86120000	-3.37230000	1.56370000
H	0.91250000	-2.48260000	2.18600000
C	1.47320000	-4.55350000	1.97790000
H	1.97630000	-4.58230000	2.94300000
C	1.45350000	-5.70490000	1.17510000
C	0.79100000	-5.62580000	-0.05300000
H	0.75880000	-6.50010000	-0.70010000
C	0.16140000	-4.44800000	-0.46840000
H	-0.34680000	-4.43750000	-1.42610000
C	2.14170000	-6.97400000	1.62020000
H	1.89020000	-7.22330000	2.65790000
H	3.23440000	-6.87540000	1.56950000
H	1.85890000	-7.82440000	0.99130000
C	4.00330000	0.59820000	0.48860000

H	3.93150000	0.19390000	1.50460000
C	4.00350000	-0.59740000	-0.49460000
H	3.93450000	-0.19310000	-1.51080000
C	5.24480000	1.47150000	0.38920000
C	5.57650000	2.12730000	-0.80630000
H	4.95630000	1.99660000	-1.69080000
C	6.69890000	2.95160000	-0.88050000
H	6.94030000	3.45060000	-1.81530000
C	7.51100000	3.13500000	0.24140000
H	8.38530000	3.77760000	0.18360000
C	7.19160000	2.48840000	1.43580000
H	7.81610000	2.62480000	2.31470000
C	6.06650000	1.66440000	1.50610000
H	5.82340000	1.16360000	2.44050000
C	5.24350000	-1.47250000	-0.39250000
C	6.06710000	-1.66740000	-1.50760000
H	5.82680000	-1.16650000	-2.44270000
C	7.19060000	-2.49340000	-1.43470000
H	7.81660000	-2.63130000	-2.31230000
C	7.50640000	-3.14010000	-0.23950000
H	8.37940000	-3.78430000	-0.17970000
C	6.69240000	-2.95480000	0.88070000
H	6.93100000	-3.45390000	1.81620000
C	5.57170000	-2.12850000	0.80390000
H	4.94980000	-1.99630000	1.68710000
H	1.15050000	-0.30890000	1.68500000
H	1.14700000	0.31220000	-1.69110000

RuH₂[(R)-Xyl-P-Phos][(R,R)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	1.05700000	-0.00090000	-0.00020000
P	-0.49830000	1.66430000	0.11020000
P	-0.49990000	-1.66410000	-0.11050000
O	-3.42220000	2.57770000	-4.08590000
O	-4.87400000	-0.78230000	-1.27430000
O	-4.87270000	0.79190000	1.26610000
O	-3.42900000	-2.56540000	4.08520000
N	2.78120000	1.37240000	0.21000000
H	2.85800000	1.93700000	-0.63520000
H	2.62430000	2.02540000	0.97510000
N	2.77970000	-1.37570000	-0.21210000
H	2.85670000	-1.94180000	0.63210000
H	2.62120000	-2.02740000	-0.97810000
N	-4.15570000	0.88690000	-2.68440000
N	-4.15920000	-0.87640000	2.67960000
C	-2.00740000	1.41530000	-0.95980000
C	-2.18530000	2.14930000	-2.13540000
H	-1.51210000	2.94190000	-2.43130000
C	-3.27290000	1.84340000	-2.95510000
C	-3.98340000	0.19670000	-1.55940000
C	-2.93710000	0.40290000	-0.63270000
C	-2.93860000	-0.39820000	0.62740000
C	-2.01040000	-1.41120000	0.95720000
C	-2.18970000	-2.14250000	2.13470000

H	-1.51690000	-2.93500000	2.43270000
C	-3.27780000	-1.83350000	2.95300000
C	-3.98490000	-0.18850000	1.55340000
C	-4.53250000	2.26620000	-4.92340000
H	-4.46390000	2.95900000	-5.76470000
H	-5.48170000	2.40760000	-4.39570000
H	-4.48370000	1.23230000	-5.28060000
C	-5.92450000	-1.00370000	-2.21060000
H	-6.51820000	-1.81780000	-1.78940000
H	-5.52600000	-1.29280000	-3.18830000
H	-6.54360000	-0.10910000	-2.33330000
C	-4.54250000	-2.25420000	4.91860000
H	-4.47550000	-2.94540000	5.76140000
H	-5.48970000	-2.39800000	4.38800000
H	-4.49670000	-1.21950000	5.27420000
C	-5.91770000	1.02480000	2.20530000
H	-6.50190000	1.84720000	1.78710000
H	-5.51330000	1.30630000	3.18270000
H	-6.54810000	0.13790000	2.32780000
C	-1.30700000	2.21110000	1.69920000
C	-2.41200000	3.08100000	1.70300000
H	-2.84160000	3.41350000	0.76140000
C	-2.97360000	3.52810000	2.90080000
C	-2.41790000	3.07830000	4.10930000
C	-1.32970000	2.20390000	4.13610000
C	-0.77770000	1.77950000	2.91660000
H	0.05900000	1.08330000	2.89720000
C	0.22530000	3.27910000	-0.50380000
C	0.22110000	4.45750000	0.25080000
H	-0.28220000	4.48440000	1.21160000
C	0.85990000	5.62260000	-0.20680000
C	1.49670000	5.59630000	-1.44780000
C	1.52180000	4.43260000	-2.23180000
C	0.89900000	3.28160000	-1.74200000
H	0.93810000	2.35740000	-2.31330000
C	-1.30660000	-2.21230000	-1.70020000
C	-2.41960000	-3.07030000	-1.70300000
H	-2.85680000	-3.39210000	-0.76090000
C	-2.98510000	-3.51440000	-2.90140000
C	-1.32380000	-2.21200000	-4.13680000
C	-0.77080000	-1.78900000	-2.91860000
H	0.06860000	-1.09640000	-2.89940000
C	-2.42420000	-3.07240000	-4.10930000
C	0.21750000	-3.28090000	0.50710000
C	0.89790000	-3.28140000	1.74160000
H	0.94560000	-2.35430000	2.30780000
C	1.52290000	-4.43220000	2.23060000
C	1.49010000	-5.59800000	1.45080000
C	0.84070000	-5.62840000	0.21600000
C	0.20590000	-4.46240000	-0.24350000
H	-0.29840000	-4.48950000	-1.20380000
C	4.03930000	0.62010000	0.45880000
H	3.96910000	0.26920000	1.49450000
C	4.03870000	-0.62470000	-0.46100000
H	3.96910000	-0.27380000	-1.49660000
C	5.27990000	1.48820000	0.31280000
C	5.61290000	2.07580000	-0.91730000
H	4.99470000	1.89390000	-1.79400000
C	6.73380000	2.89680000	-1.03610000
H	6.97620000	3.34240000	-1.99730000

C	7.54300000	3.14550000	0.07530000
H	8.41600000	3.78570000	-0.01710000
C	7.22230000	2.56740000	1.30380000
H	7.84460000	2.75490000	2.17480000
C	6.09880000	1.74600000	1.41860000
H	5.85500000	1.29840000	2.37940000
C	5.27820000	-1.49440000	-0.31480000
C	6.09550000	-1.75500000	-1.42100000
H	5.85130000	-1.30860000	-2.38230000
C	7.21780000	-2.57790000	-1.30630000
H	7.83890000	-2.76770000	-2.17770000
C	7.53900000	-3.15470000	-0.07720000
H	8.41120000	-3.79610000	0.01520000
C	6.73140000	-2.90310000	1.03470000
H	6.97430000	-3.34750000	1.99630000
C	5.61160000	-2.08060000	0.91580000
H	4.99460000	-1.89640000	1.79300000
H	1.18810000	-0.21850000	1.70260000
H	1.18530000	0.21670000	-1.70240000
H	1.98700000	-6.49660000	1.81390000
H	-2.86410000	-3.40340000	-5.04930000
H	1.98860000	6.49660000	-1.81360000
H	-2.85100000	3.41690000	5.04990000
C	-0.76400000	1.69990000	5.44510000
H	-0.98190000	0.63320000	5.58550000
H	0.32660000	1.80930000	5.47910000
H	-1.18450000	2.24060000	6.29980000
C	-4.14180000	4.48920000	2.90360000
H	-4.94510000	4.14600000	3.56700000
H	-3.84150000	5.48550000	3.25500000
H	-4.56250000	4.60630000	1.89970000
C	2.19390000	4.43370000	-3.58700000
H	1.57860000	4.95170000	-4.33470000
H	3.16210000	4.94780000	-3.55690000
H	2.35890000	3.41450000	-3.95130000
C	0.86120000	6.87210000	0.64570000
H	1.51310000	6.75760000	1.52180000
H	1.21550000	7.74140000	0.08210000
H	-0.14290000	7.10020000	1.02230000
C	2.21330000	-4.42740000	3.57660000
H	1.63020000	-4.98150000	4.32400000
H	3.20090000	-4.90180000	3.52520000
H	2.34320000	-3.40810000	3.95450000
C	0.79500000	-6.89530000	-0.60890000
H	1.58120000	-7.59710000	-0.31080000
H	-0.16710000	-7.41180000	-0.49150000
H	0.91670000	-6.68320000	-1.67720000
C	-4.15920000	-4.46860000	-2.89640000
H	-4.80800000	-4.31270000	-3.76580000
H	-3.82570000	-5.51510000	-2.92660000
H	-4.76620000	-4.34720000	-1.99290000
C	-0.73610000	-1.73700000	-5.44700000
H	0.27560000	-2.13500000	-5.60040000
H	-1.34790000	-2.05170000	-6.29910000
H	-0.65650000	-0.64380000	-5.47330000

RuH₂[(S)-tolbinap][(S)-dmapen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-1.36890000	0.50860000	-0.67940000
P	0.65810000	1.59100000	-0.33220000
P	-0.41660000	-1.51670000	-0.25130000
C	0.63110000	-2.41490000	-1.49670000
C	0.64220000	-1.98420000	-2.82740000
C	2.01530000	-1.27890000	3.78480000
C	0.65120000	-1.54620000	1.29380000
C	6.04650000	-2.77750000	-1.10060000
C	4.54620000	-0.89240000	-1.44250000
C	2.10870000	-3.82400000	-3.46300000
C	0.90900000	3.08880000	-1.42790000
C	-1.83440000	-3.99800000	-0.69140000
C	1.17650000	4.37660000	-0.94390000
C	-1.71130000	-2.83340000	0.08160000
C	1.16930000	5.31120000	-3.19670000
C	1.08320000	2.29940000	1.33820000
C	0.75290000	2.94040000	-2.81960000
C	2.23900000	0.61710000	-0.69240000
C	1.89630000	-0.91310000	1.32600000
C	0.12830000	-2.09180000	2.50050000
C	4.47160000	0.06990000	3.90430000
C	2.58430000	-0.74630000	2.58390000
C	-3.72940000	-3.52100000	1.28210000
C	3.83140000	-0.06610000	2.69240000
C	2.62290000	3.40720000	2.86400000
C	-2.87670000	-4.90440000	-0.47540000
C	0.78400000	-1.97150000	3.69940000
C	5.27880000	-3.16770000	0.02210000
C	5.68140000	-1.66150000	-1.81660000
C	1.36330000	-3.56590000	-1.16130000
C	1.37140000	-2.68190000	-3.79360000
C	2.08700000	-4.25790000	-2.12860000
C	3.04600000	0.97390000	-1.81100000
C	4.15790000	0.25540000	-2.17140000
C	3.76930000	-1.27070000	-0.30180000
C	1.65600000	3.42420000	3.88030000
C	1.29480000	5.46620000	-1.81350000
C	2.34600000	2.84940000	1.61820000
C	2.69900000	-1.12550000	5.02090000
C	2.61500000	-0.48780000	0.07670000
C	-3.83750000	-4.69210000	0.51780000
C	-2.69670000	-2.61050000	1.06410000
C	0.11670000	2.31690000	2.34970000
C	1.33280000	6.48040000	-4.13940000
C	3.90500000	-0.46700000	5.08440000
C	4.17630000	-2.43810000	0.40830000
C	0.89550000	4.02320000	-3.68280000
C	0.40140000	2.87250000	3.59940000
C	2.92960000	-4.55650000	-4.49850000
C	-4.94510000	-5.68790000	0.76990000
C	1.97880000	3.98360000	5.24590000
H	0.07830000	-1.09080000	-3.08750000
H	6.91690000	-3.35910000	-1.39300000
H	-1.11740000	-4.21040000	-1.47540000
H	1.28530000	4.54910000	0.12050000

