

简单的配体改变调控钌配合物催化还原 CO₂ 的活性：硼基配体的对位效应和 Ru—H 键的性质

刘甜¹, 黎军^{1,*}, 刘维佳², 朱育丹^{1,*}, 陆小华¹

¹南京工业大学化工学院、材料化学工程国家重点实验室, 南京 210009

²南京市锅炉压力容器检验研究院, 南京 210019

Simple Ligand Modifications to Modulate the Activity of Ruthenium Catalysts for CO₂ Hydrogenation: *Trans* Influence of Boryl Ligands and Nature of Ru—H Bond

LIU Tian¹, LI Jun^{1,*}, LIU Weijia², ZHU Yudan^{1,*}, LU Xiaohua¹

¹ College of Chemical Engineering, State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University, Nanjing 210009, Jiangsu Province, P. R. China.

² Nanjing Boiler and Pressure Vessel Inspection Institute, Nanjing 210019, Jiangsu Province, P. R. China.

*Corresponding author. Email: lijun@njtech.edu.cn (L.J.). Email: ydzh@njtech.edu.cn; Tel.: +86-25-83172287 (Z.Y.).

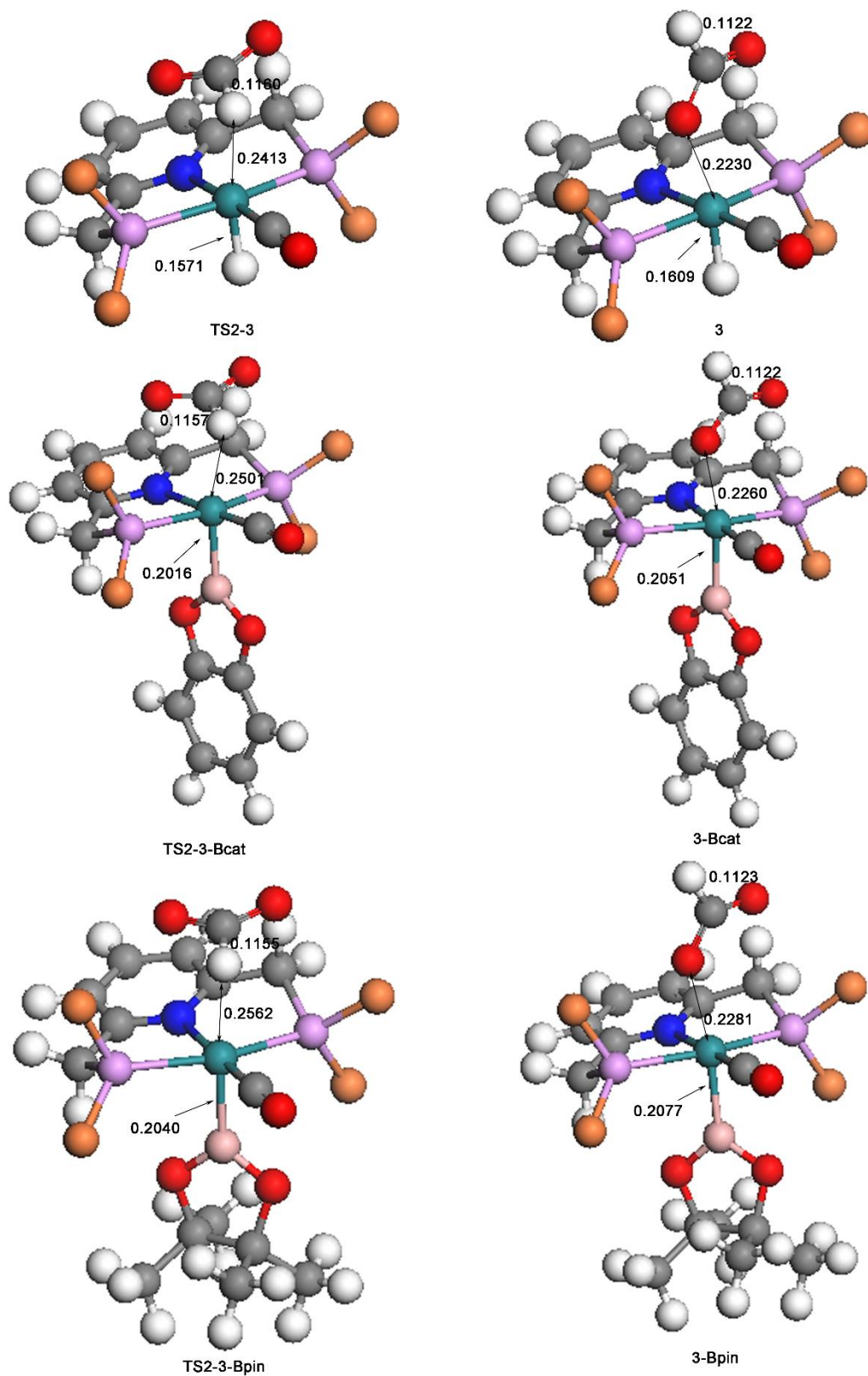


Fig. S1 Optimized transition states and O-bound formate intermediates.

