

Trans Influence of Boryl Ligands in CO₂ Hydrogenation on Ruthenium Complexes: Theoretical Prediction of Highly Active Catalysts for CO₂ Reduction

Tian Liu, Zhangyong Liu, Lipeng Tang, Jun Li,* and Zhuhong Yang

State Key Laboratory of Materials-Oriented Chemical Engineering, College of Chemical Engineering, Nanjing Tech University, Nanjing 211816, China

E-mail: lijun@njtech.edu.cn

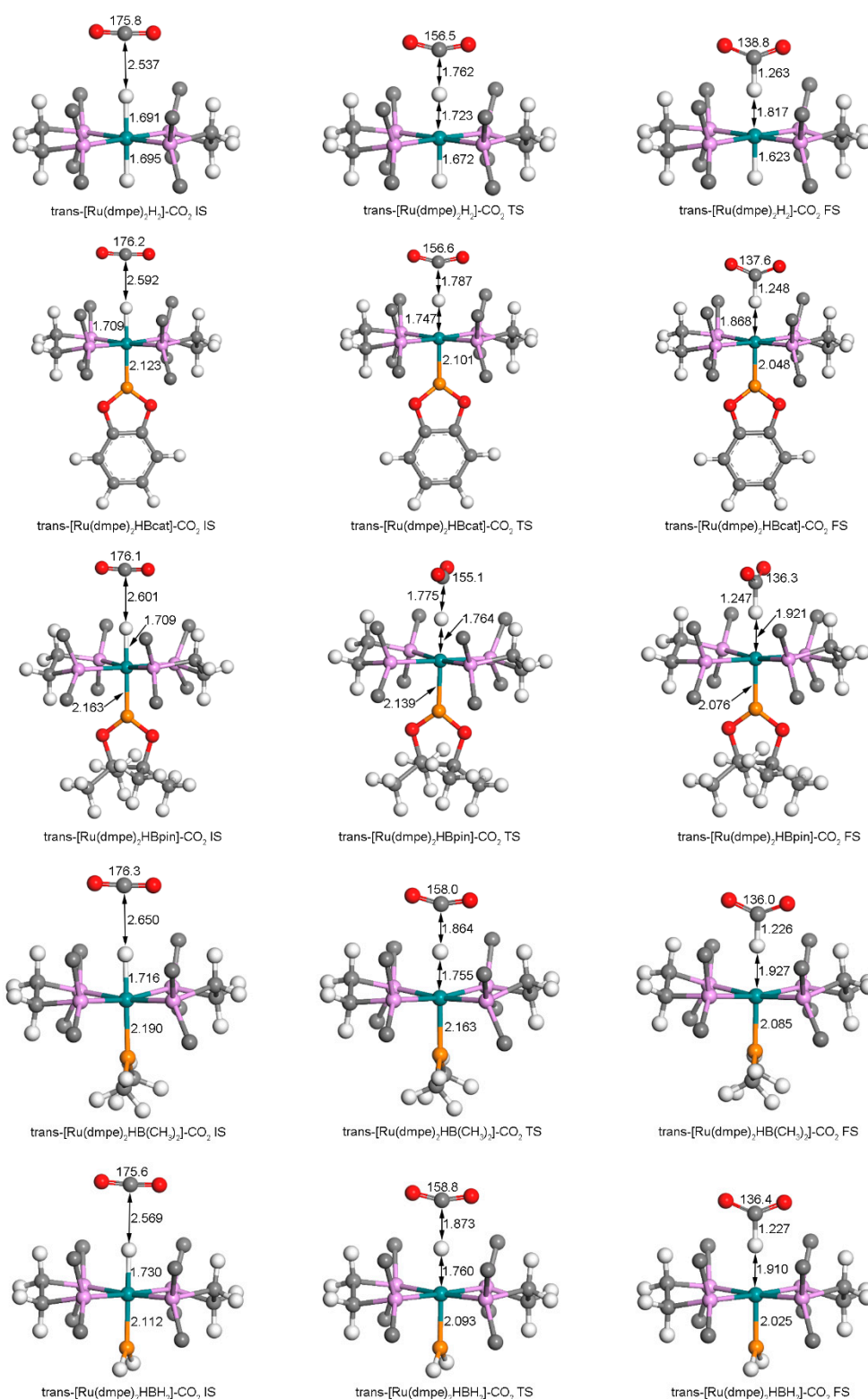


Figure S1. Optimized geometries of the species involved in the addition of hydride to CO₂ on trans-[Ru(dmpe)₂HX] complexes (X may be hydride or B ligand). H atoms on the methyl groups are omitted. Bond distances are given in angstrom (Å) and bond angles are in degree (°). (Green balls: Ru; violet: P; red: O; blue: N; grey: C; orange: B; white: H)

Table S1. Cartesian coordinates for the optimized geometries of all the species

Ru(PNP)(CO)₂H₂

Ru	0.00014500	-0.83570200	-0.00005600
P	-2.27829800	-0.50129000	0.06118800
P	2.27848100	-0.50056300	-0.06103400
N	-0.00019800	1.34840300	-0.00015300
C	-1.14035400	2.03641100	-0.27645300
C	-1.16931800	3.43403100	-0.26612400
C	-0.00076100	4.14476100	-0.00002000
C	1.16807900	3.43447300	0.26600500
C	1.13967100	2.03683700	0.27620100
H	-2.10391800	3.95271000	-0.48480900
H	-0.00098000	5.23677200	0.00002900
H	2.10247500	3.95350300	0.48472800
C	-2.36182200	1.23346000	-0.64653500
C	2.36148500	1.23436900	0.64625400
H	-2.35406900	1.08347000	-1.74104200
H	-3.28634200	1.77394500	-0.38709200
H	3.28576400	1.77511800	0.38649800
H	2.35400800	1.08470900	1.74080800
H	-0.16031200	-0.77294000	-1.68830800
C	-3.46713800	-1.42961100	-1.00831900
C	-3.21709400	-0.36848800	1.65454800
C	3.21755500	-0.36795300	-1.65425000
C	3.46726400	-1.42841700	1.00893500
H	-3.06187400	-1.47050300	-2.02944500
H	-4.24810700	-0.00733400	1.50532200
H	4.24846100	-0.00652700	-1.50494700
H	3.06170600	-1.46926600	2.02994400
C	0.00043900	-2.67720500	-0.00012200
O	0.00066000	-3.84334200	-0.00019900
H	3.24190500	-1.36046000	-2.13019400
H	2.67240300	0.31225500	-2.32512100
H	4.46785200	-0.96657600	1.01458000
H	3.54944000	-2.45893700	0.63020400
H	-3.54896400	-2.46009800	-0.62943000
H	-4.46782800	-0.96799200	-1.01374300
H	-3.24118300	-1.36089000	2.13073300
H	-2.67196800	0.31198500	2.32516300
H	0.16050500	-0.77235700	1.68819600

Ru(PNP)(CO)HBr₂

Ru	-0.06841000	0.12047300	-1.03249000
P	0.68820400	2.30588700	-0.80278800
P	-0.12609800	-2.19897200	-1.15097700
N	1.81721500	-0.32462300	-0.00762300
C	2.75290000	0.64640200	0.15761100
C	3.94595600	0.40097300	0.84272000
C	4.20800800	-0.87655400	1.33135300
C	3.26424600	-1.87857500	1.12194800
C	2.07062500	-1.57461300	0.46190400
H	4.66735300	1.20931200	0.96960600
H	5.13824900	-1.08972900	1.86188100
H	3.43374100	-2.89380900	1.48304400
C	2.50529200	1.98521500	-0.49272900
C	1.00337200	-2.62477700	0.27676400
H	2.96256900	1.95925600	-1.49826200
H	2.99249700	2.79565600	0.07190300
H	1.44917100	-3.62854100	0.19127600
H	0.35771800	-2.62071700	1.17302200
H	0.87895300	0.17595300	-2.45592400
C	0.70602900	3.46004600	-2.24425500
C	0.18085800	3.42395200	0.58080500
C	0.63414300	-3.05618700	-2.60437800
C	-1.62942200	-3.22104800	-0.83334800
H	1.10168100	2.92657500	-3.11986900
H	0.78303100	4.34671600	0.60033800
H	0.70352600	-4.14601500	-2.45437200
H	-2.13650400	-2.85257500	0.06959500
C	-1.57742100	0.47721700	-2.03671500
O	-2.50521100	0.70171300	-2.69798000
H	0.02068100	-2.84559600	-3.49381400
H	1.63376500	-2.63188300	-2.77707900
H	-1.37722600	-4.28745900	-0.72085700
H	-2.31852400	-3.10156000	-1.68352800
H	-0.32919800	3.76435200	-2.46282300
H	1.30820200	4.35971200	-2.03965700
H	-0.88111000	3.68421100	0.45126200
H	0.28453900	2.88460700	1.53345600
B	-1.16227700	0.11410500	0.77303400
Br	-3.14853600	0.14530000	1.00742000
Br	-0.31859600	0.08906700	2.63368800