H	0.48390000	1.96540000	-3.21520000
H	-0.80510000	-2.63710000	2.47660000
H	5.42060000	0.59730000	3.95450000
H	-4.47140000	-3.30900000	2.04910000
H	4.27900000	0.35850000	1.80210000
H	3.60860000	3.82670000	3.05630000
H	-2.93920000	-5.79500000	-1.09760000
H	0.36150000	-2.41250000	4.59980000
H	5.56040000	-4.05380000	0.58510000
H	6.25570000	-1.34710000	-2.68520000
H	1.36720000	-3.92530000	-0.13540000
H	1.37100000	-2.32650000	-4.82240000
H	2.65310000	-5.14220000	-1.84320000
H	2.79000000	1.84650000	-2.39530000
H	4.75280000	0.56540000	-3.02790000
H	1.49210000	6.45370000	-1.40090000
H	3.11990000	2.84610000	0.85490000
H	2.24690000	-1.54240000	5.91810000
H	-2.65380000	-1.69790000	1.64990000
H	-0.85010000	1.86170000	2.14800000
H	0.57990000	6.46270000	-4.93590000
H	2.31670000	6.46390000	-4.62720000
H	1.24510000	7.43610000	-3.61210000
H	4.42230000	-0.35700000	6.03400000
H	3.60310000	-2.76280000	1.26770000
H	0.77550000	3.86990000	-4.75380000
H	-0.36490000	2.86840000	4.37240000
H	2.81070000	-5.64320000	-4.41290000
H	3.99920000	-4.33940000	-4.37790000
H	2.64650000	-4.26410000	-5.51510000
H	-4.71680000	-6.32480000	1.63510000
H	-5.09430000	-6.34770000	-0.09110000
H	-5.89590000	-5.18590000	0.98210000
H	2.49270000	3.23550000	5.86460000
H	1.07200000	4.28360000	5.78190000
H	2.63870000	4.85610000	5.17880000
H	-1.83180000	0.51040000	0.96890000
H	-1.09130000	0.52390000	-2.38210000
N	-3.32560000	-0.43230000	-1.21330000
N	-2.82900000	2.41150000	-1.01770000
C	-3.98240000	1.85870000	-1.76980000
C	-2.29770000	3.50910000	-1.85440000
C	-3.24890000	3.01650000	0.26710000
H	-3.09970000	-0.80970000	-2.12980000
H	-3.55660000	-1.22380000	-0.61460000
H	-3.63940000	1.74960000	-2.80290000
H	-4.81980000	2.57700000	-1.77090000
H	-1.49810000	4.02170000	-1.32320000
H	-3.09230000	4.24010000	-2.08460000
H	-1.89500000	3.10090000	-2.77970000
H	-3.67750000	2.26760000	0.92430000
H	-3.98670000	3.82050000	0.09790000
H	-2.36900000	3.43840000	0.75650000
C	-4.49630000	0.47630000	-1.33190000
H	-5.12050000	0.14000000	-2.17330000
C	-5.41630000	0.44310000	-0.11670000
C	-6.78980000	0.64180000	-0.31850000
C	-4.95990000	0.20900000	1.18780000
C	-7.68560000	0.62160000	0.75130000
H	-7.16550000	0.80760000	-1.32650000

C	-5.85660000	0.18010000	2.25860000
H	-3.89390000	0.08570000	1.36120000
C	-7.22080000	0.38710000	2.04670000
H	-8.74580000	0.77810000	0.57020000
H	-5.48260000	0.00200000	3.26380000
H	-7.91570000	0.36450000	2.88200000

RuH₂[(S)-Tol-SDP][(R,R)-dpen]

Coordinates (Angstroms)

X	Y	Z	
Ru	-0.87050000	0.16110000	0.00040000
P	0.45500000	-1.73130000	-0.08630000
P	0.89370000	1.60860000	-0.00150000
C	1.03590000	-2.59430000	1.46100000
C	0.65110000	-2.12640000	2.72050000
C	1.03140000	-2.80560000	3.88180000
C	1.79590000	-3.97540000	3.82370000
C	2.18610000	-4.44210000	2.55790000
C	1.81800000	-3.76260000	1.39870000
C	-0.60880000	-3.09880000	-0.82690000
C	-1.28320000	-2.84770000	-2.04040000
C	-2.16360000	-3.77700000	-2.58930000
C	-2.42910000	-4.99690000	-1.94740000
C	-1.78370000	-5.23750000	-0.73210000
C	-0.89110000	-4.31130000	-0.18110000
C	0.43730000	3.42670000	0.18800000
C	0.99010000	4.35160000	1.08600000
C	0.61010000	5.69670000	1.06630000
C	-0.32550000	6.18060000	0.14700000
C	-0.84930000	5.26880000	-0.78010000
C	-0.47300000	3.92740000	-0.76230000
C	1.95240000	1.91710000	-1.51000000
C	2.95850000	2.89850000	-1.52050000
C	3.64020000	3.21340000	-2.69370000
C	3.32900000	2.57390000	-3.90400000
C	2.31710000	1.60810000	-3.89190000
C	1.63410000	1.28640000	-2.71640000
H	-1.01200000	0.18180000	-1.71850000
H	-0.84550000	0.19590000	1.69850000
H	0.06290000	-1.21330000	2.77360000
H	0.73000000	-2.41290000	4.85080000
H	2.78910000	-5.34510000	2.48130000
H	2.14050000	-4.14510000	0.43330000
H	-1.13350000	-1.89070000	-2.53060000
H	-2.66720000	-3.54060000	-3.52450000
H	-1.97840000	-6.16490000	-0.19710000
H	-0.42450000	-4.54890000	0.76710000
H	1.73770000	4.03840000	1.80570000
H	1.06140000	6.38260000	1.78070000
H	-1.55090000	5.61610000	-1.53630000
H	-0.85580000	3.26150000	-1.53170000
H	3.20370000	3.43600000	-0.60780000
H	2.05610000	1.09580000	-4.81570000
H	0.83510000	0.55100000	-2.72300000
H	4.41690000	3.97580000	-2.67430000

C	4.23230000	-1.03220000	-1.87820000
C	3.23510000	-1.07370000	-0.87890000
C	2.02440000	-1.77330000	-1.14400000
C	1.92760000	-2.43770000	-2.38280000
C	2.93670000	-2.40800000	-3.34400000
C	4.09700000	-1.68320000	-3.09960000
C	3.07260000	0.31330000	1.49480000
C	3.66350000	0.00710000	2.74360000
C	3.22580000	0.57310000	3.93300000
C	2.13680000	1.44300000	3.89860000
C	1.53750000	1.74510000	2.68140000
C	2.01070000	1.24240000	1.44900000
C	3.84460000	-0.44260000	0.39760000
C	4.53950000	-1.58580000	1.21550000
C	4.78530000	-0.99430000	2.61000000
C	5.44490000	-0.23470000	-1.45770000
C	4.97360000	0.47010000	-0.17800000
H	1.03320000	-2.99950000	-2.61400000
H	2.80220000	-2.94310000	-4.28080000
H	4.88930000	-1.62510000	-3.84260000
H	3.70420000	0.31270000	4.87450000
H	1.73820000	1.86800000	4.81650000
H	0.64540000	2.35960000	2.69000000
H	5.45310000	-1.93150000	0.72100000
H	3.86450000	-2.43790000	1.29730000
H	4.76380000	-1.75400000	3.39980000
H	5.76380000	-0.49640000	2.67460000
H	5.75920000	0.47300000	-2.23380000
H	6.30180000	-0.89700000	-1.26800000
H	5.77390000	0.61950000	0.55430000
H	4.56620000	1.45030000	-0.42540000
C	-0.76030000	7.62720000	0.15280000
H	-1.70270000	7.75800000	0.70190000
H	-0.01300000	8.26810000	0.63240000
H	-0.92530000	8.00130000	-0.86400000
C	4.04220000	2.94720000	-5.18290000
H	3.96860000	2.14960000	-5.92980000
H	3.61150000	3.85380000	-5.62980000
H	5.10490000	3.15020000	-5.00720000
C	2.18060000	-4.72750000	5.07680000
H	1.57820000	-5.63820000	5.19570000
H	3.23120000	-5.04010000	5.05260000
H	2.03040000	-4.11590000	5.97240000
C	-3.37710000	-6.00460000	-2.55360000
H	-2.93580000	-6.48510000	-3.43690000
H	-3.63020000	-6.79580000	-1.84040000
H	-4.31060000	-5.53100000	-2.87980000
N	-2.51150000	1.69330000	0.04320000
N	-2.77660000	-1.02220000	0.24180000
C	-4.05710000	-0.27650000	0.06470000
H	-2.24880000	2.50720000	0.59620000
H	-2.55670000	2.00430000	-0.92280000
H	-2.78150000	-1.84690000	-0.35650000
H	-2.70580000	-1.34790000	1.20270000
H	-4.80480000	-0.68290000	0.75660000
C	-3.86660000	1.22660000	0.46000000
H	-4.61840000	1.78420000	-0.11210000
C	-4.17020000	1.50080000	1.92730000
C	-5.46350000	1.92870000	2.26600000
C	-3.23110000	1.32100000	2.95280000

C	-5.81790000	2.16400000	3.59450000
H	-6.20020000	2.08400000	1.47990000
C	-3.58540000	1.56600000	4.28220000
H	-2.22730000	0.98270000	2.69900000
C	-4.87630000	1.98350000	4.60980000
H	-6.82460000	2.49680000	3.83410000
H	-2.84430000	1.42530000	5.06520000
H	-5.14660000	2.17070000	5.64580000
C	-4.63360000	-0.43880000	-1.33540000
C	-3.88220000	-0.19290000	-2.49510000
C	-5.97990000	-0.80740000	-1.47170000
C	-4.47280000	-0.31310000	-3.75510000
H	-2.82700000	0.06400000	-2.40210000
C	-6.57000000	-0.92230000	-2.73160000
H	-6.57370000	-1.00860000	-0.58220000
C	-5.81650000	-0.67290000	-3.87970000
H	-3.87610000	-0.12280000	-4.64400000
H	-7.61480000	-1.21060000	-2.81410000
H	-6.27200000	-0.76170000	-4.86270000

RuH₂[(*S*)-An-SDP][(*R,R*)-dpen]