Bond distances are in nanometer (nm). H atoms on methyl group are omitted for clarity. Green balls: Ru; violet: P; red: O; pink: B; blue: N; gray: C; white: H; orange: methyl groups, color online.

Cartesian coordinates:

1

Ru	-0.12477200	-0.85289600	-0.40884800
P	2.14000300	-0.58164500	-0.75297800
P	-2.37622700	-0.46187700	-0.09641300
N	-0.07416800	1.33319300	-0.47998300
C	1.10766400	1.99951000	-0.38241400
C	1.16487600	3.39521400	-0.44252500
C	-0.01310200	4.12810300	-0.57027500
C	-1.22198200	3.44075400	-0.65486100
C	-1.22491200	2.04298800	-0.62595700
H	2.13163700	3.89545900	-0.36871500
H	0.01080600	5.21933100	-0.60442100
H	-2.16591400	3.97688700	-0.76359400
C	2.35177100	1.18065300	-0.14917600
C	-2.50179700	1.26491100	-0.81678300
H	2.49814600	1.08138800	0.94102200
H	3.24082600	1.68464800	-0.56128800
H	-3.37246500	1.83331500	-0.45227600
H	-2.63865200	1.09824900	-1.90046300
H	0.20817700	-0.75894600	1.25035100
H	-0.45902200	-0.83477000	-2.06908500
C	3.42818300	-1.49101000	0.21181600
C	2.86554400	-0.56435000	-2.45813600
C	-3.12193000	-0.30549000	1.59284600
C	-3.69991400	-1.36990000	-1.01459900
H	3.16897300	-1.43518700	1.27854000
H	3.91843300	-0.23744800	-2.46623500
H	-4.13831400	0.12097600	1.56502400
H	-3.41932000	-1.42224100	-2.07632700
C	-0.16343400	-2.69276000	-0.35706200
O	-0.18622800	-3.85806000	-0.32311700
C	0.87414600	0.15708500	3.62278500
O	-0.23977800	0.17868200	3.96922500
O	2.00842900	0.16664200	3.33660100
H	-3.16062200	-1.30841000	2.04625300
H	-2.46356600	0.31443200	2.21823700
H	-4.68496000	-0.88813400	-0.90403900
H	-3.75680700	-2.39728500	-0.62304600
H	3.41715300	-2.54805400	-0.09569900
H	4.43611200	-1.07759000	0.04553700
H	2.79415500	-1.58084900	-2.87523200
H	2.25766100	0.09974700	-3.09008500
TS1-2			
Ru	-0.03826100	-0.82571400	-0.33285300
P	2.23367100	-0.43596200	-0.58445600

P	-2.33591000	-0.56869100	-0.19302800
N	-0.09009000	1.35862400	-0.36542200
C	1.05193400	2.07738900	-0.19023800
C	1.03867600	3.47536100	-0.19743900
C	-0.16908900	4.15141800	-0.35370700
C	-1.33549400	3.40952000	-0.52466500
C	-1.26772800	2.01350900	-0.54658700
H	1.97304600	4.02073700	-0.05812100
H	-0.20069800	5.24289400	-0.34434000
H	-2.29921600	3.90236700	-0.65995400
C	2.32850700	1.31620600	0.06938900
C	-2.49370400	1.18488500	-0.83876700
H	2.44040700	1.19018200	1.16063900
H	3.20428600	1.87498500	-0.29728800
H	-3.40711200	1.69364000	-0.49224400
H	-2.57231500	1.07223000	-1.93518200
H	0.18470800	-0.73448300	1.39831500
H	-0.25646000	-0.81505500	-1.97902800
C	3.51885000	-1.31536100	0.40487300
C	2.99200400	-0.34428800	-2.26996300
C	-3.23604700	-0.55935700	1.42106100
C	-3.49436500	-1.50425500	-1.28792800
H	3.20361900	-1.30342200	1.45781800
H	4.02507100	0.03888400	-2.24049900
H	-2.64899900	0.01375000	2.15221900
H	-3.11113300	-1.47736100	-2.31803900
C	0.01509900	-2.66828800	-0.34052100
O	0.05007400	-3.83179600	-0.35577900
C	0.47932300	-0.07880300	2.91712900
O	-0.59833600	0.27172400	3.28247300
O	1.65939000	-0.20585300	3.04882600
H	-3.29877100	-1.59751300	1.78388700
H	-4.25358200	-0.14782900	1.32135500
H	-3.51757700	-2.55386300	-0.95664300
H	-4.51638700	-1.09392200	-1.25148900
H	2.98894000	-1.35400900	-2.70880700
H	2.36754100	0.30095000	-2.90517500
H	3.57649700	-2.35894500	0.05944100
H	4.50898300	-0.84357800	0.29889600
Ru	-0.03319700	-0.84493400	-0.27145300
P	2.26066900	-0.46491100	-0.50323700
P	-2.34383200	-0.58255400	-0.17018300
N	-0.07686400	1.33566900	-0.38014200
C	1.06678600	2.05738300	-0.22274400
C	1.05353700	3.45461300	-0.26974100