Ru(PNP)(CO)HBCl₂

Ru	-0.50688900	0.25714300	-0.60035300
P	0.66762600	2.25694600	-0.49850000
P	-1.02624400	-1.99701800	-0.76021900
N	1.46662800	-0.57889900	-0.14686800
C	2.57443600	0.20527100	-0.21254100
C	3.84063400	-0.29233200	0.10706700
C	3.98459800	-1.63223100	0.45895400
C	2.85156300	-2.44125300	0.48535500
C	1.60202300	-1.88795900	0.19255800
H	4.70553700	0.37065000	0.05777400
H	4.96708600	-2.04134400	0.70306500
H	2.92141700	-3.49693600	0.75095400
C	2.41125100	1.61651100	-0.72118200
C	0.34903600	-2.72346300	0.27969100
H	2.56565200	1.59854200	-1.81508100
H	3.17319200	2.28423100	-0.28901500
H	0.56058300	-3.77828900	0.04229400
H	-0.01966500	-2.68165700	1.31997100
H	0.02150700	0.26848300	-2.23016100
C	0.51087700	3.52453000	-1.83292100
C	0.76172200	3.30833300	1.02167100
C	-0.87267400	-2.86485300	-2.38793700
C	-2.54828600	-2.76531900	-0.05084800
H	0.55806200	3.01846600	-2.80749600
H	1.50365500	4.11632300	0.91526500
H	-0.96674600	-3.95851200	-2.28744900
H	-2.70630900	-2.38438400	0.96790100
C	-2.14177200	0.94221200	-1.11643400
O	-3.16273100	1.37154900	-1.46803100
H	-1.65998000	-2.48800400	-3.05874200
H	0.09939200	-2.60560100	-2.83182500
H	-2.48070500	-3.86488200	-0.04004300
H	-3.41122000	-2.46419400	-0.66473500
H	-0.47405400	4.00803000	-1.74184000
H	1.29604900	4.29439500	-1.76237700
H	-0.23097400	3.74742500	1.20642500
H	1.01723500	2.67263500	1.88171300
B	-1.04810700	0.28272800	1.44717700
Cl	-2.69868700	0.60834300	2.16567000
Cl	0.14446400	-0.02593300	2.84465600

Ru(PNP)(CO)HB(OCH)₂

Ru	-0.25485300	-0.42334900	-0.71656700
P	-2.18659300	0.82787100	-0.49990800
P	1.96427600	-1.05616900	-0.82935000
N	0.65812700	1.43176000	0.00902900
C	-0.06183600	2.58461900	0.04216000
C	0.48811700	3.77544600	0.52476700
C	1.81712300	3.79933000	0.94254000
C	2.56055800	2.62367000	0.87280700
C	1.95536500	1.44900000	0.41626200
H	-0.12396700	4.67824600	0.54779800
H	2.26825500	4.72261300	1.31206100
H	3.60503300	2.60066800	1.18695800
C	-1.45552800	2.55241800	-0.53257500
C	2.70686100	0.14316400	0.40162700
H	-1.38153400	2.79944100	-1.60706500
H	-2.09954400	3.31016000	-0.05823700
H	3.78717000	0.30629000	0.26096200
H	2.55069000	-0.33986500	1.38170800
H	-0.17304900	0.28042700	-2.27634400
C	-3.46613300	0.90268300	-1.83132700
C	-3.23293800	0.81759100	1.03057000
C	2.94258600	-0.78651900	-2.37995900
C	2.61078800	-2.68912600	-0.25005100
H	-2.95781800	1.01517500	-2.79934000
H	-4.02054900	1.58818100	1.00024600
H	4.02278800	-0.94766200	-2.22920600
H	2.20355700	-2.89936700	0.74902500
C	-1.00930900	-1.97316900	-1.37072200
O	-1.48176100	-2.95104900	-1.79186300
H	2.57133400	-1.47992400	-3.15043300
H	2.75639800	0.23771700	-2.73435700
H	3.71212200	-2.70887300	-0.21864100
H	2.25608000	-3.47067800	-0.93957400
H	-4.01806700	-0.04989000	-1.83963300
H	-4.17707200	1.72950100	-1.67263700
H	-3.69133300	-0.17743300	1.13394000
H	-2.58638500	0.97901900	1.90599200
B	-0.39984200	-1.17316200	1.29697700
O	-1.35258400	-2.09518500	1.81121100
O	0.41303100	-0.80270500	2.41654900
C	-1.10510700	-2.24960400	3.15871100
C	-0.06421300	-1.48711600	3.52078500
H	-1.73809600	-2.92563500	3.72757500
H	0.42711100	-1.33561100	4.47817600

Ru(PNP)(CO)HBcat

Ru	0.90387000	0.03374300	-0.92762700
P	1.21617200	2.27713600	-0.45410200
P	0.90399600	-2.27268200	-0.78514900
N	1.50228900	-0.17312900	1.16802600
C	2.05633800	0.87711600	1.83020500
C	2.42273600	0.78093700	3.17550700
C	2.25727500	-0.42723700	3.84898700
C	1.72003200	-1.50962000	3.15644200
C	1.33740500	-1.35391600	1.82124200
H	2.85398700	1.64843700	3.67710300
H	2.54783800	-0.52518400	4.89700500
H	1.57705500	-2.47407800	3.64582400
C	2.33334500	2.13241300	1.04154600
C	0.68928000	-2.48507200	1.06382300
H	3.35077600	2.04697900	0.61895300
H	2.31281500	3.02258700	1.69021500
H	1.03893300	-3.46154400	1.43523400
H	-0.40032700	-2.43004000	1.23452100
H	2.58099400	0.06507300	-1.28269500
C	2.16618800	3.39936100	-1.57259000
C	-0.15117700	3.38448600	0.12880600
C	2.43511400	-3.24155000	-1.17319000
C	-0.42043800	-3.35507800	-1.48666200
H	3.07672200	2.87907200	-1.90184300
H	0.22655600	4.35978500	0.47660600
H	2.34810900	-4.30064800	-0.87933400
H	-1.40456200	-2.93883600	-1.22813600
C	0.44954900	0.18861000	-2.70845100
O	0.17230200	0.28238000	-3.83516400
H	2.62411000	-3.17424700	-2.25563900
H	3.28394600	-2.77179300	-0.65536200
H	-0.33949800	-4.39119000	-1.12095800
H	-0.32737800	-3.35275100	-2.58373600
H	1.55038800	3.61281600	-2.45988400
H	2.42541700	4.34924400	-1.07790300
H	-0.85676000	3.54220400	-0.70160400
H	-0.69271200	2.88008500	0.94255600
B	-1.15288300	0.06871900	-0.34777400
O	-2.31649900	0.08215800	-1.17695200
O	-1.62731700	0.10053500	1.01342100
C	-3.41688500	0.12512300	-0.36085100
C	-2.99947700	0.13524300	0.97426400
C	-4.76116300	0.15354100	-0.70487400
C	-3.90690700	0.17367500	2.02363800
C	-5.69013200	0.19235200	0.35027600
H	-5.07498600	0.14604200	-1.75000400
C	-5.27231300	0.20201800	1.68675900
H	-3.57007900	0.18173200	3.06192100
H	-6.75774300	0.21552900	0.12063600
H	-6.01849100	0.23254900	2.48386900

Ru(PNP)(CO)HB(OCH₂)₂

Ru	0.15741000	-0.45683800	-0.76013600
P	-1.97976700	-1.30427200	-0.51029600
P	1.95889300	0.97529400	-0.92039600
N	-0.79557300	1.35935100	-0.00308100
C	-2.15006600	1.44226900	0.07394000
C	-2.78451400	2.57537500	0.59138700
C	-2.02060300	3.66521200	1.00212100
C	-0.63397900	3.58775700	0.89036400
C	-0.04486600	2.41983400	0.39875100
H	-3.87374800	2.60028200	0.64784300
H	-2.49857800	4.56339800	1.39863500
H	0.00120800	4.41993800	1.19760900
C	-2.95168300	0.29794400	-0.49161400
C	1.45546100	2.27600900	0.33341700
H	-3.13980800	0.51609300	-1.55851300
H	-3.92864200	0.21122700	0.00989800
H	1.93886900	3.25334900	0.17291400
H	1.81046200	1.88562200	1.30424200
H	-0.41951000	0.00173000	-2.30866400
C	-2.81080800	-2.26241000	-1.85601800
C	-2.56497000	-2.19662900	1.00460400
C	2.26756700	1.95356600	-2.46490200
C	3.67503600	0.53394900	-0.39678800
H	-2.63682600	-1.74836000	-2.81183700
H	-3.66294900	-2.28818000	1.03265100
H	3.04380100	2.72398300	-2.32437900
H	3.61705600	-0.03176800	0.54354500
C	0.97823600	-1.97728500	-1.40348800
O	1.49856600	-2.93645700	-1.81280700
H	2.57992600	1.25814700	-3.25914200
H	1.32284100	2.41984500	-2.78067100
H	4.31281100	1.42533000	-0.28305400
H	4.11180100	-0.12391500	-1.16424200
H	-2.34823800	-3.25995400	-1.91237500
H	-3.89156900	-2.37777100	-1.67355400
H	-2.11843800	-3.20367800	1.00977400
H	-2.19387200	-1.65385800	1.88534700
B	0.75889700	-0.94281600	1.25766200
O	1.94463400	-1.56915600	1.67665700
O	-0.01658600	-0.63920900	2.40053700
C	1.99641200	-1.63922300	3.10893700
C	0.59888300	-1.19201200	3.57476500
H	2.24463500	-2.66706100	3.41932900
H	2.79496800	-0.96939900	3.47741800
H	0.63217900	-0.42925500	4.36999400
H	-0.01035200	-2.03914200	3.93892000