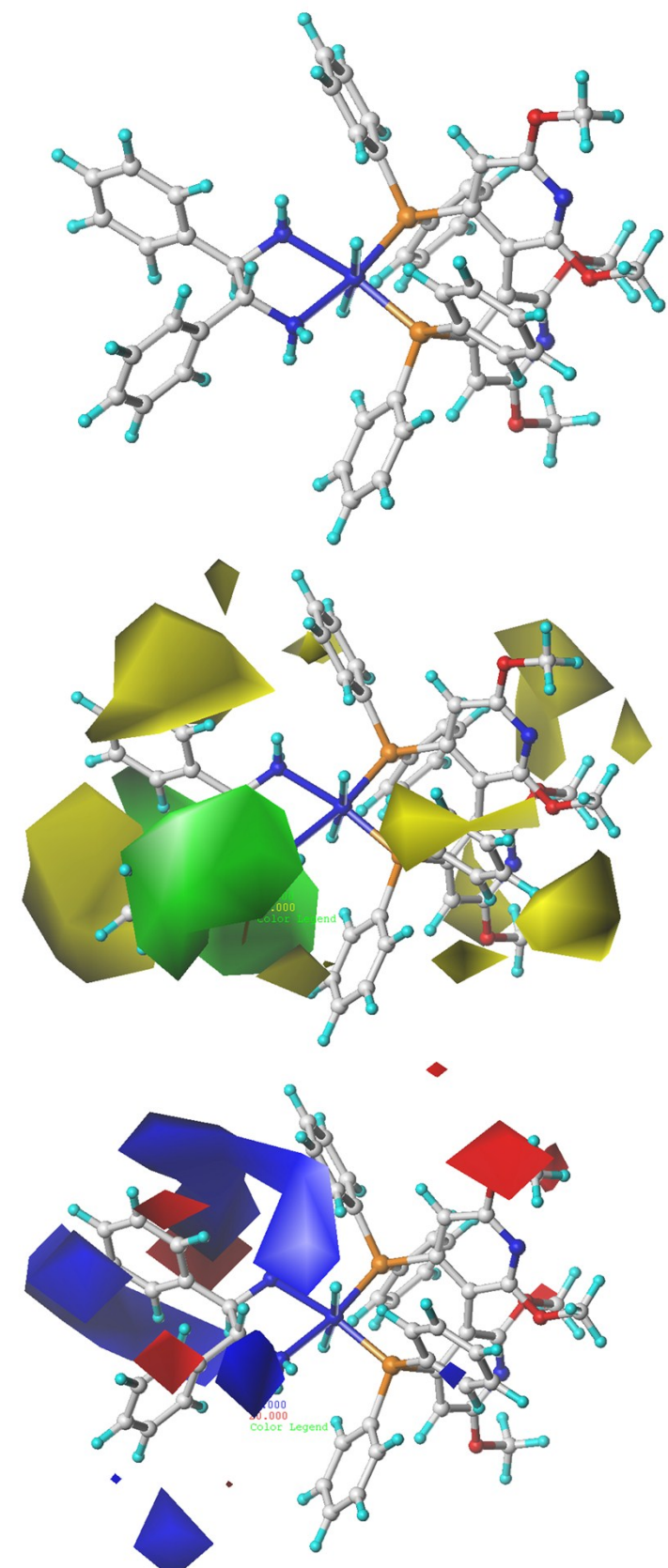
Coordinates (Angstroms)

X	Y	Z	
Ru	-0.40740000	0.86290000	0.01430000
P	-1.16570000	-1.31100000	-0.21340000
P	1.79120000	0.26890000	0.15940000
C	-1.62860000	-2.34180000	1.26550000
C	-1.59580000	-1.78920000	2.55480000
C	-2.00920000	-2.52090000	3.66290000
C	-2.47630000	-3.83360000	3.51030000
C	-2.51540000	-4.40760000	2.23200000
C	-2.08860000	-3.66010000	1.13070000
C	-2.83610000	-1.21930000	-1.07390000
C	-2.95220000	-0.44030000	-2.24800000
C	-4.16990000	-0.26160000	-2.89060000
C	-5.33590000	-0.84920000	-2.37390000
C	-5.25410000	-1.60320000	-1.20050000
C	-4.01610000	-1.77930000	-0.56840000
C	2.97920000	1.68210000	0.51800000
C	3.97820000	1.72790000	1.49760000
C	4.85890000	2.81170000	1.60940000
C	4.76330000	3.88380000	0.71850000
C	3.79540000	3.84310000	-0.29650000
C	2.93240000	2.76010000	-0.39150000
C	2.77270000	-0.34700000	-1.30320000
C	4.15090000	-0.58740000	-1.22180000
C	4.90960000	-0.90950000	-2.34940000
C	4.28530000	-0.97760000	-3.60260000
C	2.91200000	-0.71950000	-3.70390000
C	2.17120000	-0.40590000	-2.56960000
H	-0.35800000	1.03970000	-1.70080000
H	-0.47950000	0.80980000	1.71200000
H	-1.22280000	-0.77410000	2.66870000
H	-1.97340000	-2.09650000	4.66190000
H	-2.86660000	-5.42270000	2.08290000
H	-2.12240000	-4.12140000	0.14660000

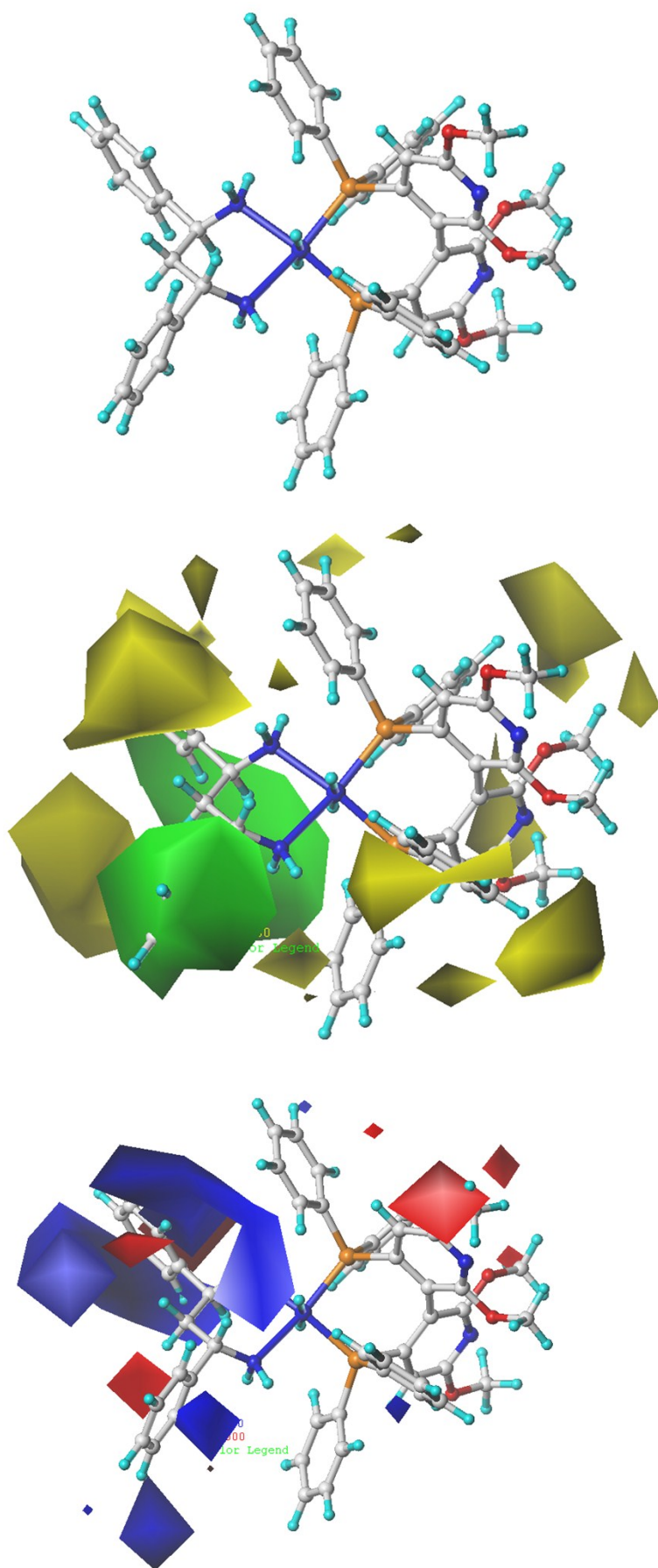
H	-2.06490000	0.05500000	-2.63080000
H	-4.24510000	0.34440000	-3.78840000
H	-6.13650000	-2.05730000	-0.76320000
H	-3.99540000	-2.36470000	0.34280000
H	4.09870000	0.90620000	2.19440000
H	5.61200000	2.79870000	2.38970000
H	3.75070000	4.66410000	-1.00590000
H	2.22680000	2.72390000	-1.21740000
H	4.66040000	-0.50650000	-0.26490000
H	2.44510000	-0.76960000	-4.68290000
H	1.11170000	-0.18430000	-2.65140000
H	5.97420000	-1.08570000	-2.24200000
C	1.73810000	-3.88450000	-1.92420000
C	1.04810000	-3.15100000	-0.93410000
C	-0.20340000	-2.55810000	-1.26320000
C	-0.70030000	-2.79390000	-2.56070000
C	-0.01520000	-3.54440000	-3.51450000
C	1.22650000	-4.08460000	-3.20170000
C	1.89730000	-2.32660000	1.55020000
C	1.90180000	-3.04320000	2.77040000
C	2.00830000	-2.41440000	4.00320000
C	2.07090000	-1.02200000	4.03940000
C	2.05570000	-0.30260000	2.85020000
C	2.02500000	-0.92070000	1.58050000
C	1.81990000	-3.34170000	0.39450000
C	1.24520000	-4.61150000	1.11270000
C	1.76420000	-4.53110000	2.55430000
C	3.05910000	-4.42800000	-1.43060000
C	3.25980000	-3.69830000	-0.09460000
H	-1.65610000	-2.37620000	-2.84620000
H	-0.45260000	-3.69040000	-4.49900000
H	1.79240000	-4.65290000	-3.93640000
H	2.00550000	-2.99860000	4.92050000
H	2.10600000	-0.49390000	4.98920000
H	2.02400000	0.77860000	2.90720000
H	1.53800000	-5.53020000	0.59400000
H	0.15600000	-4.56620000	1.11700000
H	1.08240000	-4.99720000	3.27510000
H	2.73580000	-5.03460000	2.66570000
H	3.87270000	-4.23530000	-2.14000000
H	3.00830000	-5.51830000	-1.29750000
H	3.79400000	-4.29790000	0.64990000
H	3.83220000	-2.78480000	-0.25520000
O	5.55930000	4.99270000	0.73850000
O	4.92680000	-1.27340000	-4.77250000
O	-2.86490000	-4.46710000	4.65610000
O	-6.48280000	-0.61570000	-3.07480000
C	-3.33980000	-5.79880000	4.55980000
H	-2.57340000	-6.47470000	4.15720000
H	-3.58860000	-6.10360000	5.57840000
H	-4.23950000	-5.86450000	3.93300000
C	-7.69100000	-1.17540000	-2.58840000
H	-7.93690000	-0.79810000	-1.58670000
H	-8.46860000	-0.86750000	-3.29010000
H	-7.64520000	-2.27230000	-2.55690000
C	6.32040000	-1.52360000	-4.72860000
H	6.55770000	-2.39140000	-4.09810000
H	6.62100000	-1.73420000	-5.75710000
H	6.87780000	-0.65170000	-4.36050000
C	6.56240000	5.07860000	1.73640000

H	7.29420000	4.26450000	1.64590000
H	7.06550000	6.03400000	1.57540000
H	6.13070000	5.06180000	2.74610000
N	-0.12760000	3.08750000	0.15330000
N	-2.49620000	1.71870000	0.15220000
C	-2.62560000	3.19870000	0.01220000
H	0.64540000	3.32850000	0.77120000
H	0.16490000	3.34130000	-0.78600000
H	-3.13890000	1.26220000	-0.49360000
H	-2.76830000	1.44220000	1.09240000
H	-3.43600000	3.54970000	0.66300000
C	-1.32340000	3.90510000	0.51640000
H	-1.27110000	4.85800000	-0.02450000
C	-1.37490000	4.26680000	1.99500000
C	-1.74240000	5.57570000	2.34370000
C	-1.10550000	3.34830000	3.02020000
C	-1.84820000	5.96130000	3.68030000
H	-1.94450000	6.30280000	1.55950000
C	-1.20340000	3.73890000	4.35810000
H	-0.81660000	2.33100000	2.75840000
C	-1.57770000	5.04080000	4.69470000
H	-2.13250000	6.98100000	3.92720000
H	-0.98700000	3.01600000	5.14100000
H	-1.65420000	5.33800000	5.73750000
C	-3.00130000	3.61520000	-1.40370000
C	-2.27520000	3.19990000	-2.53070000
C	-4.08990000	4.48020000	-1.58600000
C	-2.63750000	3.64380000	-3.80440000
H	-1.44810000	2.50180000	-2.40420000
C	-4.44810000	4.92660000	-2.85920000
H	-4.66550000	4.80700000	-0.72220000
C	-3.72000000	4.50980000	-3.97450000
H	-2.06820000	3.30850000	-4.66800000
H	-5.29740000	5.59450000	-2.97800000
H	-3.99640000	4.85370000	-4.96790000