C	-0.15341100	4.12606600	-0.44316200
C	-1.32104300	3.38176400	-0.59200000
C	-1.25456700	1.98647400	-0.57593800
H	1.98751400	4.00301500	-0.14183800
H	-0.18442100	5.21741200	-0.46164800
H	-2.28456800	3.87200000	-0.73649300
C	2.34356800	1.31108700	0.07178000
C	-2.48755800	1.15884100	-0.84441100
H	2.44026000	1.22532200	1.16967800
H	3.22014500	1.85463900	-0.31425800
H	-3.39299300	1.67702400	-0.49187200
H	-2.58430900	1.03569300	-1.93825800
H	0.10723800	-0.75435100	1.57821000
H	-0.19312600	-0.91264800	-1.87798600
C	3.50530600	-1.31218200	0.55625700
C	3.02142200	-0.46152600	-2.18729600
C	-3.21307600	-0.55314100	1.45441500
C	-3.48688700	-1.53954600	-1.26018300
H	3.14515800	-1.23387900	1.59325500
H	4.05730700	-0.08647400	-2.16650000
H	-4.20886300	-0.08822900	1.37497800
H	-3.10285900	-1.52493900	-2.29052600
C	0.01826100	-2.69047000	-0.26014400
O	0.05162800	-3.85182000	-0.28091300
C	0.37303300	0.01215000	2.56877700
O	-0.63109000	0.59927200	2.95303800
O	1.56320200	-0.05501500	2.86842200
H	-3.32420400	-1.59229000	1.80271500
H	-2.56964300	-0.01565300	2.17013100
H	-4.51046500	-1.13287900	-1.23322700
H	-3.50756800	-2.58433700	-0.91425000
H	3.01429100	-1.49012200	-2.57940900
H	2.40978700	0.16199400	-2.85586200
H	3.56484800	-2.37100600	0.26182400
H	4.50048500	-0.84945400	0.45954500
TS2-3			
Ru	-0.05276600	-0.82411700	-0.25053600
P	2.24082400	-0.38385200	-0.54252200
P	-2.37085900	-0.57408600	-0.09274600
N	-0.11769100	1.36367900	-0.30843600
C	1.01793500	2.08822100	-0.12152100
C	0.99137000	3.48661000	-0.11866100
C	-0.22208200	4.15107000	-0.26482600
C	-1.38405200	3.40121900	-0.43406500
C	-1.30213500	2.00768300	-0.46855300
H	1.91991700	4.03865700	0.03044100

H	-0.26406200	5.24207200	-0.24327700
H	-2.35356400	3.88689200	-0.55136300
C	2.29587300	1.34336600	0.15691000
C	-2.53370500	1.17655300	-0.73552600
H	2.35694500	1.16854700	1.25148500
H	3.17707900	1.91911400	-0.16610200
H	-3.43637400	1.68139300	-0.35741800
H	-2.65282800	1.07174000	-1.82909200
H	0.26863300	-1.45992700	2.05464100
H	-0.21734600	-0.83687900	-1.81297900
C	3.56592000	-1.28242500	0.36165600
C	2.88180400	-0.23487300	-2.26988000
C	-3.18105100	-0.58555600	1.56087400
C	-3.53710700	-1.51513000	-1.17252300
H	3.26800100	-1.28522500	1.42247400
H	3.90753700	0.16700400	-2.28342000
H	-4.16753900	-0.09575800	1.53827900
H	-3.18092500	-1.48210000	-2.21264000
C	0.01591200	-2.66514000	-0.35606800
O	0.05695600	-3.81968700	-0.48003300
C	0.58156700	-0.41075800	2.43760200
O	-0.34731800	0.43777100	2.43714200
O	1.78550600	-0.29196900	2.74597600
H	-3.30148600	-1.63374500	1.87748100
H	-2.48279600	-0.08799900	2.25287700
H	-4.55989900	-1.10978200	-1.11521000
H	-3.55000200	-2.56592000	-0.84500500
H	2.87666400	-1.23086000	-2.73873300
H	2.21794700	0.42173900	-2.85123100
H	3.62649200	-2.31263800	-0.02098800
H	4.54100200	-0.78581700	0.23422900
Ru	-0.08792200	-0.77481800	-0.24716300
P	2.18188200	-0.35095500	-0.62974200
P	-2.39315200	-0.51517400	-0.09537900
N	-0.12837300	1.41524600	-0.19670700
C	1.02431300	2.12005600	-0.03006600
C	1.00971800	3.51812000	0.05150000
C	-0.20097600	4.20045100	-0.01133500
C	-1.37593300	3.47141500	-0.18813200
C	-1.31009900	2.08051800	-0.29996500
H	1.95010500	4.05447300	0.18441400
H	-0.23016600	5.28920500	0.06953200
H	-2.34210300	3.97266500	-0.26043800
C	2.31572100	1.35894000	0.10758900
C	-2.54923500	1.27753500	-0.61794600