Ru(PNP)(CO)HB(OH)₂

Ru	0.13415900	-0.70660000	-0.33909100
P	-2.16850400	-0.90402800	-0.27001100
P	2.27222500	0.14279800	-0.48207000
N	-0.34176000	1.41718400	-0.13659400
C	-1.61853100	1.85314200	-0.30294200
C	-1.95761400	3.19967600	-0.14309000
C	-0.96407700	4.12989100	0.15335900
C	0.34823300	3.68290000	0.29004000
C	0.63146700	2.32101500	0.15473700
H	-2.99545000	3.50999700	-0.27329200
H	-1.20804800	5.18780900	0.27068900
H	1.15728100	4.37831400	0.51851000
C	-2.64864100	0.84417500	-0.74217800
C	2.02884900	1.79523900	0.36970500
H	-2.65994900	0.83583600	-1.84709600
H	-3.65577300	1.12898300	-0.39853700
H	2.78266500	2.54934400	0.09101600
H	2.15436500	1.57999700	1.44598600
H	-0.11904500	-0.49514300	-2.02204700
C	-3.10215700	-1.92578600	-1.49632300
C	-3.12193800	-1.21875300	1.28891800
C	3.00418700	0.59790900	-2.12401700
C	3.73002900	-0.57117600	0.40214800
H	-2.70096400	-1.72329200	-2.49938800
H	-4.19779900	-1.01087100	1.16833600
H	3.94852300	1.15870600	-2.02511800
H	3.41635300	-0.86311900	1.41402200
C	0.54809600	-2.49150400	-0.53617400
O	0.80985100	-3.61938200	-0.66916500
H	3.18481400	-0.32888700	-2.69020300
H	2.26586900	1.19201300	-2.68227000
H	4.57572400	0.13432100	0.43948500
H	4.04579100	-1.48138300	-0.13121100
H	-2.93241500	-2.98905000	-1.26608700
H	-4.18451300	-1.72017200	-1.46779800
H	-2.98766300	-2.27476500	1.57249700
H	-2.68980900	-0.59378500	2.08326000
B	0.37049100	-0.84661500	1.81526800
O	1.21371600	-1.76910900	2.44248200
H	1.17963100	-1.71271100	3.41485700
O	-0.32577700	0.03723800	2.66109000
H	-0.14825800	-0.13086200	3.60506000

Ru(PNP)(CO)HBpin

Ru	0.73095800	0.23331800	-0.97688400
P	1.11137900	2.36495000	-0.16829800
P	0.83043300	-2.05585600	-1.29007500
N	1.75497300	-0.31968700	0.87828900
C	2.42411500	0.61938200	1.60011000
C	3.06801800	0.29766300	2.79831000
C	3.06648700	-1.02120600	3.24807000
C	2.41491300	-1.98641200	2.48339800
C	1.75684900	-1.61073900	1.30841800
H	3.58450500	1.08037800	3.35597600
H	3.57286300	-1.29396200	4.17635800
H	2.39660100	-3.03160900	2.79560900
C	2.51593200	2.00842400	1.02013500
C	0.98879200	-2.61502800	0.48972800
H	3.42530500	2.04920200	0.39356200
H	2.62101300	2.76576000	1.81344800
H	1.41104700	-3.62646500	0.60144900
H	-0.05401300	-2.62022500	0.85231200
H	2.30369500	0.40070400	-1.64366300
C	1.81369300	3.69464100	-1.24402400
C	-0.09215500	3.32463600	0.86555800
C	2.28711300	-2.81885100	-2.14435700
C	-0.56591800	-3.09550900	-1.91336200
H	2.62817900	3.26614700	-1.84489200
H	0.35834800	4.25039300	1.25917400
H	2.30249900	-3.91701200	-2.04586300
H	-1.47155000	-2.82521500	-1.35315400
C	-0.11209000	0.69680100	-2.54747300
O	-0.65045200	0.98771500	-3.54023000
H	2.24772500	-2.54532200	-3.21013100
H	3.20488900	-2.38525100	-1.72147400
H	-0.35770500	-4.17168600	-1.79991400
H	-0.72576600	-2.87037100	-2.97915700
H	1.02417200	4.04103800	-1.92885300
H	2.18033100	4.55162200	-0.65604200
H	-0.97363800	3.56316700	0.25330000
H	-0.43276400	2.68914400	1.69552600
B	-1.23022200	0.06522200	-0.06414500
O	-1.74778400	-1.04394400	0.64966500
O	-2.22177200	1.05820800	-0.09348300
C	-3.01478600	-0.68920800	1.27000400
C	-3.48155100	0.52723300	0.39103200
C	-3.93652000	-1.90756800	1.23797700
C	-2.71341300	-0.30917000	2.72685700
C	-4.29731800	0.11135600	-0.84187800
C	-4.21980500	1.63157200	1.14728200
H	-4.06154800	-2.29917000	0.21968600
H	-4.93281800	-1.66007500	1.64006300
H	-3.51374900	-2.71176000	1.86068100
H	-2.19579100	-1.14885200	3.21598300
H	-2.05483500	0.57034700	2.78127800
H	-3.63176000	-0.09357300	3.29575100
H	-3.78862100	-0.68454400	-1.40550700
H	-4.39667500	0.98050800	-1.50927500
H	-5.30759000	-0.23635700	-0.57296900
H	-5.16024100	1.25577400	1.58338400
H	-3.60646500	2.05524500	1.95370200
H	-4.47276300	2.44738000	0.45253900

Ru(PNP)(CO)HB(NHCH₂)₂

Ru	0.25484900	-0.32945500	-0.80730100
P	-1.28793400	-2.00495300	-0.43676300
P	1.27986200	1.72844000	-0.97249900
N	-1.32692200	0.89528700	0.08066500
C	-2.58622500	0.39792100	0.22103000
C	-3.61355700	1.15787500	0.78756300
C	-3.36204100	2.47030200	1.18318600
C	-2.07881100	2.98519000	1.00995900
C	-1.07467400	2.17571500	0.47057900
H	-4.60782700	0.72094500	0.89222100
H	-4.15509300	3.08379600	1.61576800
H	-1.84020700	4.00786500	1.30581100
C	-2.85334100	-0.98000400	-0.32851700
C	0.34325200	2.66961600	0.34849600
H	-3.17420900	-0.86357900	-1.37958400
H	-3.66992000	-1.47696200	0.21970400
H	0.37625400	3.76357900	0.22345200
H	0.86554500	2.40606300	1.28601400
H	-0.57490600	-0.11222600	-2.29470900
C	-1.71739100	-3.26328200	-1.72164900
C	-1.32491600	-3.02504200	1.11324300
C	1.10047000	2.77832100	-2.49121700
C	3.04563500	2.03799700	-0.51380000
H	-1.84146600	-2.74958300	-2.68550500
H	-2.24703400	-3.62280400	1.20146800
H	1.48687500	3.80070800	-2.34455000
H	3.26211200	1.52081400	0.43195400
C	1.59319600	-1.34557900	-1.54505600
O	2.46399600	-1.98806600	-1.98814000
H	1.64703800	2.29348000	-3.31495600
H	0.03674900	2.81023800	-2.76892600
H	3.26478900	3.11372400	-0.41906200
H	3.68924200	1.60917600	-1.29774800
H	-0.87729900	-3.96902100	-1.81299300
H	-2.63143100	-3.82287600	-1.46496400
H	-0.45120800	-3.69489500	1.11229000
H	-1.22599600	-2.35244300	1.97810200
B	1.20045000	-0.56641500	1.16083900
N	2.41135400	-1.26809800	1.50698700
N	0.74669300	-0.01447500	2.43816900
C	2.81505500	-1.03930300	2.89260800
H	3.11513400	-1.57466200	0.84834600
C	1.49566300	-0.59905600	3.55691300
H	-0.22345000	0.21230000	2.62249000
H	3.57550000	-0.23316000	2.97981900
H	3.23747400	-1.93751200	3.37631100
H	1.66848400	0.11535500	4.38101600
H	0.97660900	-1.48102500	3.98855600

Ru(PNP)(CO)HB(OCH₃)₂

Ru	0.31988200	-0.37642400	-0.75213600
P	-1.34326100	-1.96318000	-0.50396600
P	1.44442400	1.62829700	-0.94539700
N	-1.26357700	0.96364000	-0.06326300
C	-2.54981600	0.52808500	-0.00019300
C	-3.57613800	1.34606800	0.48143300
C	-3.29041700	2.65256700	0.87104500
C	-1.97611700	3.10483900	0.77350000
C	-0.97933700	2.23838200	0.31618700
H	-4.59445500	0.95702700	0.52673500
H	-4.08053700	3.31020900	1.23946500
H	-1.70998700	4.12249500	1.06349600
C	-2.84726200	-0.84559700	-0.54390300
C	0.46299600	2.67766000	0.25944400
H	-3.07656700	-0.73604800	-1.61939900
H	-3.73189100	-1.28385500	-0.05500500
H	0.53734100	3.75961700	0.06238400
H	0.92743000	2.48888000	1.24396600
H	-0.35976900	-0.21029100	-2.32333100
C	-1.71818500	-3.19149300	-1.83478900
C	-1.59268800	-2.98301200	1.02409700
C	1.38024900	2.60319500	-2.52225800
C	3.19106200	1.89451800	-0.40391600
H	-1.72525800	-2.66966400	-2.80202000
H	-2.57458800	-3.48399300	1.03265700
H	1.80322900	3.61544200	-2.40946800
H	3.34259800	1.36886200	0.54906200
C	1.66824200	-1.49019600	-1.32669700
O	2.52627600	-2.19468300	-1.68467100
H	1.94357900	2.05297300	-3.29166300
H	0.33322200	2.66311700	-2.85365000
H	3.43337800	2.96529100	-0.30971100
H	3.85737900	1.44085800	-1.15415600
H	-0.91247600	-3.94171200	-1.85441200
H	-2.68026000	-3.70235200	-1.66689900
H	-0.79801200	-3.74467600	1.06720600
H	-1.48195400	-2.32376300	1.89617100
B	1.03411400	-0.54152100	1.29713300
O	2.39386000	-0.68043600	1.61415000
O	0.09874700	-0.47369700	2.35134300
C	2.91121200	-1.40168300	2.72377000
H	3.84124500	-1.89802400	2.40235200
H	3.15277300	-0.74000200	3.57506900
H	2.21172900	-2.17875000	3.07711300
C	0.39730200	-0.07165500	3.68214900
H	0.63274100	-0.93056300	4.33514200
H	1.24574800	0.63350400	3.72161600
H	-0.49211600	0.43392000	4.09307900