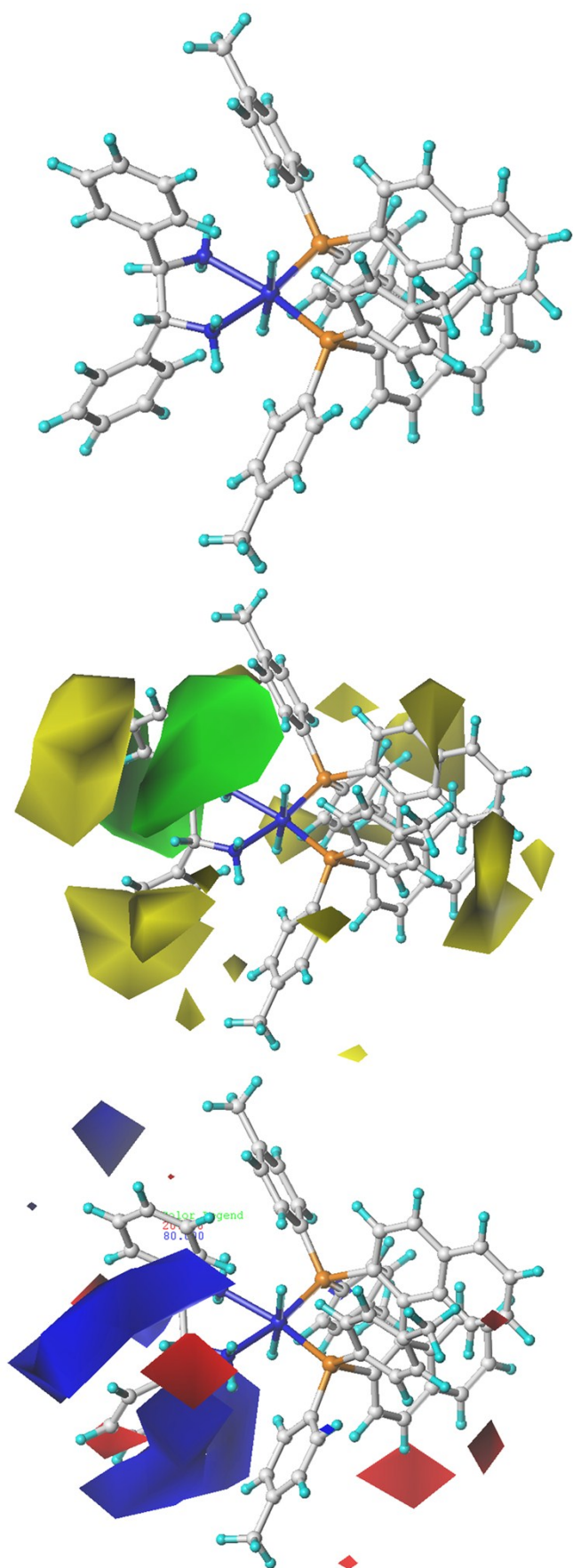
The structure, steric and electrostatic contour maps from CoMFA of catalysts in training set.



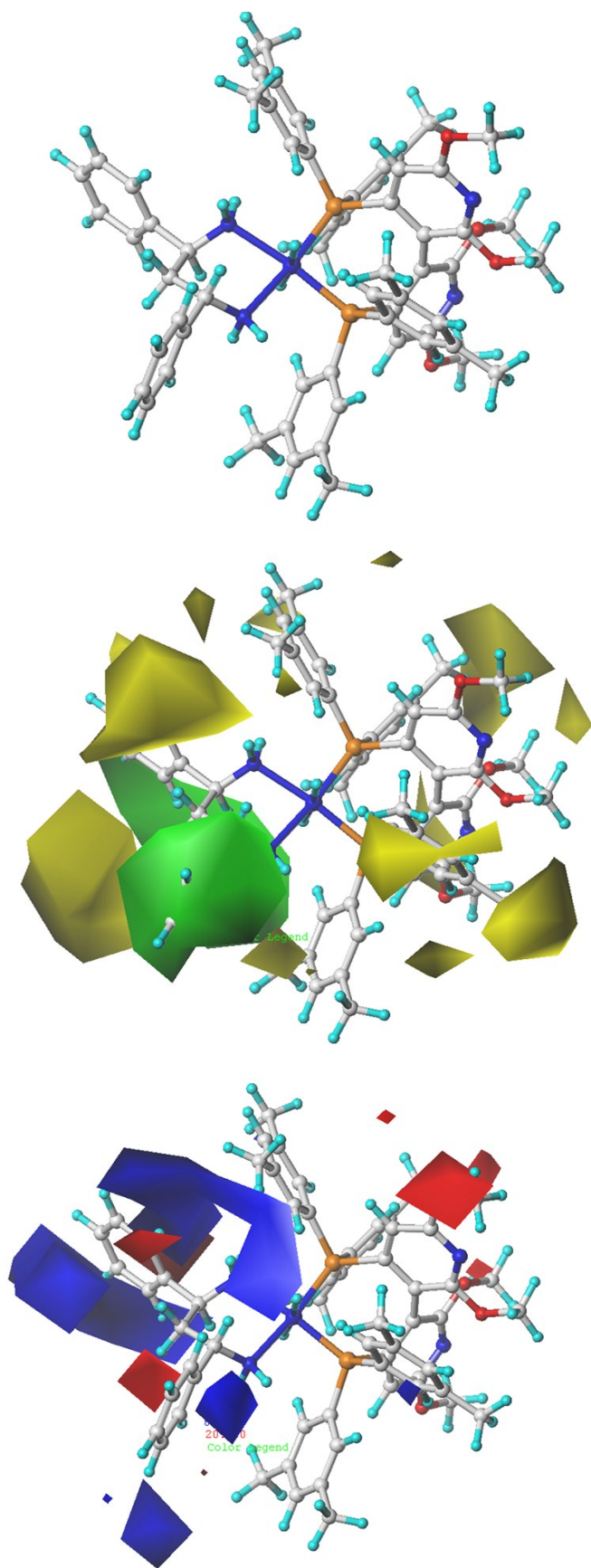




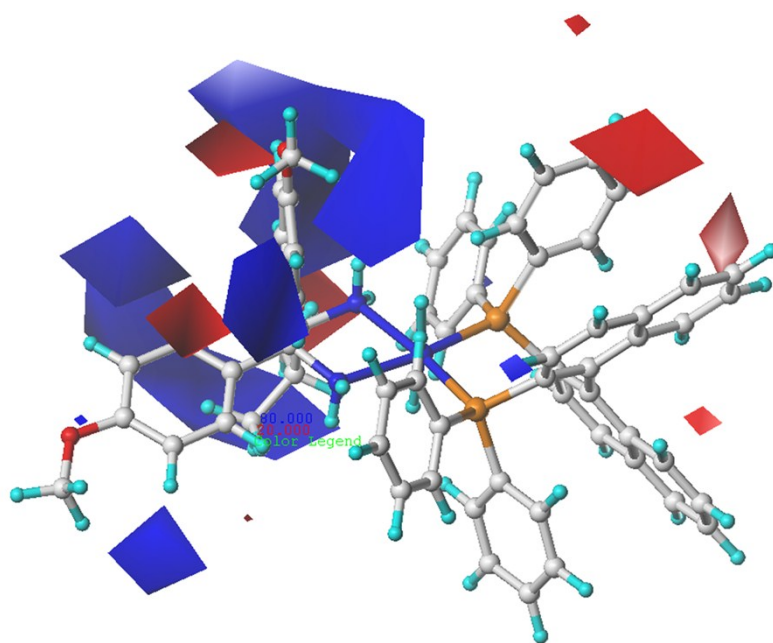
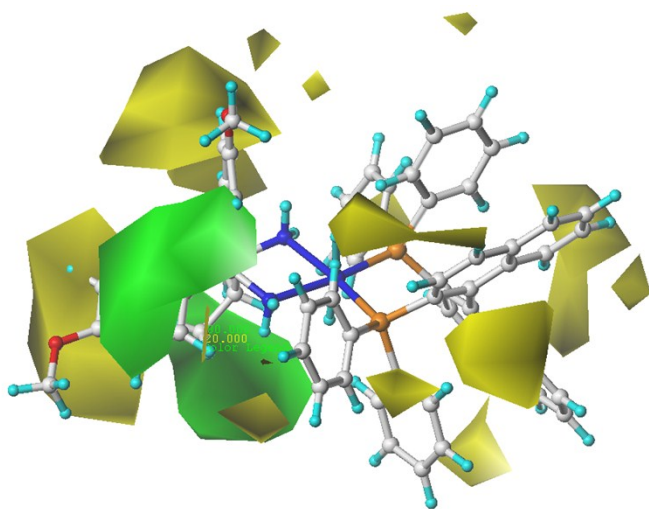
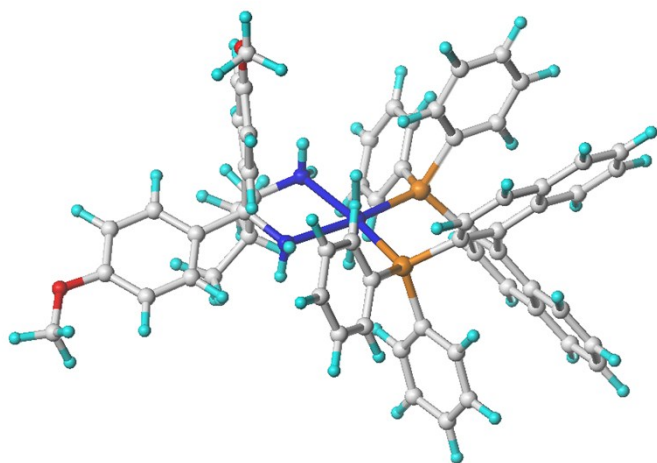
$\text{RuH}_2[(R)\text{-P-Phos}][(S,S)\text{-dppen}]$



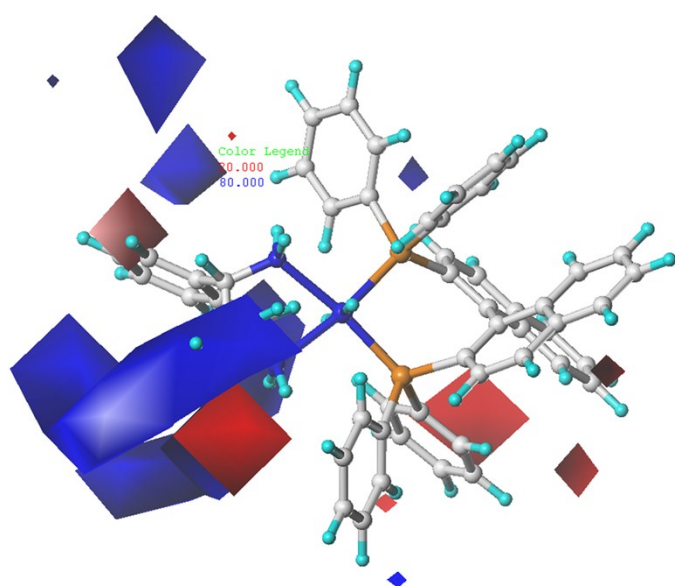
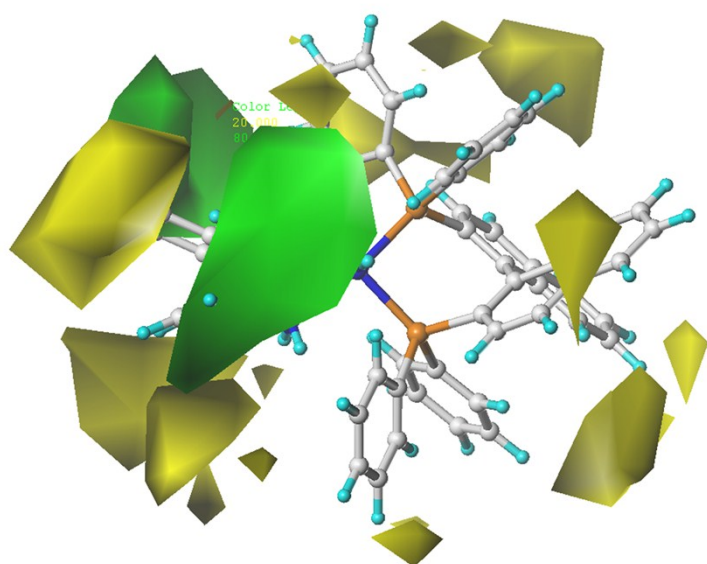
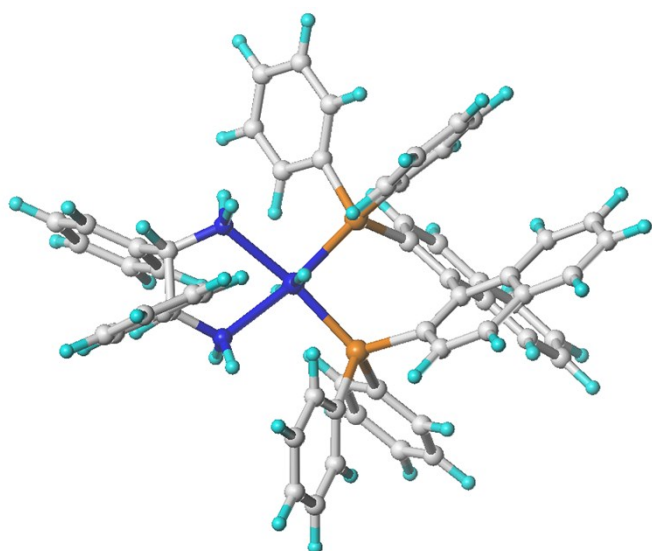
$\text{RuH}_2[(R)\text{-Tol-P-Phos}][(\text{R,R})\text{-dpen}]$