3

H	2.48107400	1.13949500	1.17914700
H	3.16363300	1.94486800	-0.28130600
H	-3.45040000	1.76560900	-0.21396800
H	-2.66020800	1.24757800	-1.71694600
H	0.51067400	-0.64929300	3.87918700
H	-0.25750000	-0.71662100	-1.84618600
C	3.62029500	-1.26908700	0.06570400
C	2.67637400	-0.12236900	-2.40048800
C	-3.23316100	-0.59818600	1.54676200
C	-3.58084600	-1.37032100	-1.22179500
H	3.46889200	-1.34217000	1.15036200
H	3.70218800	0.27087000	-2.48992900
H	-4.23990800	-0.15172600	1.51901000
H	-3.21319900	-1.29266600	-2.25535200
C	-0.03967400	-2.60806300	-0.40586200
O	-0.01364900	-3.76325000	-0.54285200
C	0.84077300	-0.56809300	2.80987100
O	2.04153600	-0.37257800	2.57376900
O	-0.12902500	-0.69022100	1.98082600
H	-3.30807700	-1.65571000	1.84336800
H	-2.59158900	-0.09462600	2.28277800
H	-3.61735200	-2.43622900	-0.94921900
H	-4.59502900	-0.94573500	-1.15027100
H	2.61393300	-1.09443900	-2.91357500
H	1.96831600	0.56344700	-2.88807700
H	3.64126800	-2.27538500	-0.38054400
1-Bcat			
Ru	-0.54803700	0.12874300	-0.80594700
P	-0.48388600	2.37307600	-0.24730700
P	-0.84988300	-2.16661000	-0.73375900
N	-0.94471000	-0.05876500	1.34210800
C	-0.70966000	0.98478000	2.18067000
C	-0.95525800	0.88873700	3.55337200
C	-1.42169300	-0.31034700	4.08636900
C	-1.65364000	-1.37915100	3.22366100
C	-1.42565800	-1.22323400	1.85333800
H	-0.76049000	1.74987600	4.19409200
H	-1.60472000	-0.40985900	5.15828100
H	-2.02967500	-2.33198800	3.59896400
C	-0.12509500	2.24184600	1.58714100
C	-1.77870700	-2.32437200	0.88493400
H	0.97488100	2.17081800	1.66093700
H	-0.43975600	3.13096500	2.15662600
H	-1.66500400	-3.31478800	1.35361000
H	-2.84128500	-2.20678200	0.60795800
C	0.81914100	3.54478400	-0.83747500

C	-2.00428000	3.42627300	-0.33911100
C	0.56058100	-3.35504400	-0.55807100
C	-1.95205000	-3.04418800	-1.92835400
H	1.80643200	3.07066900	-0.74387200
H	-1.86792400	4.39533800	0.16852300
H	0.21416500	-4.38235900	-0.36006300
H	-2.90049000	-2.49351100	-1.99730600
C	-0.24345500	0.29916700	-2.61661200
O	-0.05944300	0.40894600	-3.76078300
H	-2.24712400	0.18191300	-1.02153800
C	3.49062700	-0.37739500	0.69705700
C	3.80076700	0.02293500	-0.60683300
C	4.47878600	-0.67878800	1.62370900
C	5.11360200	0.13972900	-1.04145800
C	5.81329100	-0.56364500	1.19437100
H	4.22569000	-0.99122000	2.63849800
C	6.12371300	-0.16264100	-0.11088100
H	5.34324700	0.45168900	-2.06162700
H	6.62074600	-0.79235200	1.89349800
H	7.16993800	-0.08337500	-0.41444000
B	1.54449300	-0.00890600	-0.41453900
O	2.63820000	0.25469500	-1.29562100
O	2.12526900	-0.40424700	0.84356700
C	-4.85569600	0.06867600	-0.37609300
O	-4.90241900	1.21542000	-0.16546500
O	-4.86950600	-1.08544200	-0.56427500
H	-2.23919600	3.60080700	-1.40069900
H	-2.84788000	2.87698300	0.10182200
H	0.79820200	4.49343300	-0.27743400
H	0.64162400	3.75399300	-1.90375000
H	-1.47065300	-3.03855500	-2.91837000
H	-2.13900300	-4.08663400	-1.62419500
H	1.14725200	-3.34247300	-1.48996000
H	1.21298600	-3.01211700	0.25826700
TS1-2-Bcat			
Ru	0.64975600	-0.43126700	-0.53998200
P	0.52167800	-2.10401100	1.06919200
P	0.92009400	1.62873500	-1.59839400
N	0.93949600	0.80575800	1.24083900
C	0.64224500	0.31930200	2.47472800
C	0.83831000	1.08637000	3.62634900
C	1.32072600	2.38775800	3.50975400
C	1.61769400	2.88272800	2.24213000
C	1.43659900	2.06606400	1.12226100
H	0.59598700	0.66251200	4.60173700
H	1.46814400	3.00745500	4.39668600