Ru(PNP)(CO)HB(CH₃)₂

Ru	0.12054800	-0.69202700	-0.34071500
P	-2.18792500	-0.82315200	-0.31576200
P	2.28161500	0.10161200	-0.47842100
N	-0.29250800	1.44598500	-0.10588900
C	-1.55648400	1.92256100	-0.26846700
C	-1.85507000	3.27759300	-0.09945000
C	-0.83402900	4.17732200	0.19924300
C	0.46558100	3.69092600	0.32422100
C	0.70852400	2.32228600	0.18020200
H	-2.88369200	3.61897700	-0.22536500
H	-1.04651300	5.24090300	0.32505200
H	1.29615800	4.36137600	0.55015500
C	-2.61835500	0.95323800	-0.72415400
C	2.09551900	1.75975200	0.37210800
H	-2.64275100	0.98286700	-1.82848900
H	-3.61382500	1.25380600	-0.36045700
H	2.86194900	2.49250300	0.07209400
H	2.24230900	1.54923600	1.44627200
H	-0.13282600	-0.40512900	-2.02334500
C	-3.11399300	-1.77457300	-1.60263400
C	-3.20407700	-1.18028200	1.19740500
C	3.00796200	0.52807100	-2.13072200
C	3.74225400	-0.64149300	0.38173000
H	-2.67446300	-1.55174200	-2.58491400
H	-4.27929800	-1.00960400	1.02317500
H	3.96856800	1.06282000	-2.04574700
H	3.48468000	-0.84438800	1.43108000
C	0.48589300	-2.47184700	-0.61209800
O	0.72584000	-3.59970300	-0.79399000
H	3.15514700	-0.40606500	-2.69451300
H	2.27819600	1.13870900	-2.68194600
H	4.62642300	0.01422500	0.33068500
H	3.98059200	-1.60125000	-0.10247800
H	-2.98607600	-2.84988300	-1.40347200
H	-4.18936800	-1.53381500	-1.59889400
H	-3.04751700	-2.23118500	1.48667200
H	-2.85583100	-0.54408400	2.02401700
B	0.31335900	-0.95033200	1.82134800
C	0.83472300	-2.28309300	2.53358500
H	1.27148400	-2.12280400	3.54000900
H	-0.06937800	-2.90817200	2.70140700
H	1.52052600	-2.91432000	1.94647400
C	-0.11647300	0.15712900	2.90006300
H	-0.69098700	-0.29261700	3.73529800
H	0.81132700	0.53517300	3.38125200
H	-0.67212700	1.03858900	2.54039400

Ru(PNP)(CO)HBH₂

Ru	-0.01156300	-0.80917200	-0.04900500
P	-2.29829200	-0.45301900	-0.07825600
P	2.27148700	-0.49493700	-0.19378300
N	0.02367700	1.38103200	-0.02475500
C	-1.11383800	2.08966900	-0.25506600
C	-1.13369400	3.48523600	-0.18283500
C	0.04415000	4.17713800	0.09147200
C	1.21441400	3.44829900	0.29006200
C	1.17625000	2.05179800	0.23900100
H	-2.06857700	4.01829800	-0.36218500
H	0.05087400	5.26778500	0.14347500
H	2.15949000	3.95117900	0.50066700
C	-2.34223500	1.32027500	-0.67340800
C	2.42017300	1.23758100	0.50344900
H	-2.32816900	1.23992500	-1.77539900
H	-3.26303700	1.85236100	-0.38652900
H	3.31863400	1.76971600	0.15117200
H	2.52181500	1.10273800	1.59471400
H	-0.19083600	-0.67207000	-1.77312300
C	-3.40928500	-1.32151400	-1.27162900
C	-3.33633100	-0.43286800	1.45854300
C	3.10940700	-0.39191200	-1.84375500
C	3.50745700	-1.44682500	0.79982900
H	-2.93955500	-1.29816200	-2.26487000
H	-4.35843400	-0.06715900	1.26648900
H	4.15463800	-0.04975800	-1.76409300
H	3.18592400	-1.46800000	1.85156700
C	-0.02770000	-2.64780200	-0.00559800
O	-0.03429600	-3.81241600	0.04661800
H	3.08264600	-1.38962500	-2.30844300
H	2.53184200	0.29046500	-2.48405900
H	4.51879100	-1.01604000	0.72339600
H	3.52949100	-2.48325700	0.42911900
H	-3.50447700	-2.37306900	-0.95977200
H	-4.41155500	-0.86479600	-1.30810500
H	-3.38579300	-1.45579000	1.86301400
H	-2.84743700	0.20511300	2.21046200
B	0.08324100	-0.77509800	2.05960100
H	0.07228000	-1.73493500	2.81577600
H	0.12212100	0.29113600	2.67547800

Ru(PNP)(CO)H₂-CO₂ IS

Ru	-0.12485200	-0.85327100	-0.40834000
P	-2.37628200	-0.46165700	-0.09635500
P	2.13996800	-0.58260100	-0.75244900
N	-0.07381800	1.33275000	-0.48062700
C	-1.22440600	2.04267500	-0.62720400
C	-1.22120800	3.44042500	-0.65697300
C	-0.01221300	4.12760000	-0.57261900
C	1.16560800	3.39456400	-0.44424100
C	1.10812900	1.99891200	-0.38329900
H	-2.16502400	3.97666500	-0.76618300
H	0.01190800	5.21880200	-0.60742800
H	2.13245100	3.89467100	-0.37058900
C	-2.50142200	1.26473800	-0.81774800
C	2.35205500	1.17994200	-0.14947300
H	-2.63814900	1.09745100	-1.90134700
H	-3.37202100	1.83355400	-0.45371600
H	3.24124200	1.68356500	-0.56176000
H	2.49834200	1.08122800	0.94078700
H	-0.45898500	-0.83577800	-2.06863400
C	-3.70001200	-1.36997600	-1.01418100
C	-3.12217100	-0.30411300	1.59270300
C	2.86564700	-0.56613900	-2.45755800
C	3.42785300	-1.49185500	0.21283200
H	-3.41930000	-1.42299300	-2.07584400
H	-4.13839500	0.12270700	1.56449900
H	3.91859000	-0.23941100	-2.46567400
H	3.16860700	-1.43543000	1.27952100
C	-0.16377700	-2.69310900	-0.35550400
O	-0.18669700	-3.85838400	-0.32084100
H	0.20785500	-0.75871700	1.25084400
H	-3.75712800	-2.39711900	-0.62202500
H	-4.68499500	-0.88798500	-0.90402300
H	-3.16130000	-1.30677800	2.04663900
H	-2.46367300	0.31590800	2.21785600
H	2.79412700	-1.58277700	-2.87428900
H	3.41647200	-2.54905200	-0.09415100
H	4.43593100	-1.07886500	0.04639600
H	2.25794000	0.09783600	-3.08980700
C	0.87349400	0.16029600	3.62259800
O	-0.24057900	0.18277400	3.96850700
O	2.00789700	0.16902200	3.33687500

Ru(PNP)(CO)H₂-CO₂ TS

Ru	-0.03816900	-0.82555900	-0.33298900
P	2.23369300	-0.43536500	-0.58468900
P	-2.33587000	-0.56888400	-0.19322800
N	-0.09034300	1.35878700	-0.36496200
C	1.05160800	2.07766400	-0.18967000
C	1.03817400	3.47563000	-0.19663900
C	-0.16967800	4.15156800	-0.35278800
C	-1.33598900	3.40956100	-0.52387000
C	-1.26804900	2.01355700	-0.54602300
H	1.97247500	4.02110100	-0.05723500
H	-0.20141300	5.24303900	-0.34324300
H	-2.29977200	3.90230900	-0.65909200
C	2.32825600	1.31658100	0.06979800
C	-2.49391200	1.18484300	-0.83845700
H	2.44001300	1.19011400	1.16101200
H	3.20399400	1.87562900	-0.29655800
H	-3.40739400	1.69335400	-0.49176700
H	-2.57251500	1.07255900	-1.93491200
H	0.18489600	-0.73501200	1.39823900
H	-0.25644500	-0.81431000	-1.97913400
C	3.51900900	-1.31498100	0.40427500
C	2.99198100	-0.34291200	-2.27018100
C	-3.23594000	-0.56003300	1.42089100
C	-3.49420600	-1.50432000	-1.28834700
H	3.20394900	-1.30319200	1.45727600
H	4.02489400	0.04065500	-2.24052100
H	-4.25350100	-0.14852200	1.32139900
H	-3.11103300	-1.47706100	-2.31847000
C	0.01556400	-2.66812300	-0.34110600
O	0.05085900	-3.83161700	-0.35662000
C	0.47945400	-0.08022500	2.91704500
O	-0.59824900	0.26981700	3.28277200
O	1.65955800	-0.20708400	3.04879900
H	-2.64884900	0.01288600	2.15216500
H	-3.29857300	-1.59828200	1.78346400
H	-3.51721700	-2.55402700	-0.95736600
H	-4.51629500	-1.09417200	-1.25173800
H	4.50917000	-0.84329100	0.29818500
H	3.57647500	-2.35852500	0.05869200
H	2.36730900	0.30229500	-2.90521600
H	2.98934700	-1.35249400	-2.70934800