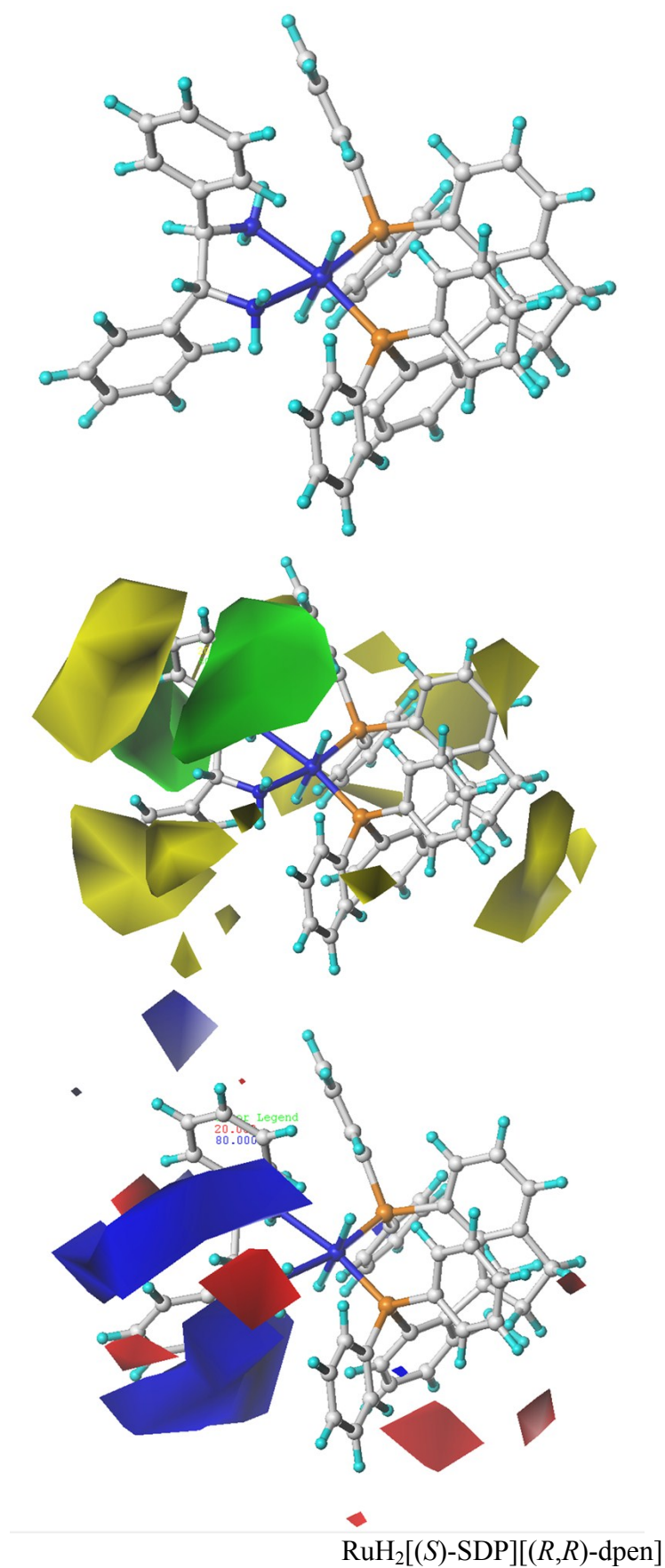
$\text{RuH}_2[(R)\text{-Xyl-P-Phos}][(S,S)\text{-dppen}]$

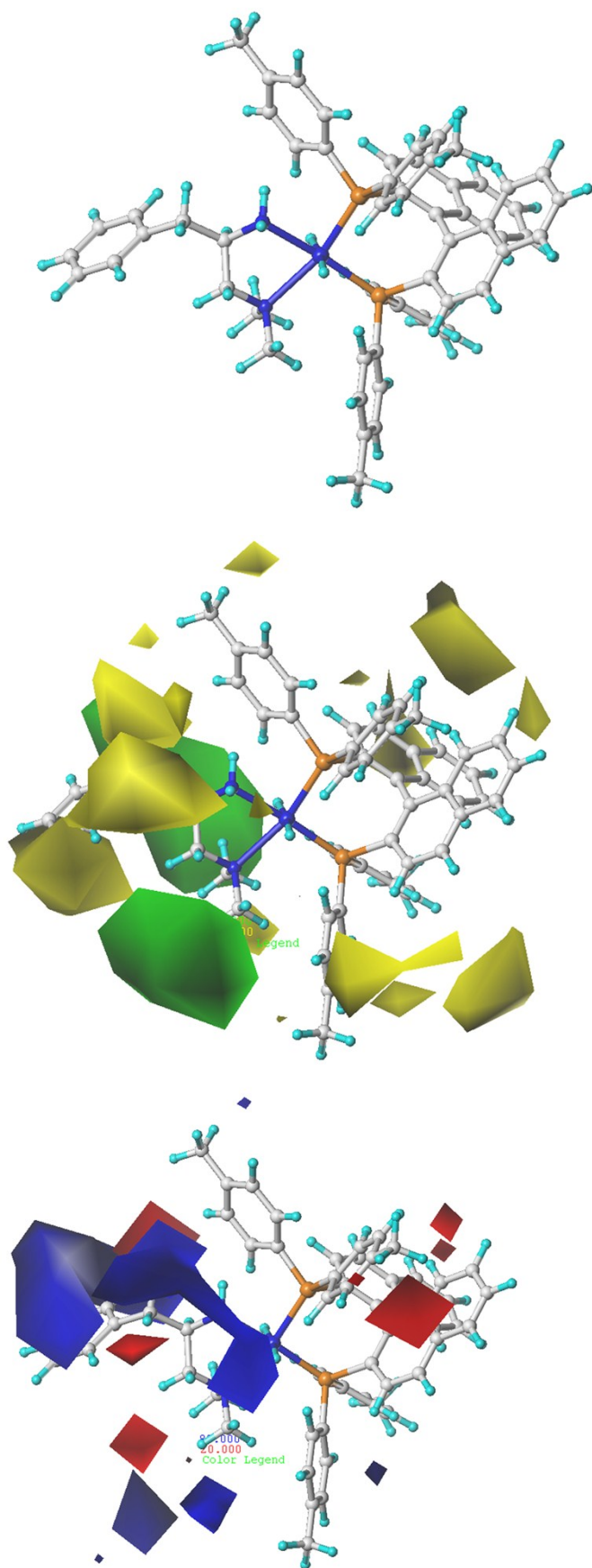


$\text{RuH}_2[(S)\text{-binap}][(S)\text{-daipen}]$

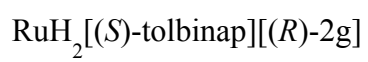
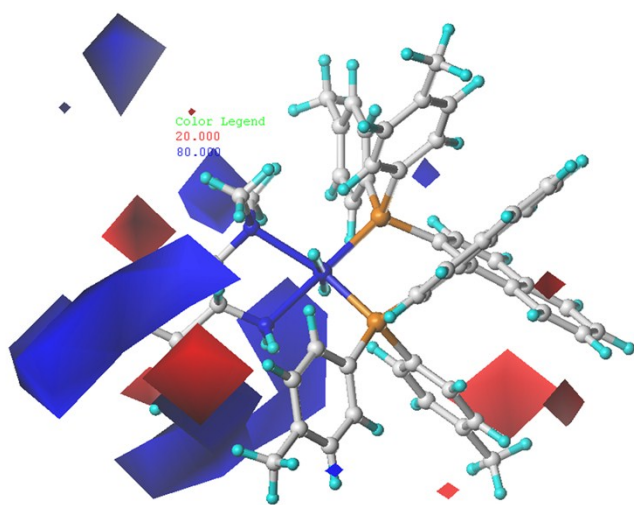
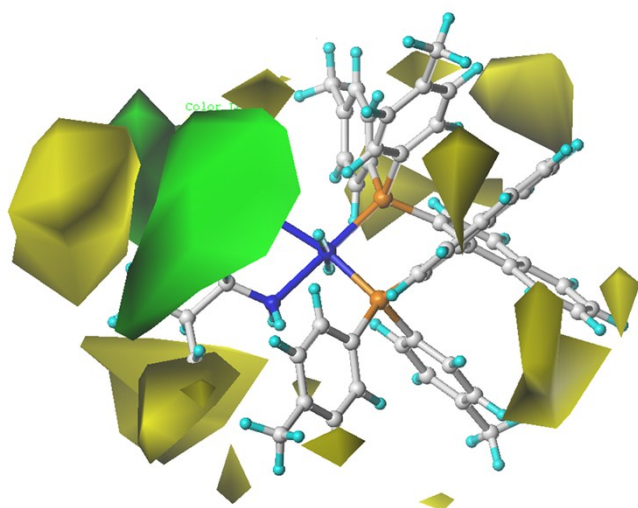
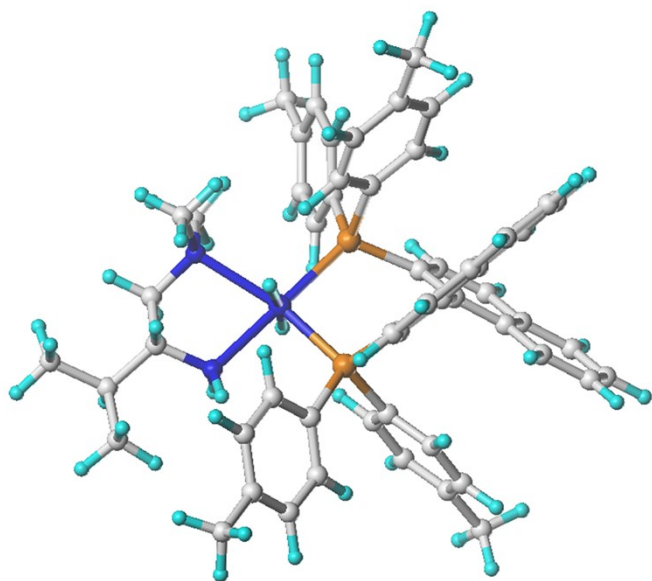