H	2.01061700	3.89176200	2.11153200
C	0.05163800	-1.06620000	2.55758000
C	1.85388600	2.52709300	-0.25059900
H	-1.04791400	-0.97348200	2.51181400
H	0.30522700	-1.54671600	3.51577800
H	1.79928600	3.62357700	-0.33761800
H	2.90339900	2.21933700	-0.40665300
C	-0.76640400	-3.42738700	1.05208300
C	2.02426200	-3.03322500	1.61287500
C	-0.50955400	2.73590300	-1.99033000
C	2.01064900	1.82781600	-3.07222100
H	-1.74457400	-2.98630000	0.81481200
H	1.82903800	-3.61089000	2.53078700
H	-0.17256700	3.74166000	-2.28883200
H	2.96604700	1.32623300	-2.86508400
C	0.43565300	-1.49002900	-2.03921700
O	0.30973400	-2.15896700	-2.98069900
H	2.40935700	-0.51674800	-0.61590600
C	-3.45550500	0.59488800	0.26751300
C	-3.67140500	-0.43444800	-0.65377400
C	-4.50671400	1.28419100	0.85485900
C	-4.94970500	-0.82111300	-1.03053500
C	-5.80717500	0.90077700	0.48105300
H	-4.32663000	2.08641800	1.57262400
C	-6.02350800	-0.12994000	-0.44201200
H	-5.10605200	-1.62482400	-1.75174400
H	-6.66296300	1.41844700	0.91972100
H	-7.04574600	-0.40350700	-0.71214200
B	-1.43840200	-0.20046200	-0.39218600
O	-2.46026200	-0.93478700	-1.06281800
O	-2.10184600	0.75762300	0.44753400
C	4.05552900	-0.65207500	-0.71159200
O	4.26607100	-1.79384900	-0.45257900
O	4.40122800	0.45778300	-0.99801000
H	2.32765200	-3.71406800	0.80372900
H	2.85286500	-2.32909300	1.76773400
H	-0.81152800	-3.96071300	2.01483000
H	-0.51410700	-4.14471300	0.25591300
H	1.52868200	1.34498800	-3.93600500
H	2.18544600	2.89074300	-3.30279400
H	-1.08954300	2.28909900	-2.81283600
H	-1.16316000	2.80245600	-1.10866700
2-Beat			
Ru	-0.58053600	-0.26517500	-0.75353400
P	-0.54252900	1.99543000	-1.35235300
P	-0.78267200	-2.28131900	0.43499200