Ru(PNP)(CO)H₂-CO₂ FS

Ru	-0.03314200	-0.84471200	-0.27183600
P	2.26081600	-0.46433700	-0.50348000
P	-2.34383700	-0.58294100	-0.17004400
N	-0.07731400	1.33586800	-0.37971200
C	1.06630400	2.05768700	-0.22247100
C	1.05292800	3.45489600	-0.26969600
C	-0.15413000	4.12620500	-0.44303000
C	-1.32173200	3.38180200	-0.59146800
C	-1.25512000	1.98650000	-0.57527600
H	1.98686200	4.00343600	-0.14208100
H	-0.18522300	5.21754700	-0.46174200
H	-2.28533400	3.87195900	-0.73571800
C	2.34308200	1.31146100	0.07224100
C	-2.48816200	1.15877600	-0.84333500
H	2.43913900	1.22510700	1.17016400
H	3.21978500	1.85543800	-0.31293100
H	-3.39340100	1.67669000	-0.48987400
H	-2.58574800	1.03620300	-1.93716700
H	0.10842000	-0.75474500	1.57796200
C	3.50489500	-1.31185000	0.55644100
C	3.02196700	-0.46065500	-2.18730900
C	-3.21272800	-0.55510800	1.45476900
C	-3.48656300	-1.53967300	-1.26064100
H	3.14417000	-1.23356800	1.59325000
H	4.05770600	-0.08522900	-2.16652500
H	-4.20868300	-0.09039900	1.37612600
H	-3.10207500	-1.52486200	-2.29079800
C	0.01865800	-2.69022500	-0.26098600
O	0.05314600	-3.85155200	-0.28159800
H	-0.19372800	-0.91198200	-1.87829400
H	3.56440200	-2.37067900	0.26201200
H	4.50020100	-0.84929300	0.46029500
H	3.01520100	-1.48932400	-2.57923800
H	2.41009000	0.16249600	-2.85600100
H	-3.32350600	-1.59465700	1.80192100
H	-3.50749100	-2.58450800	-0.91486800
H	-4.51012700	-1.13294200	-1.23401500
H	-2.56926300	-0.01793900	2.17068200
C	0.37346500	0.01148100	2.56863400
O	-0.63099300	0.59802800	2.95286800
O	1.56361700	-0.05536200	2.86888300

Ru(PNP)(CO)HB(OCH₃)₂-CO₂ IS

Ru	-0.21417600	-0.21556000	0.68941200
P	-0.25227800	2.05001500	1.14027000
P	0.23002600	-2.28553400	-0.23797600
N	0.79099300	0.48152800	-1.12739200
C	0.77741700	1.79996800	-1.46181600
C	1.42226300	2.26837300	-2.61122200
C	2.07322300	1.37005600	-3.45271300
C	2.08617300	0.02083300	-3.10427100
C	1.45742600	-0.39530100	-1.92730700
H	1.39407800	3.33423400	-2.84256000
H	2.56914100	1.71614100	-4.36205500
H	2.60049800	-0.71452600	-3.72487300
C	0.00735700	2.74707700	-0.57738400
C	1.57063700	-1.82752800	-1.46378500
H	-1.01154400	2.82826300	-0.99095800
H	0.46666100	3.74845200	-0.57628600
H	1.62712500	-2.51683900	-2.32156500
H	2.51423800	-1.92469500	-0.89846900
C	-1.75179300	2.97186500	1.71604700
C	1.07310500	2.83390500	2.17062400
C	-0.98206500	-3.25028700	-1.25926700
C	1.02385100	-3.62919300	0.75419500
H	-2.60188800	2.70066100	1.07428800
H	1.03845700	3.93512000	2.12696500
H	-0.52636500	-4.16067700	-1.68173200
H	1.87084600	-3.19986500	1.30700100
C	-1.04692800	-0.79761400	2.22357100
O	-1.57868500	-1.16302100	3.19515600
H	1.35766200	-0.34697700	1.37629000
B	-2.15178100	-0.10023500	-0.29308600
O	-2.42539400	0.91328400	-1.23857600
O	-3.14326400	-1.05304100	-0.03055700
C	-4.54414300	-0.83358800	-0.10420700
H	-4.80826800	0.22967500	0.03018200
H	-4.96966400	-1.17732100	-1.06435900
H	-5.02086000	-1.40959600	0.70548500
C	-3.34334800	0.78941800	-2.31882900
H	-3.46296500	-0.25887000	-2.64134500
H	-2.94887100	1.36961400	-3.16953600
H	-4.34116200	1.18912100	-2.06601400
H	-1.35539800	-2.60994100	-2.07181300
H	-1.84121400	-3.51693000	-0.62673500
H	1.36533900	-4.46449900	0.12158300
H	0.28701600	-4.00604600	1.48034000
H	2.05167200	2.46654900	1.83185300
H	0.93619400	2.50609300	3.21315400
H	-1.97884400	2.66337500	2.74831200
H	-1.59687800	4.06289600	1.69379100
C	4.04639500	-0.28558100	1.36262400
O	4.09087600	-1.42680100	1.11160900
O	4.07485200	0.85584000	1.60488600

Ru(PNP)(CO)HB(OCH₃)₂-CO₂ TS

Ru	-0.19785700	0.22226800	-0.65428300
P	-0.27203300	-2.04430300	-1.15171200
P	0.24438800	2.27983300	0.33139700
N	0.97116800	-0.49958900	1.05117600
C	1.02298400	-1.82706700	1.33982900
C	1.79576300	-2.31266000	2.39971300
C	2.50674900	-1.42201200	3.19904600
C	2.44864400	-0.06255100	2.89976300
C	1.69295000	0.37218700	1.80753000
H	1.82083800	-3.38551300	2.59559600
H	3.10451900	-1.78207800	4.03903200
H	3.00665700	0.66641000	3.48908900
C	0.18441100	-2.76894800	0.51354600
C	1.72217700	1.82128400	1.38448100
H	-0.78174300	-2.89065100	1.02986800
H	0.66472900	-3.75684500	0.43394900
H	1.85893700	2.48395400	2.25398300
H	2.59079800	1.96429500	0.71810000
C	-1.83419900	-2.94959900	-1.55984900
C	0.92016500	-2.79902500	-2.34604400
C	-0.90798300	3.10866700	1.52189600
C	0.86092800	3.70371500	-0.66853400
H	-2.59697800	-2.69640300	-0.81029400
H	0.91495000	-3.89960400	-2.28650800
H	-0.46594500	4.02784600	1.93901300
H	1.65866200	3.33922900	-1.33000600
C	-1.15014500	0.83682700	-2.10574000
O	-1.75344600	1.22278900	-3.02418500
H	1.36184400	0.38197200	-1.46860900
B	-2.04474700	0.05650400	0.43498100
O	-2.22084400	-0.97337900	1.38057800
O	-3.07159800	0.98352700	0.23909200
C	-4.46009000	0.73812500	0.41376600
H	-4.71572300	-0.32730600	0.28182100
H	-4.81662400	1.06089600	1.40816900
H	-5.00363500	1.31798100	-0.34919300
C	-3.07282500	-0.89816100	2.51882500
H	-3.19528400	0.13861400	2.87515700
H	-2.61233100	-1.48945200	3.32713300
H	-4.07430600	-1.31598100	2.31658000
H	-1.14625700	2.40945500	2.33709200
H	-1.84506100	3.34377400	0.99725900
H	1.23800000	4.51828300	-0.02937100
H	0.02954300	4.08210300	-1.28310400
H	1.92413000	-2.40171200	-2.14484700
H	0.63016700	-2.48956500	-3.36260500
H	-2.18581700	-2.61787500	-2.54899000
H	-1.67801800	-4.04031800	-1.58270400
C	3.12901700	0.45281700	-1.70635400
O	3.42618600	-0.69528400	-1.76564900
O	3.33327900	1.62468900	-1.69943600