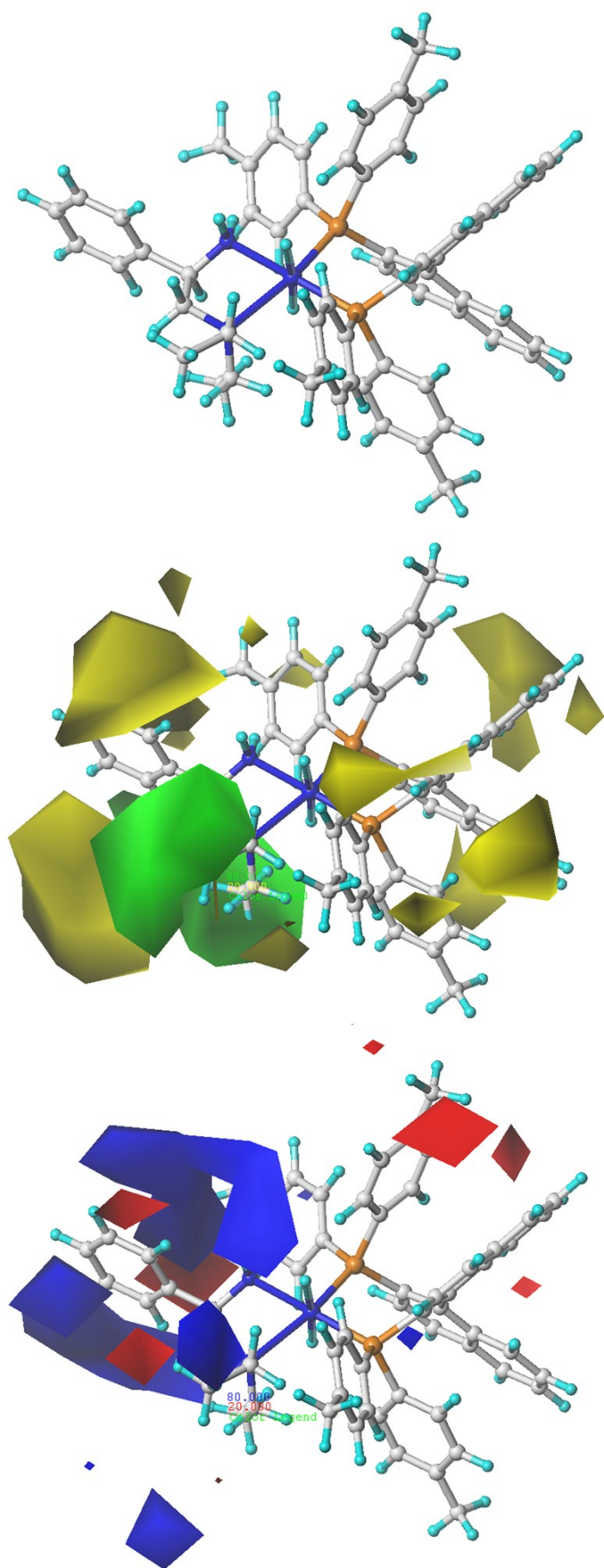
$\text{RuH}_2[(S)\text{-binap}][(\text{S,S})\text{-dpen}]$

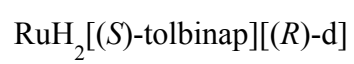
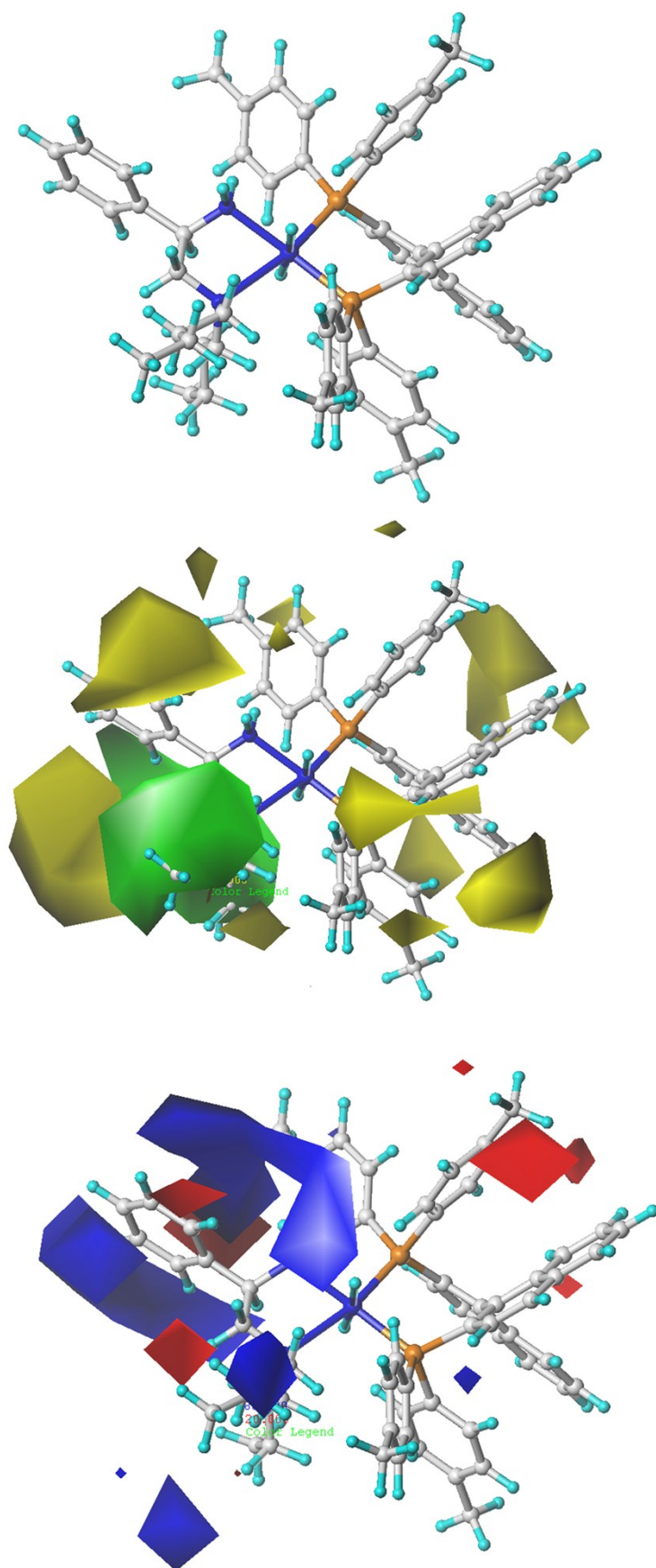


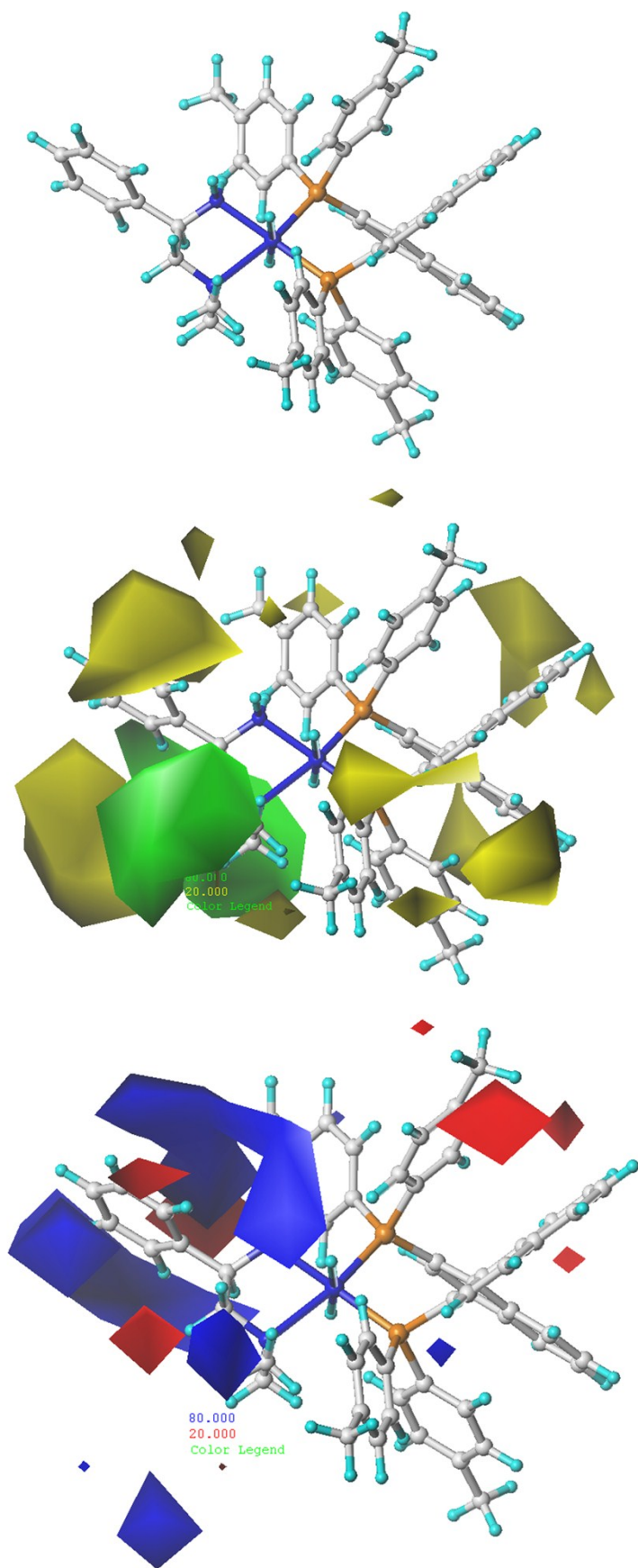


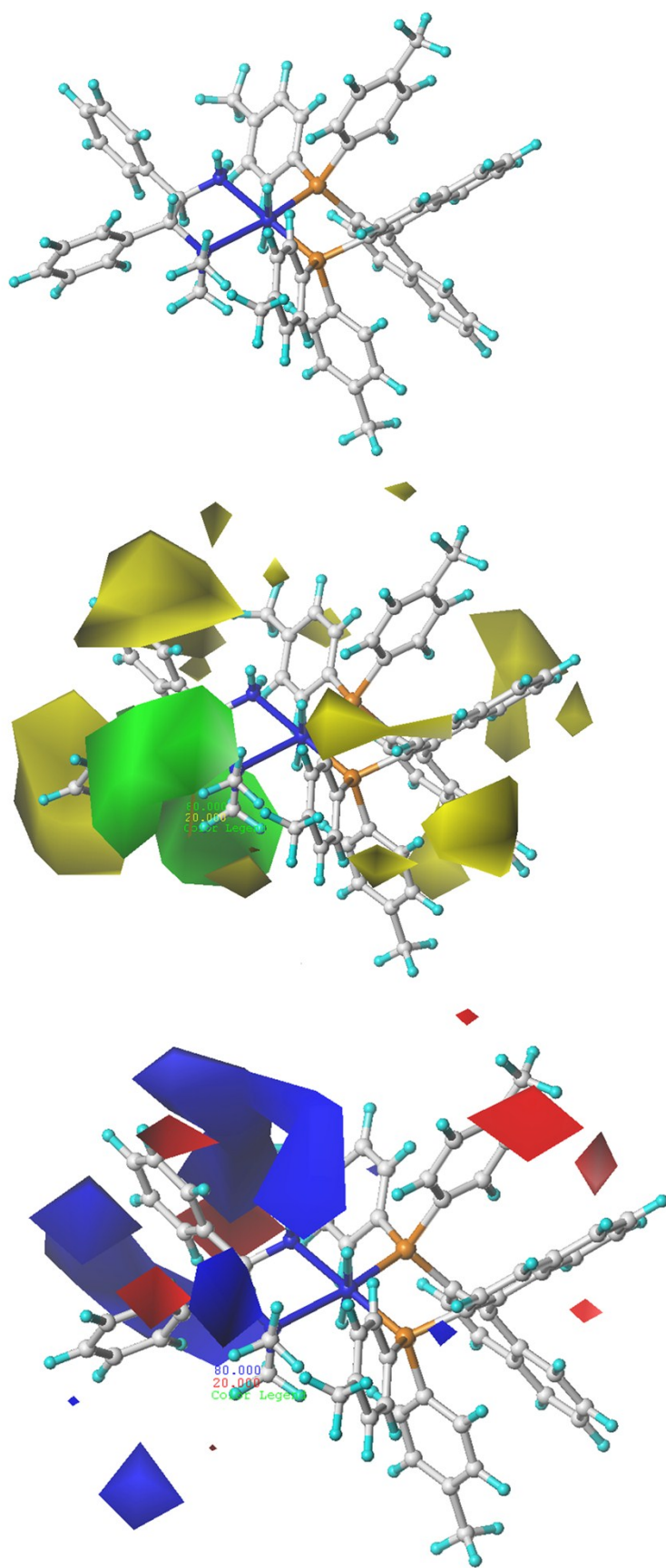
$\text{RuH}_2[(S)\text{-tolbinap}][(R)\text{-1g}]$