N	-1.12352800	0.56794100	1.19201900
C	-1.01352000	1.90369200	1.42073300
C	-1.41064200	2.46935100	2.63436700
C	-1.89822200	1.64809000	3.64739800
C	-1.99514500	0.27952200	3.41391100
C	-1.62152600	-0.23726900	2.17015400
H	-1.32113400	3.54650600	2.77927500
H	-2.20393900	2.07100800	4.60654600
H	-2.38665000	-0.39406300	4.17695200
C	-0.39343300	2.76262200	0.34684000
C	-1.84213200	-1.69576900	1.85587800
H	0.69099500	2.81996100	0.54584900
H	-0.79560000	3.78683800	0.38206000
H	-1.73501700	-2.31811500	2.75787600
H	-2.87436000	-1.80509500	1.47502600
C	0.85351200	2.76443200	-2.28529000
C	-2.03747700	2.75362500	-2.11479100
C	0.69429900	-3.06023700	1.22621700
C	-1.72434000	-3.69987100	-0.26168700
H	1.81270600	2.47351600	-1.83310700
H	-2.01410300	3.85207800	-2.03287900
H	0.40190600	-3.90080900	1.87530200
H	-2.68281700	-3.29824600	-0.62457000
C	-0.15475800	-0.98866800	-2.40307700
O	0.10313800	-1.44513500	-3.43763900
H	-2.44085900	-0.33663400	-1.13807900
C	3.34818300	0.28840300	0.78720100
C	3.66956900	-0.39374300	-0.38982700
C	4.32299900	0.70644900	1.68132200
C	4.98185800	-0.69017200	-0.72843300
C	5.65720700	0.41201800	1.34887100
H	4.06127100	1.23748500	2.59803700
C	5.97920100	-0.27162500	0.16964900
H	5.22029000	-1.22271200	-1.65028100
H	6.45614100	0.72346400	2.02504700
H	7.02552500	-0.48470500	-0.05903200
B	1.42977500	-0.16646900	-0.31451500
O	2.51391400	-0.67918000	-1.07585800
O	1.98137600	0.44145600	0.85773100
C	-3.62828200	-0.31691000	-0.69928100
O	-4.05717200	0.83004200	-0.62020700
O	-4.03629500	-1.45406000	-0.46148400
H	-2.06282600	2.46869900	-3.17843700
H	-2.92589400	2.32901600	-1.61782700
H	0.76662400	3.86247500	-2.30032300
H	0.83161200	2.38903000	-3.31978000

H	-1.15422400	-4.12915600	-1.09944900
H	-1.89722900	-4.47717300	0.49955400
H	1.37017200	-3.42552600	0.43817300
H	1.23104800	-2.30366600	1.81716800
TS2-3-Bcat			
Ru	0.58987700	0.27368600	-0.73949800
P	0.50031200	-1.96751800	-1.43801000
P	0.83487700	2.22401400	0.58268400
N	1.15438800	-0.66061400	1.15337800
C	1.01625400	-2.00092100	1.32580100
C	1.43863400	-2.63174400	2.49699900
C	1.98964100	-1.86992800	3.52478200
C	2.12593900	-0.49754600	3.34520400
C	1.72373800	0.08448400	2.13907600
H	1.32368300	-3.71149600	2.59795200
H	2.31715500	-2.34382400	4.45247900
H	2.57344300	0.12879100	4.11745200
C	0.35218200	-2.79742800	0.22991500
C	1.99238800	1.54015400	1.86932100
H	-0.73046800	-2.83784900	0.44124800
H	0.72842500	-3.83192100	0.21487000
H	2.00358700	2.12816400	2.79989300
H	2.98417300	1.61523200	1.37455500
C	-0.92734400	-2.65987200	-2.38275400
C	1.97472400	-2.70803300	-2.25368400
C	-0.62556000	2.85270200	1.52539600
C	1.65847700	3.74367600	-0.04210600
H	-1.87368700	-2.36028900	-1.90927800
H	1.94786300	-3.80829200	-2.20767100
H	-0.32390400	3.63337400	2.24145300
H	2.59894700	3.41868800	-0.51403000
C	0.13614400	1.09263700	-2.33887400
O	-0.14582500	1.60832800	-3.33766200
H	2.76279900	0.58543700	-1.93734100
C	-3.28688200	-0.27569500	0.79885500
C	-3.60740100	0.45969700	-0.34587800
C	-4.26057900	-0.72192600	1.68008700
C	-4.91788400	0.78326000	-0.66485300
C	-5.59324500	-0.40016400	1.36751100
H	-3.99942900	-1.29413800	2.57175200
C	-5.91441000	0.33622400	0.22030700
H	-5.15563700	1.35698100	-1.56174000
H	-6.39175100	-0.73225900	2.03419700
H	-6.95967200	0.56897900	0.00676800
B	-1.37445400	0.20326600	-0.29299400
O	-2.45201900	0.76272200	-1.02636500