Ru(PNP)(CO)HB(OCH₃)₂-CO₂ FS

Ru	-0.28987800	-0.15606400	0.63382200
P	-0.18352300	2.15129800	1.00517900
P	0.06947200	-2.32755800	-0.18419000
N	1.15065400	0.33525500	-0.93979200
C	1.38980100	1.63246600	-1.27079400
C	2.35454700	1.97413000	-2.22213500
C	3.06866700	0.96918500	-2.86881600
C	2.81833500	-0.35703800	-2.52854700
C	1.87243100	-0.65023300	-1.54193500
H	2.53012400	3.02530800	-2.45377500
H	3.81954400	1.21736700	-3.62186900
H	3.37476500	-1.17125900	-2.99417300
C	0.55229000	2.70543700	-0.62153800
C	1.70059400	-2.06695700	-1.05397900
H	-0.31942300	2.88986200	-1.27070100
H	1.12177200	3.64302800	-0.52789900
H	1.88086400	-2.79130700	-1.86360600
H	2.45073300	-2.23529200	-0.25872400
C	-1.67764400	3.22690700	1.16511300
C	0.94614000	2.79622900	2.30865400
C	-1.02150200	-3.10017100	-1.46221500
C	0.41297400	-3.70441200	0.98812100
H	-2.36718000	3.01011300	0.33725900
H	1.13427100	3.87380700	2.17622800
H	-0.62421700	-4.07802000	-1.77743900
H	1.18333900	-3.34037900	1.68568000
C	-1.46867000	-0.59046100	1.98522700
O	-2.21306700	-0.86008700	2.83583200
H	1.25034000	-0.37734400	1.79910400
B	-1.95333500	0.07649700	-0.61181500
O	-1.93363800	1.07004000	-1.60197000
O	-3.05957500	-0.75694600	-0.47563200
C	-4.39870400	-0.42262100	-0.81946100
H	-4.57610500	0.66557700	-0.79144100
H	-4.66923200	-0.79694500	-1.82219800
H	-5.06367100	-0.89999900	-0.08292800
C	-2.65169600	1.00529600	-2.83106200
H	-2.84002400	-0.03482900	-3.14476900
H	-2.04122600	1.49631400	-3.60577600
H	-3.61894900	1.53252500	-2.76879900
H	-1.09322400	-2.43331700	-2.33439700
H	-2.03025200	-3.21930700	-1.04245100
H	0.76864000	-4.60335500	0.45962300
H	-0.51178900	-3.94330800	1.53504600
H	1.88201500	2.21311000	2.26313500
H	0.47353800	2.62718800	3.28914800
H	-2.17905100	2.99477800	2.11712700
H	-1.40509200	4.29444900	1.15555800
C	2.48072100	-0.54031800	1.87261800
O	3.09181400	0.52884300	1.87609000
O	2.78662500	-1.73709400	1.91344700

Ru(PNP)(CO)HB(NHCH₂)₂-CO₂ IS

Ru	-0.13849200	0.14498500	-0.73435000
P	0.48897600	2.27079100	-0.09383500
P	-0.46605400	-2.13959200	-0.81288100
N	0.67237400	-0.36028800	1.23433100
C	1.42024800	0.54396900	1.92481500
C	1.94711500	0.24522100	3.18484700
C	1.73984800	-1.01719800	3.73786900
C	0.99305500	-1.94665000	3.01696900
C	0.45581300	-1.59089200	1.77615600
H	2.53483200	0.99882900	3.71127900
H	2.15549700	-1.27292400	4.71473800
H	0.80390600	-2.94462800	3.41503500
C	1.72724600	1.85903500	1.25213300
C	-0.43710000	-2.53761400	1.01691400
H	2.68701400	1.74908000	0.71705100
H	1.85152400	2.66390400	1.99434000
H	-0.18614900	-3.58716000	1.23820700
H	-1.47316900	-2.34785100	1.35160400
H	1.46750600	-0.00050700	-1.32053700
C	1.45779400	3.38718700	-1.20434000
C	-0.67172900	3.46715600	0.72126500
C	0.79946400	-3.27491300	-1.55129000
C	-2.04179100	-2.93123000	-1.37361100
H	2.29256000	2.81352100	-1.63092800
H	-0.14451400	4.33862800	1.14287800
H	0.60199800	-4.33322300	-1.31259000
H	-2.89010600	-2.38548100	-0.93694700
C	-0.84158100	0.56495600	-2.37670700
O	-1.31741700	0.82769900	-3.41183500
B	-2.13874300	0.33113300	0.14695800
N	-3.39685200	0.59577200	-0.50534300
C	-4.53677200	0.46091300	0.39891700
C	-3.88560300	0.63045500	1.78593700
N	-2.50589300	0.18624400	1.55558900
H	-5.01775600	-0.53817800	0.32045700
H	-4.40603000	0.03895700	2.55957700
H	-5.32385700	1.21465700	0.22159100
H	-3.93185500	1.69536000	2.09821500
H	-1.85355900	0.34883700	2.31345900
H	-3.56380400	0.52757000	-1.50048200
H	-1.22654700	2.94041000	1.51163200
H	-1.40339100	3.80829300	-0.02731600
H	0.80291900	3.71523100	-2.02624800
H	1.83863500	4.27335100	-0.67118200
H	0.78707800	-3.13940000	-2.64418300
H	1.79514400	-2.97950400	-1.19160500
H	-2.10215100	-2.84439500	-2.46977000
H	-2.08983000	-3.99654400	-1.09632100
C	4.10174900	-0.33814500	-1.26990400
O	4.00622400	-1.49357000	-1.40380200
O	4.27165600	0.81019100	-1.12641700

Ru(PNP)(CO)HB(NHCH₂)₂-CO₂ TS

Ru	-0.02618000	-0.07501700	0.68587300
P	0.72865300	-2.20410400	0.15050500
P	-0.55582600	2.18108600	0.59393800
N	0.65685600	0.33620100	-1.35606500
C	1.47006500	-0.54834100	-1.99559600
C	1.93595000	-0.30129000	-3.29058300
C	1.59700800	0.88997800	-3.92911700
C	0.78280800	1.80153500	-3.26001200
C	0.31141400	1.49542800	-1.97998200
H	2.58156600	-1.03441100	-3.77601100
H	1.96535700	1.10650800	-4.93407200
H	0.49319900	2.74412400	-3.72643500
C	1.91507400	-1.76907900	-1.23114400
C	-0.64729000	2.40945800	-1.26246800
H	2.84985000	-1.50944900	-0.70339700
H	2.12745800	-2.60962200	-1.91077000
H	-0.52227800	3.45472500	-1.58586200
H	-1.67002900	2.08066000	-1.52149100
H	1.63017700	0.25127000	1.17690900
C	1.78156900	-3.18677800	1.30611900
C	-0.37161700	-3.50051200	-0.58382500
C	0.63439300	3.47553900	1.16971900
C	-2.17114200	2.87404200	1.16878600
H	2.59048600	-2.53826900	1.67006000
H	0.20390600	-4.35872200	-0.96689200
H	0.33568700	4.48181800	0.83370700
H	-2.98730300	2.22757100	0.81661200
C	-0.61355500	-0.40606300	2.39379300
O	-1.01646100	-0.61105200	3.47011500
B	-2.02447800	-0.50748900	-0.03447600
N	-3.19952500	-0.86748000	0.71605500
C	-4.40309500	-0.88944800	-0.11308500
C	-3.82960600	-1.06116600	-1.53360900
N	-2.48980200	-0.47125700	-1.41949800
H	-4.97572000	0.06018200	-0.04267300
H	-4.45587100	-0.56179900	-2.29315600
H	-5.09606800	-1.70722500	0.15030600
H	-3.78586500	-2.13877500	-1.79729600
H	-1.87332300	-0.61070200	-2.21115100
H	-3.30946000	-0.76241000	1.71599900
H	-0.96079200	-3.04839100	-1.39487100
H	-1.07502000	-3.84477700	0.18956100
H	1.16313400	-3.50218200	2.16041000
H	2.20329500	-4.07862500	0.81545400
H	0.66991800	3.45062000	2.26951700
H	1.64258900	3.22986400	0.80959800
H	-2.17753500	2.87216700	2.26986600
H	-2.32393700	3.90554500	0.81286300
C	3.29442300	0.55166200	1.57353700
O	3.23934500	1.60115600	2.12396500
O	3.84554100	-0.41113900	1.13365600

Ru(PNP)(CO)HB(NHCH₂)₂-CO₂ FS

Ru	0.21058400	-0.17685000	-0.69263400
P	-0.52871400	-2.28820000	0.00545300
P	0.59198600	2.12066400	-0.86785600
N	-1.00200000	0.46242100	1.01496500
C	-1.88934000	-0.39817200	1.58629600
C	-2.70954300	0.00506700	2.64462900
C	-2.65397300	1.32081200	3.09552400
C	-1.76166000	2.20254400	2.49024400
C	-0.93297000	1.74613200	1.46251100
H	-3.40802600	-0.70920900	3.08207100
H	-3.30322400	1.65773100	3.90630400
H	-1.69119700	3.24112300	2.81546300
C	-2.03027200	-1.77726100	0.99440200
C	0.11226700	2.65101700	0.86032900
H	-2.83302600	-1.73085200	0.23448500
H	-2.31690200	-2.51349700	1.76158200
H	-0.20201200	3.70488300	0.91134500
H	1.03688500	2.53765700	1.45363000
H	-1.37152000	0.00551000	-1.77273400
C	-1.21016600	-3.49960300	-1.20125400
C	0.47594200	-3.32495800	1.16117600
C	-0.45295700	3.12880400	-2.00192200
C	2.27578300	2.85102000	-1.07496200
H	-1.92832200	-2.94881300	-1.82859400
H	-0.10648800	-4.17706100	1.54640700
H	-0.39464300	4.20119900	-1.75545600
H	2.97668600	2.36077100	-0.38465900
C	1.23296900	-0.71620400	-2.12189000
O	1.90759200	-1.05337000	-3.01005100
B	1.94442300	-0.32717300	0.50528500
N	3.27568000	-0.72376600	0.13414000
C	4.23075800	-0.50604100	1.21989700
C	3.32379500	-0.46687000	2.46652900
N	2.03670000	-0.01304600	1.92469700
H	4.77354600	0.45634800	1.10829000
H	3.72257700	0.20677500	3.24407200
H	4.99054100	-1.30286900	1.29164600
H	3.24822800	-1.48032200	2.91260300
H	1.24513500	-0.04937200	2.55520800
H	3.63143700	-0.77701700	-0.81105600
H	0.82831700	-2.70041400	1.99490200
H	1.36032900	-3.69756100	0.62255100
H	-0.38779000	-3.88852500	-1.82059300
H	-1.71127100	-4.33656400	-0.68930200
H	-0.09276800	2.97214800	-3.03095000
H	-1.48750200	2.75217100	-1.93194800
H	2.61233300	2.66209100	-2.10601100
H	2.26632800	3.93774100	-0.89500700
C	-2.61526000	0.09611400	-1.75497900
O	-3.15799900	-1.00718700	-1.87471200
O	-2.99202200	1.25962800	-1.61580000