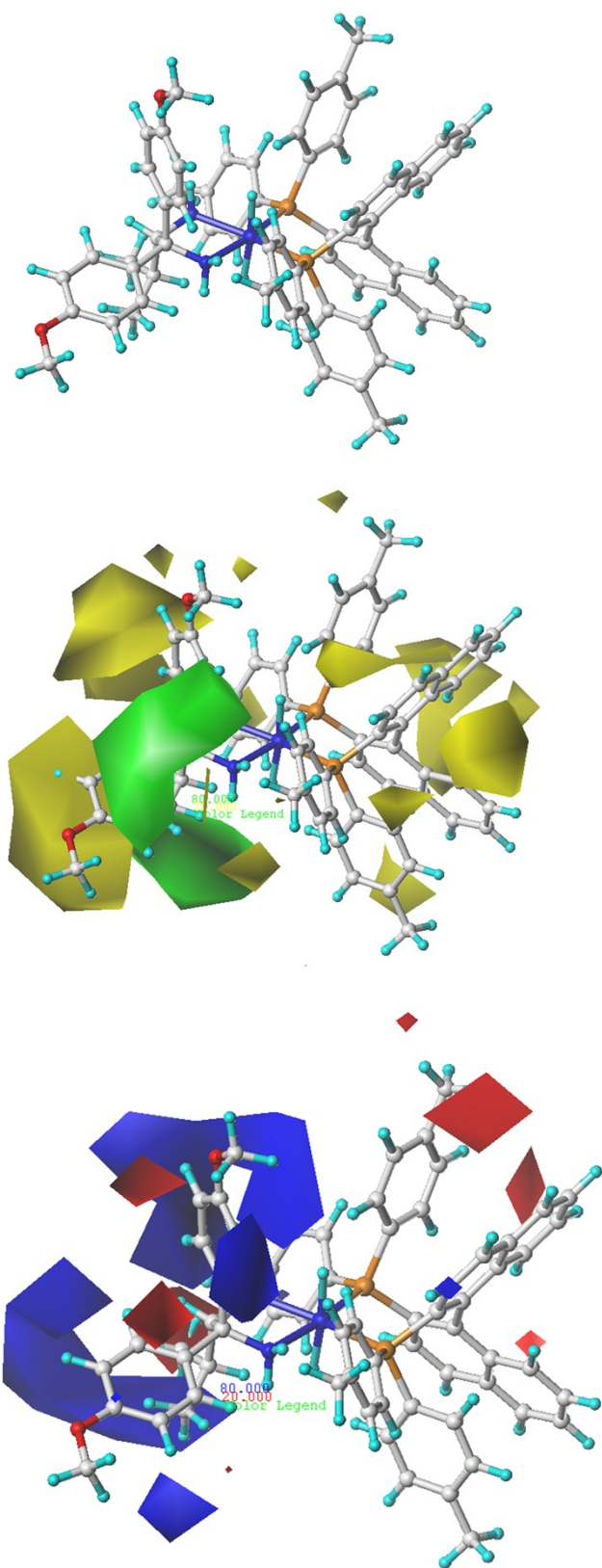




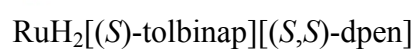
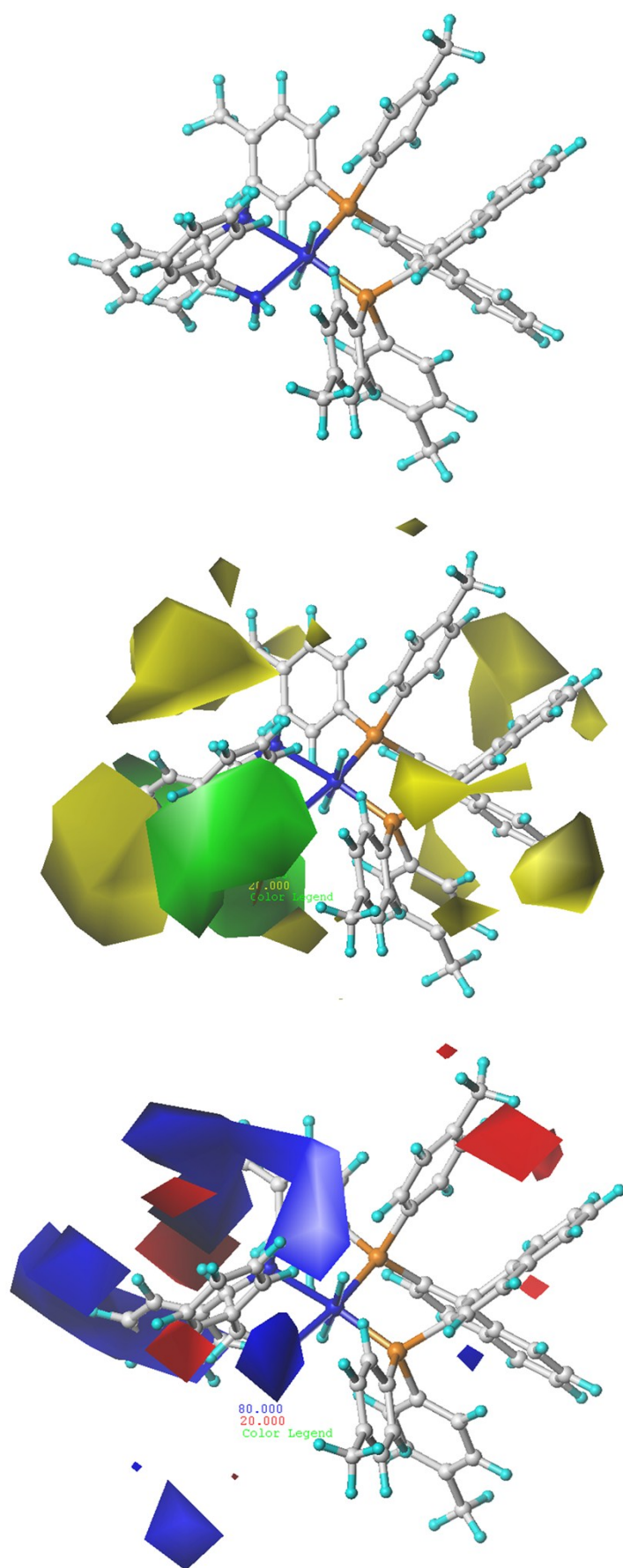