O	-1.92088700	-0.44684900	0.85537100
C	3.42926400	0.50664400	-0.99535300
O	3.58000400	-0.65959800	-0.55659200
O	3.85271800	1.59825400	-0.55338200
H	1.98410100	-2.38581600	-3.30683800
H	2.86010600	-2.28939600	-1.74620500
H	-0.87292600	-3.75864400	-2.43776500
H	-0.90598000	-2.24843400	-3.40341500
H	1.00217900	4.22563800	-0.78272900
H	1.85957400	4.44683100	0.78157400
H	-1.35783400	3.27189200	0.81872800
H	-1.10203000	2.02050400	2.06376400
3-Bcat			
Ru	-0.65152100	-0.25006200	-0.71124100
P	-0.48086700	1.95669600	-1.48627100
P	-0.85646000	-2.12962000	0.69239100
N	-1.14960500	0.77423500	1.16103500
C	-0.97421200	2.11732500	1.27921300
C	-1.35542000	2.80266300	2.43529600
C	-1.89178900	2.09195500	3.50723100
C	-2.04814600	0.71454700	3.38975000
C	-1.68702900	0.07487300	2.19800200
H	-1.21111300	3.88222900	2.49303400
H	-2.18395400	2.60773700	4.42448200
H	-2.47044200	0.12554600	4.20470800
C	-0.28998500	2.84523400	0.14864800
C	-1.94569100	-1.39604100	2.01350600
H	0.79407600	2.82971600	0.35361100
H	-0.61274600	3.89694000	0.10123300
H	-1.89883300	-1.93307300	2.97371600
H	-2.95427900	-1.51522900	1.57080900
C	0.94528500	2.59481400	-2.47089900
C	-1.93386600	2.75364800	-2.29925500
C	0.63974100	-2.72595100	1.60553600
C	-1.67938000	-3.70382400	0.20871000
H	1.88783700	2.27702900	-2.00223100
H	-1.83477300	3.85063100	-2.31277000
H	0.36550300	-3.48122400	2.35924800
H	-2.65972100	-3.44463700	-0.21251600
C	-0.25431200	-1.14046100	-2.27884300
O	-0.01461100	-1.70051500	-3.26670800
H	-4.79979100	-0.29178300	-1.47247400
C	3.34162000	0.35025500	0.63943600
C	3.57187700	-0.67211200	-0.28635100
C	4.37163300	0.91733200	1.37583200
C	4.84456000	-1.17363100	-0.51854800

C	5.66619900	0.41676000	1.14904100
H	4.18071600	1.71381100	2.09714500
C	5.89710200	-0.60663900	0.22153700
H	5.01271800	-1.96998500	-1.24518400
H	6.50569500	0.83591500	1.70778500
H	6.91436500	-0.97298400	0.06781600
B	1.35680900	-0.22378200	-0.29412900
O	2.38186900	-1.03580500	-0.86296900
O	1.99831100	0.64545200	0.65544900
C	-3.88071500	-0.66656800	-0.94874000
O	-3.98677100	-1.65652000	-0.21023600
O	-2.83803600	0.03075600	-1.21040500
H	-2.00540900	2.37757800	-3.33121400
H	-2.84148200	2.43733500	-1.76860900
H	0.92307600	3.69351600	-2.54825800
H	0.89685600	2.16223000	-3.48190300
H	-1.05793400	-4.20135000	-0.55170000
H	-1.79504500	-4.37255200	1.07667300
H	1.34768300	-3.16592600	0.88754600
H	1.13608000	-1.87763900	2.09959100
1-Bpin			
Ru	0.50849800	0.17588900	-0.73273400
P	0.84627600	2.26111600	0.21163800
P	0.48131300	-2.10929200	-1.10179900
N	1.07882100	-0.48965500	1.27625400
C	1.62479100	0.38808800	2.16113200
C	1.97476800	-0.00383800	3.45643100
C	1.80519200	-1.33168300	3.84371700
C	1.28188900	-2.23415200	2.92102000
C	0.91334500	-1.78755500	1.64807500
H	2.39913700	0.73110700	4.14209800
H	2.08349300	-1.65909700	4.84767700
H	1.13832500	-3.28374000	3.18169200
C	1.91748300	1.78515100	1.67289600
C	0.27469600	-2.72228100	0.65451500
H	2.94746900	1.79396100	1.27440900
H	1.87343500	2.51195000	2.49973500
H	0.62007000	-3.75775600	0.80338700
H	-0.81583500	-2.68558000	0.81853000
H	2.19170400	0.22007600	-1.06780100
C	1.86494400	3.54936000	-0.63699900
C	-0.49733100	3.28965700	0.97088500
C	1.98647400	-2.98477200	-1.73229800
C	-0.87174000	-3.00404900	-1.99137700
H	2.78691600	3.07901600	-1.00554700
H	-0.09406500	4.19641400	1.45067000