Ru(PNP)(CO)HBpin-CO₂ IS

Ru	-0.50795700	-0.17578900	-0.73360700
P	-0.84531500	-2.26211200	0.20839300
P	-0.48170600	2.10975900	-1.10062700
N	-1.08017400	0.48752000	1.27567300
C	-1.62593400	-0.39141000	2.15949900
C	-1.97726900	-0.00075600	3.45481300
C	-1.80917500	1.32693900	3.84325400
C	-1.28589100	2.23055200	2.92167600
C	-0.91603400	1.78524800	1.64865400
H	-2.40147800	-0.73660800	4.13960600
H	-2.08854000	1.65333000	4.84725100
H	-1.14336400	3.28004700	3.18328300
C	-1.91668900	-1.78857900	1.67031100
C	-0.27729500	2.72132300	0.65641100
H	-2.94704200	-1.79905800	1.27281300
H	-1.87079700	-2.51582100	2.49667400
H	-0.62366300	3.75638200	0.80587200
H	0.81311900	2.68545200	0.82138800
H	-2.19087700	-0.22047200	-1.06998600
C	-1.86351300	-3.54947300	-0.64218600
C	0.49862000	-3.29129600	0.96618000
C	-1.98664300	2.98481000	-1.73218700
C	0.87182300	3.00599800	-1.98797600
H	-2.78555000	-3.07883000	-1.01018900
H	0.09576000	-4.19901900	1.44446700
H	-1.89866400	4.08023900	-1.64336000
H	1.83529500	2.67107000	-1.57925000
C	-0.04742200	-0.73124200	-2.42755200
O	0.24538000	-1.07981400	-3.50076700
B	1.59474400	-0.14599400	-0.23157800
O	2.26627300	0.85099300	0.51686600
C	3.62129400	0.41635800	0.81705800
C	3.87827200	-0.65709700	-0.30223400
O	2.53578300	-1.11907400	-0.59951500
C	4.44822700	-0.06203300	-1.59834700
C	4.72363800	-1.85664800	0.12556100
C	4.54554500	1.63291600	0.77976200
C	3.60426600	-0.17318500	2.23459700
H	5.74087000	-1.54484400	0.41517300
H	4.27066800	-2.39599100	0.96805600
H	4.81334500	-2.56110200	-0.71571600
H	3.85721100	0.80288200	-1.93400600
H	4.39934500	-0.82511200	-2.38958000
H	5.49790100	0.25216100	-1.48315600
H	3.21103200	0.58274900	2.93163600
H	2.95051300	-1.05611900	2.29052200
H	4.61154400	-0.46344000	2.57302200
H	4.47651800	2.16953000	-0.17595100
H	5.59589600	1.33770800	0.93799100
H	4.26953600	2.33456100	1.58273800
C	-4.85700500	-0.24090600	-0.87668400
O	-4.93597300	0.85494700	-1.26928100
O	-4.84720000	-1.33815400	-0.47130500
H	-2.12435500	2.71462900	-2.79085400
H	-2.86693300	2.62421600	-1.18204800
H	0.82912400	2.74310400	-3.05619800
H	0.77806000	4.09890300	-1.88190400
H	1.21954300	-3.56703600	0.18269400
H	1.03395600	-2.68670400	1.71276700
H	-1.29499100	-3.93113200	-1.50430000
H	-2.10707300	-4.38863400	0.02929800

Ru(PNP)(CO)HBpin-CO₂ TS

Ru	-0.58686500	-0.16572200	-0.67189100
P	-0.87714000	-2.26209100	0.29635000
P	-0.55156200	2.13221000	-1.03140400
N	-1.11705900	0.49573300	1.34922700
C	-1.65592200	-0.38480900	2.23574000
C	-1.99091500	0.00547500	3.53560100
C	-1.81259100	1.33167100	3.92333300
C	-1.29367700	2.23581200	2.99984900
C	-0.93964800	1.79152500	1.72220400
H	-2.41271600	-0.72874800	4.22326300
H	-2.08154500	1.65754700	4.93034300
H	-1.14374400	3.28373600	3.26312700
C	-1.95606800	-1.77890900	1.74629000
C	-0.30394700	2.72595300	0.72592000
H	-2.97805900	-1.77238800	1.32784700
H	-1.92776500	-2.50671200	2.57249000
H	-0.63579500	3.76387100	0.88683900
H	0.78832300	2.67610800	0.87307900
H	-2.32216300	-0.20810700	-0.97770200
C	-1.86879200	-3.57432100	-0.54233300
C	0.49517700	-3.24287100	1.06075300
C	-2.05984800	3.02551400	-1.61899800
C	0.79393800	3.00810400	-1.94744800
H	-2.80653900	-3.12614100	-0.89790800
H	0.10976300	-4.14563900	1.56162500
H	-1.94108600	4.11750100	-1.52935300
H	1.76239800	2.65670100	-1.56565800
C	-0.15155000	-0.71931900	-2.37546700
O	0.12605200	-1.06379800	-3.45184100
B	1.50500900	-0.14722800	-0.23778800
O	2.19514700	0.84464000	0.49359700
C	3.56053100	0.40872500	0.74821300
C	3.78061900	-0.66314800	-0.38156600
O	2.42724400	-1.12081800	-0.64021800
C	4.31282500	-0.06759800	-1.69303600
C	4.63399800	-1.86612600	0.01884000
C	4.48190800	1.62599300	0.68179600
C	3.58957800	-0.18167700	2.16472500
H	5.65970900	-1.55703600	0.27922700
H	4.20455000	-2.40574500	0.87331900
H	4.69750200	-2.56871100	-0.82620600
H	3.71488000	0.79912000	-2.01143100
H	4.24035100	-0.82963600	-2.48337000
H	5.36575200	0.24470400	-1.60752700
H	3.22397400	0.57499600	2.87575400
H	2.93547700	-1.06250300	2.24309000
H	4.60691800	-0.47584600	2.46717700
H	4.38469200	2.16200700	-0.27172900
H	5.53636800	1.33103600	0.80892500
H	4.22977100	2.32779200	1.49230600
C	-4.01177700	-0.30091100	-1.23096600
O	-4.20320200	0.55165200	-2.03497100
O	-4.34582100	-1.18321200	-0.49802700
H	0.71784300	2.75278500	-3.01557700
H	0.71937400	4.10139000	-1.83263300
H	-1.29715900	-3.94825300	-1.40557500
H	-2.08677000	-4.41280800	0.13843800
H	1.21232600	-3.52514700	0.27650700
H	1.02517600	-2.61424900	1.79106500
H	-2.24157100	2.75770000	-2.67058500
H	-2.93168500	2.68445500	-1.04482900

Ru(PNP)(CO)HBpin-CO₂ FS

Ru	-0.49714700	-0.19489100	-0.77102500
P	-0.80032300	-2.31807000	0.17914400
P	-0.49013700	2.11816000	-1.16114600
N	-1.28494700	0.44529200	1.16359100
C	-1.88370900	-0.45657700	1.99018300
C	-2.42651900	-0.06503200	3.21725500
C	-2.40003400	1.27743300	3.58427300
C	-1.81689400	2.19901000	2.71885600
C	-1.25238800	1.75766000	1.51944400
H	-2.89515800	-0.81330600	3.85742700
H	-2.83774500	1.60338200	4.53011200
H	-1.78487400	3.26031600	2.96780200
C	-2.03268900	-1.88093500	1.51455500
C	-0.54514900	2.72626400	0.60621300
H	-3.01330500	-1.96484100	1.01053200
H	-2.01639200	-2.58565000	2.36057000
H	-0.97760300	3.73496100	0.69336900
H	0.51310200	2.77068700	0.91463700
H	-2.33383100	-0.25266900	-1.36672000
C	-1.64558100	-3.63483500	-0.79093700
C	0.53725700	-3.22805600	1.07246000
C	-1.93512100	2.89092000	-2.00159100
C	0.94990700	3.03317800	-1.86769400
H	-2.55304800	-3.18165400	-1.21942100
H	0.14110200	-4.15145500	1.52411800
H	-1.95874800	3.97923000	-1.83082700
H	1.86040300	2.73407300	-1.33104400
C	0.14183700	-0.75646200	-2.41046600
O	0.54660500	-1.10899500	-3.44059500
B	1.48957900	-0.11982200	-0.15362600
O	2.05313600	0.90709300	0.62436700
C	3.39937200	0.52314800	1.03086400
C	3.77528000	-0.56058900	-0.04872600
O	2.47135600	-1.06879000	-0.44260200
C	4.42463900	0.02968000	-1.30765300
C	4.61788600	-1.72521700	0.46825100
C	4.28341000	1.76903100	1.03563400
C	3.29542500	-0.04112900	2.45378800
H	5.59365000	-1.37183500	0.83952800
H	4.11345700	-2.26903400	1.27786000
H	4.80608000	-2.43692000	-0.35016000
H	3.84013000	0.87359500	-1.70284300
H	4.45824900	-0.74668800	-2.08639100
H	5.45313800	0.37386400	-1.11701600
H	2.83045900	0.71403400	3.10567800
H	2.66803700	-0.94403500	2.48191400
H	4.28383800	-0.29226100	2.86871000
H	4.26877400	2.28712600	0.06752700
H	5.32754900	1.50863800	1.27347300
H	3.93038600	2.47421400	1.80422700
C	-3.54299200	-0.29120700	-1.04362200
O	-4.00123300	0.83108200	-0.83461900
O	-3.96737900	-1.44920500	-1.00554000
H	-1.85070900	2.69440100	-3.08214200
H	-2.84967500	2.40202000	-1.62540700
H	1.05349700	2.76335900	-2.92980400
H	0.80720900	4.12271700	-1.78759100
H	0.95584500	-2.58485000	1.85990100
H	1.34294500	-3.46926200	0.36502500
H	-0.97222100	-3.96901200	-1.59495300
H	-1.90992300	-4.49439800	-0.15457100