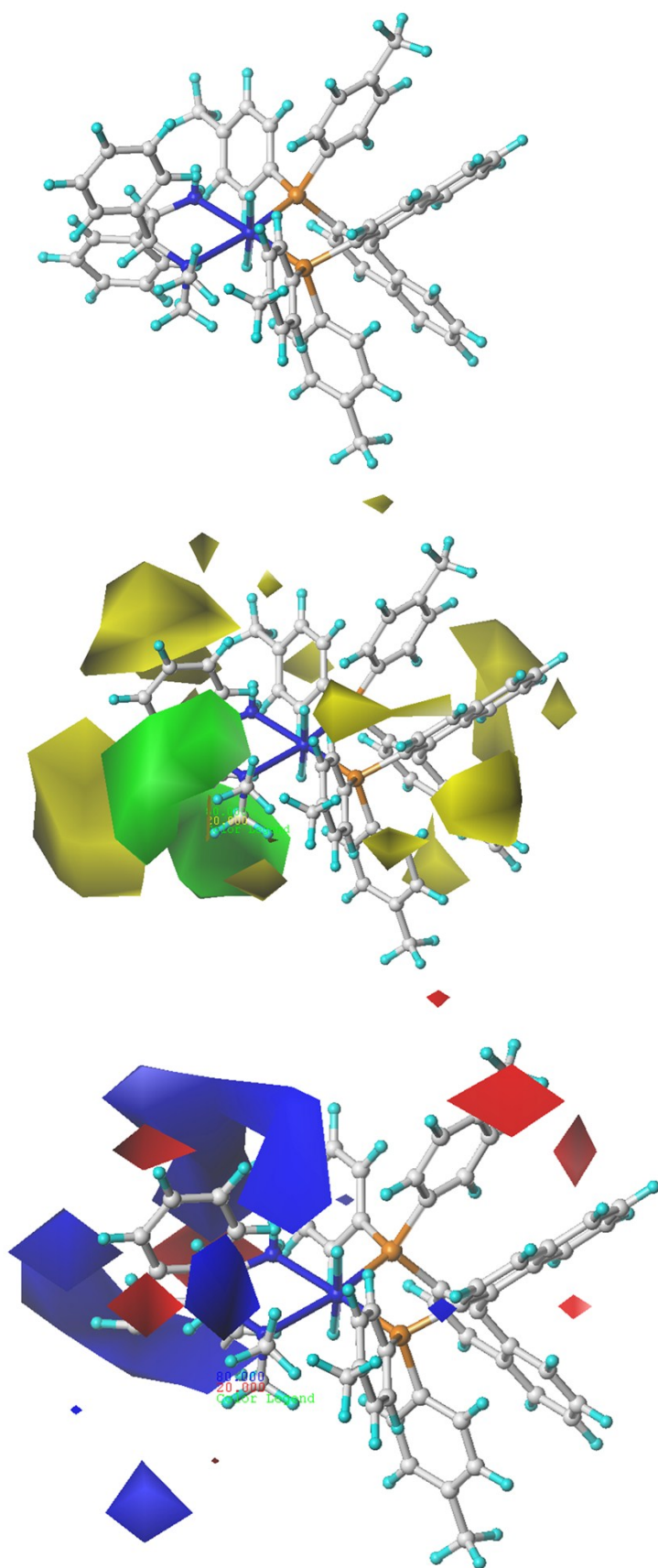


$\text{RuH}_2[(S)\text{-tolbinap}][(R,R)\text{-dmpen}]$

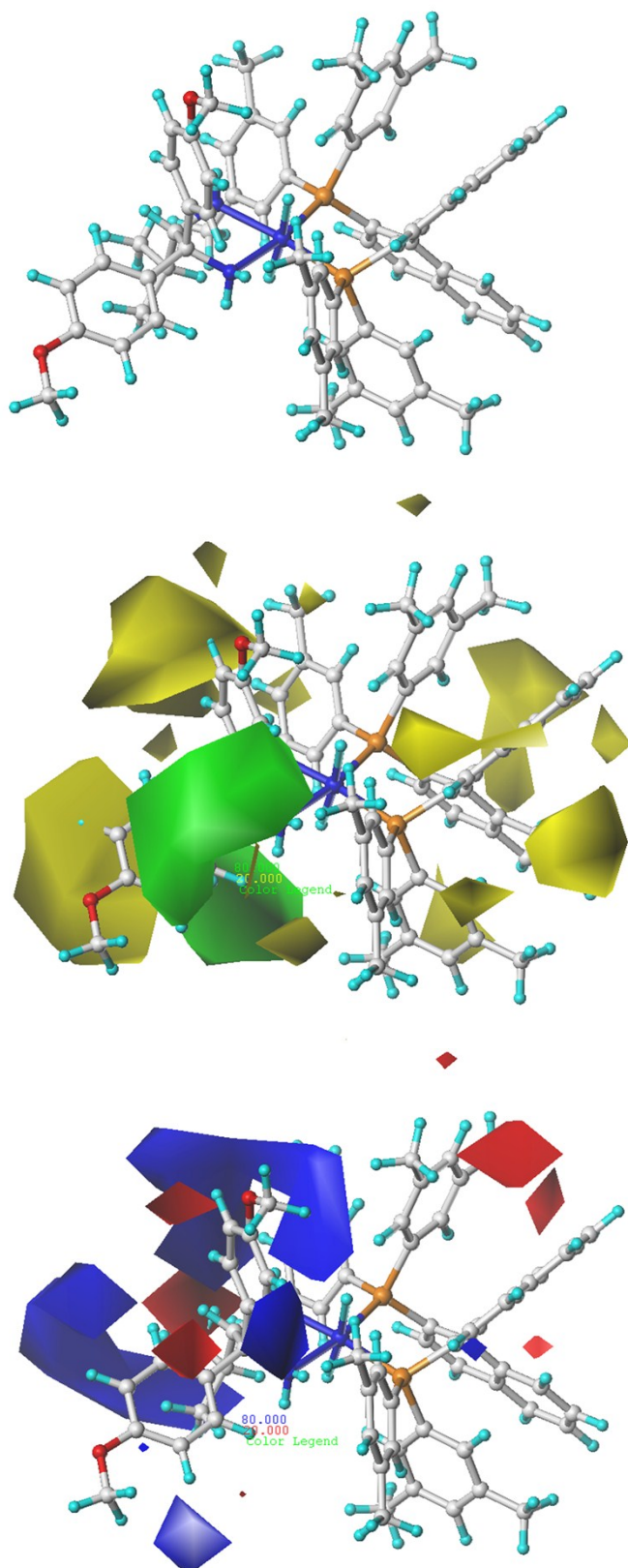


$\text{RuH}_2[(S)\text{-tolbinap}][(S)\text{-daipen}]$

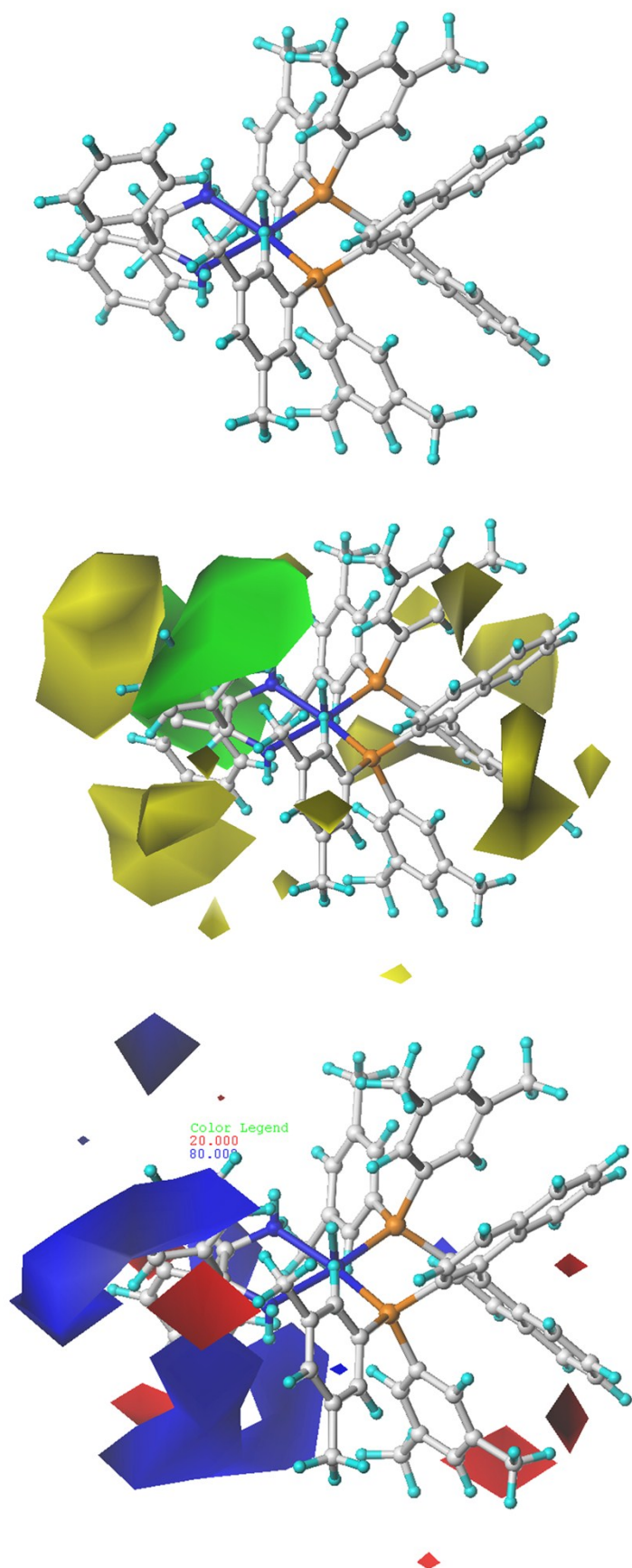




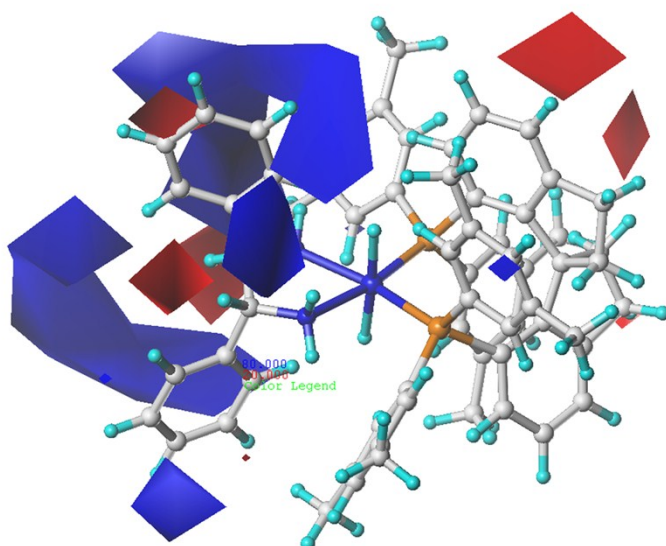
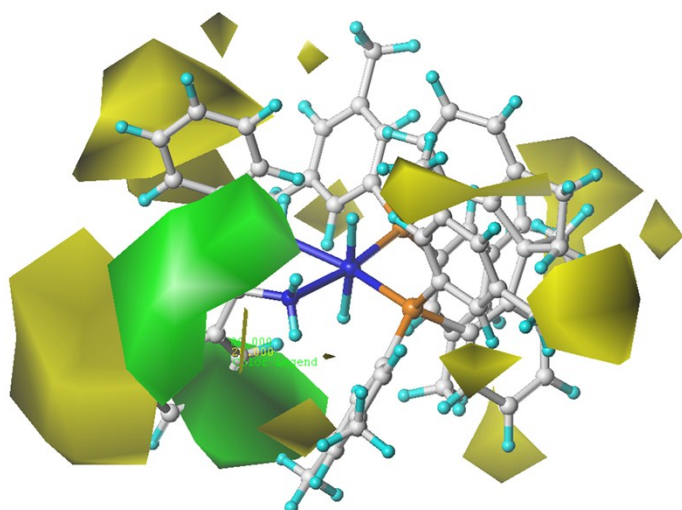
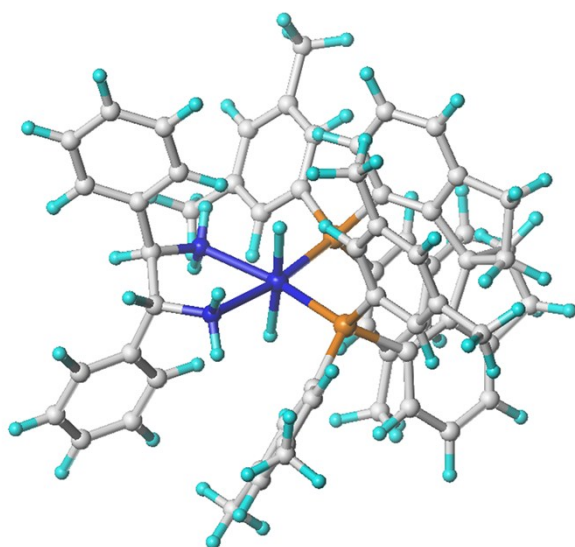
$\text{RuH}_2[(S)\text{-tolbinap}][(S,S)\text{-dmpen}]$

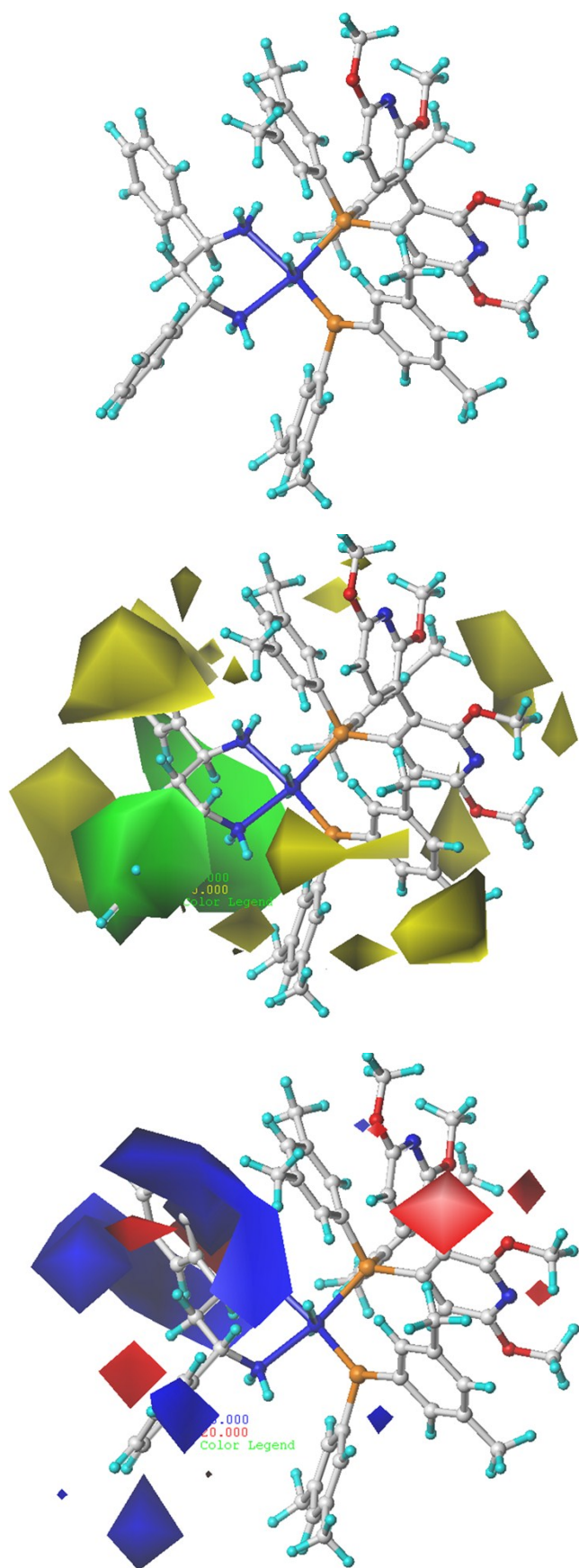


$\text{RuH}_2[(S)\text{-xylbinap}][(S)\text{-daipen}]$



$\text{RuH}_2[(S)\text{-xylbinap}][(S,S)\text{-dpen}]$





$\text{RuH}_2[(S)\text{-Xyl-P-Phos}][(S,S)\text{-dppen}]$