Ru(PNP)(CO)HBcat-CO₂ IS

Ru	-0.53163400	-0.27201400	-0.74888500
P	-0.58633400	1.95666900	-1.37712500
P	-0.73533500	-2.24333600	0.44917300
N	-0.98021500	0.60620300	1.20923000
C	-0.82815900	1.94136900	1.41738300
C	-1.12207100	2.52463600	2.65368500
C	-1.55140500	1.72338500	3.70857800
C	-1.70244800	0.35561600	3.49036800
C	-1.43040200	-0.17640900	2.22677300
H	-0.99331400	3.60023700	2.78216000
H	-1.76977200	2.15882100	4.68590300
H	-2.05079000	-0.30471000	4.28583200
C	-0.28395900	2.77025900	0.28239800
C	-1.70412000	-1.63023500	1.92900300
H	0.81469500	2.79021700	0.38360200
H	-0.65445300	3.80628200	0.33390700
H	-1.56312900	-2.25191600	2.82750800
H	-2.76182500	-1.71966800	1.62455400
C	0.68572100	2.75517800	-2.45621700
C	-2.14981100	2.72890200	-1.99740300
C	0.71609500	-3.12194900	1.19295100
C	-1.76582000	-3.64886500	-0.16439300
H	1.68684600	2.47807200	-2.09658600
H	-2.08369400	3.82875500	-2.03350000
H	0.40430800	-3.96772300	1.82690500
H	-2.73291500	-3.25098400	-0.50190600
C	-0.20385900	-1.01489300	-2.40486800
O	-0.00705800	-1.48509400	-3.45151600
H	-2.22747900	-0.39789900	-0.95778600
C	3.78527800	-0.61727700	-0.31541700
C	3.56989800	0.49076800	0.51019800
C	5.05162000	-1.15529800	-0.49759800
C	4.60918000	1.10950600	1.19026800
C	6.11315900	-0.53676100	0.18646300
H	5.20855100	-2.01857800	-1.14636800
C	5.89702600	0.57240800	1.01338600
H	4.42983700	1.97309000	1.83328100
H	7.12520600	-0.93029400	0.06856900
H	6.74252000	1.03084300	1.53105700
B	1.56876900	-0.14762800	-0.36039500
O	2.23146500	0.80155700	0.49911800
O	2.59016300	-1.01918300	-0.85213500
C	-4.85427200	-0.33807400	-0.37360600
O	-4.80340500	-1.42623000	0.05178500
O	-4.96570800	0.75119800	-0.77675500
H	0.58271100	3.85214600	-2.46884000
H	-2.34883900	2.34196200	-3.00898000
H	-2.98212900	2.41501000	-1.35212100
H	1.30119500	-2.40631800	1.78945000
H	1.36163000	-3.48519900	0.37937100
H	-1.92048900	-4.41483400	0.61247200
H	-1.25511800	-4.10711900	-1.02526400
H	0.56748400	2.37157800	-3.48133500

Ru(PNP)(CO)HBcat-CO₂ TS

Ru	-0.60542800	-0.26325300	-0.74031200
P	-0.53703800	1.98085600	-1.34193900
P	-0.80779000	-2.25547100	0.44993400
N	-1.05334500	0.59058600	1.22385200
C	-0.88415300	1.91984800	1.45062500
C	-1.20221000	2.49454500	2.68447000
C	-1.67058500	1.68801600	3.71814400
C	-1.82970900	0.32428300	3.48413600
C	-1.53287500	-0.19877600	2.22269100
H	-1.06368600	3.56686400	2.82816800
H	-1.91169800	2.11686700	4.69296600
H	-2.20534200	-0.33912600	4.26422400
C	-0.28851800	2.75611600	0.34566500
C	-1.80702100	-1.65006300	1.91049800
H	0.80516000	2.77766400	0.49475600
H	-0.65346900	3.79390800	0.39630700
H	-1.68429900	-2.27732800	2.80758200
H	-2.85686500	-1.73928000	1.58056100
C	0.83705500	2.71389700	-2.33812900
C	-2.01637100	2.83330300	-2.04683900
C	0.66146000	-3.08113800	1.21345400
C	-1.79511100	-3.67576600	-0.18852800
H	1.80496100	2.37688600	-1.94047600
H	-1.89853500	3.92884600	-2.02892700
H	0.36490700	-3.91081000	1.87513900
H	-2.75884600	-3.28929000	-0.54812800
C	-0.27001800	-0.99057200	-2.40417200
O	-0.06931800	-1.44967400	-3.45281000
H	-2.35622700	-0.33045700	-0.96979900
C	3.70475300	-0.40557600	-0.47852800
C	3.41366100	0.21551700	0.74002800
C	5.00852700	-0.68620400	-0.86209000
C	4.41190800	0.58491500	1.63022100
C	6.02901300	-0.31636500	0.03170100
H	5.22344200	-1.17105200	-1.81564600
C	5.73742200	0.30606100	1.25191600
H	4.17361800	1.06856900	2.57916800
H	7.06899000	-0.51921500	-0.23303600
H	6.55320000	0.58084000	1.92407300
B	1.46097400	-0.17856900	-0.34049000
O	2.05135700	0.36658800	0.85076600
O	2.53380600	-0.65177500	-1.15001100
C	-4.02192500	-0.28198600	-0.61308500
O	-4.27382400	0.88131400	-0.62777400
O	-4.30004700	-1.43309700	-0.46965900
H	-2.14046600	2.49874600	-3.08881600
H	-2.90846500	2.52474200	-1.48503500
H	0.79383100	3.81481400	-2.33805000
H	0.74763800	2.35192900	-3.37396200
H	-1.25106800	-4.12843100	-1.03162300
H	-1.95628400	-4.43892600	0.58954900
H	1.30696300	-3.46766200	0.40988000
H	1.23471700	-2.33514800	1.78324400

Ru(PNP)(CO)HBcat-CO₂ FS

Ru	-0.58073000	-0.26546600	-0.75349500
P	-0.54212100	1.99500700	-1.35310700
P	-0.78340700	-2.28109400	0.43586600
N	-1.12314300	0.56867100	1.19185200
C	-1.01235600	1.90437500	1.42021700
C	-1.40842900	2.47049300	2.63400500
C	-1.89574800	1.64967700	3.64750100
C	-1.99358700	0.28110600	3.41431500
C	-1.62105500	-0.23611100	2.17043000
H	-1.31826800	3.54763200	2.77862900
H	-2.20061100	2.07290500	4.60678500
H	-2.38501100	-0.39210100	4.17773300
C	-0.39255200	2.76282600	0.34575600
C	-1.84282400	-1.69443200	1.85635000
H	0.69192000	2.82029200	0.54447300
H	-0.79467900	3.78707300	0.38062400
H	-1.73688000	-2.31677600	2.75848000
H	-2.87488600	-1.80278100	1.47470600
C	0.85402600	2.76334200	-2.28643300
C	-2.03703200	2.75309500	-2.11565900
C	0.69322500	-3.06029000	1.22735900
C	-1.72586600	-3.69939000	-0.26026000
H	1.81319800	2.47175600	-1.83463100
H	-2.01347700	3.85160500	-2.03460900
H	0.40051300	-3.90075800	1.87642400
H	-2.68411100	-3.29729200	-0.62327200
C	-0.15521300	-0.98985300	-2.40267400
O	0.10258900	-1.44688400	-3.43701400
H	-2.44147200	-0.33666000	-1.13762400
C	3.66935200	-0.39433500	-0.39011700
C	3.34800700	0.28785800	0.78689600
C	4.98163000	-0.69068600	-0.72882000
C	4.32286800	0.70596200	1.68094300
C	5.97902200	-0.27197800	0.16913400
H	5.22002600	-1.22321600	-1.65068300
C	5.65707000	0.41162000	1.34839600
H	4.06117400	1.23698900	2.59767300
H	7.02534600	-0.48493700	-0.05965800
H	6.45603500	0.72312500	2.02450600
B	1.42957000	-0.16711500	-0.31469300
O	1.98120900	0.44085300	0.85753000
O	2.51365700	-0.67984000	-1.07606600
C	-3.62868000	-0.31616700	-0.69885000
O	-4.03724400	-1.45304600	-0.46043800
O	-4.05719000	0.83097500	-0.62019400
H	-1.15604400	-4.12946400	-1.09781000
H	-1.89933800	-4.47621800	0.50134200
H	1.36916500	-3.42577400	0.43946100
H	1.23001800	-2.30379300	1.81836300
H	-2.06268400	2.46732200	-3.17907300
H	-2.92542400	2.32897500	-1.61821400
H	0.76780500	3.86144300	-2.30118800
H	0.83157700	2.38820600	-3.32100600