H	1.89740800	-4.08023200	-1.64495500
H	-1.83549800	-2.66878900	-1.58359000
C	0.04962700	0.73322000	-2.42653600
O	-0.24208100	1.08297700	-3.49965600
C	4.85852200	0.24305100	-0.87849500
O	4.93726500	-0.85238800	-1.27224300
O	4.84898500	1.33992000	-0.47207400
H	2.12607700	-2.71339900	-2.79040500
H	2.86623900	-2.62569100	-1.18032900
H	-0.77879600	-4.09708100	-1.88587200
H	-0.82762100	-2.74052900	-3.05938600
H	-1.21806500	3.56704000	0.18780300
H	-1.03298800	2.68414200	1.71650200
H	1.29664700	3.93247300	-1.49861300
H	2.10865500	4.38744400	0.03577600
B	-1.59459300	0.14680700	-0.23221800
O	-2.53506000	1.12028800	-0.60047100
O	-2.26693000	-0.85013800	0.51558700
C	-3.87789500	0.65871800	-0.30412700
C	-3.62198300	-0.41515300	0.81502900
C	-3.60570100	0.17397500	2.23275000
H	-4.61309700	0.46452300	2.57057100
H	-3.21322600	-0.58230600	2.92984200
H	-2.95164600	1.05664000	2.28936700
C	-4.54657300	-1.63142800	0.77680800
H	-4.27119500	-2.33341100	1.57970600
H	-5.59693200	-1.33599200	0.93455700
H	-4.47714600	-2.16775600	-0.17903600
C	-4.72308000	1.85845200	0.12350300
H	-4.81200300	2.56320400	-0.71760700
H	-5.74060700	1.54692500	0.41237900
H	-4.27044800	2.39736500	0.96645500
C	-4.44728900	0.06421800	-1.60074400
H	-5.49712300	-0.24969300	-1.48623700
H	-4.39772500	0.82750600	-2.39173400
H	-3.85634400	-0.80078500	-1.93630300

TS1-2-Bpin

Ru	0.53193900	0.22417300	-0.75403500
P	0.83415400	2.28532000	0.27918800
P	0.49946300	-2.05217400	-1.23089800
N	1.20897400	-0.51031800	1.19332600
C	1.77644300	0.34258900	2.08902200
C	2.22406500	-0.10272900	3.33571300
C	2.13061600	-1.45498300	3.65746000
C	1.58017700	-2.32804100	2.72314100
C	1.11310100	-1.83083100	1.50245100

H	2.66576600	0.61095600	4.03256900
H	2.48867000	-1.82371400	4.62094800
H	1.49469600	-3.39478000	2.93428300
C	1.98347700	1.77882400	1.66945900
C	0.44070400	-2.74215700	0.50822500
H	2.99760700	1.87036600	1.24245700
H	1.93138800	2.45428600	2.53830500
H	0.83810800	-3.76670900	0.57944400
H	-0.63543300	-2.76412600	0.75036400
H	2.25000800	0.29412700	-1.15858100
C	1.75862900	3.64186100	-0.56402400
C	-0.51227200	3.21468700	1.14636800
C	1.94822500	-2.87865400	-2.02774300
C	-0.91955400	-2.91060100	-2.04913100
H	2.66946900	3.21675100	-1.00778600
H	-0.11289200	4.10430200	1.65972800
H	1.87715900	-3.97618900	-1.95445800
H	-1.84961600	-2.60989100	-1.54803500
C	-0.01760200	0.84948100	-2.39850100
O	-0.36705400	1.24218800	-3.43724300
B	-1.52389300	0.13969500	-0.18216300
O	-2.14219000	-0.91810200	0.52011500
C	-3.49124100	-0.53267900	0.90610100
C	-3.81095300	0.62194400	-0.11386700
O	-2.48756500	1.12278700	-0.43843900
C	-4.43739200	0.12408400	-1.42420600
C	-4.64633500	1.77128700	0.44831800
C	-4.39794100	-1.75874100	0.80656800
C	-3.42440900	-0.05928700	2.36479400
H	-5.64062100	1.41825700	0.76782400
H	-4.15680800	2.25511500	1.30403200
H	-4.79403200	2.53518400	-0.33060100
H	-3.85423100	-0.70150700	-1.85822400
H	-4.43876900	0.94904700	-2.15220200
H	-5.47568400	-0.21530500	-1.28226800
H	-2.99749400	-0.86404500	2.98284100
H	-2.77762700	0.82456300	2.46822000
H	-4.42032700	0.18939100	2.76374300
H	-4.36380900	-2.21392800	-0.19225700
H	-5.44432300	-1.49555200	1.03211600
H	-4.07829000	-2.51867100	1.53683500
C	3.98642200	0.28169700	-0.92436100
O	4.26767600	1.43051600	-1.05731800
O	4.21977500	-0.86409900	-0.70642000
H	-0.96290100	-2.59504200	-3.10296400
H	-0.80660400	-4.00596100	-2.00717700

H	1.12408700	4.04762400	-1.36702500
H	2.01722900	4.45235300	0.13630300
H	-1.27131500	3.51335800	0.40931200
H	-0.99772100	2.55245500	1.87776900
H	1.97043900	-2.58708600	-3.08967300
H	2.87083800	-2.51550800	-1.55537600
2-Bpin			
Ru	-0.49753500	-0.19484600	-0.77111000
P	-0.80115200	-2.31808800	0.17876600
P	-0.48974000	2.11809000	-1.16110300
N	-1.28435700	0.44542900	1.16382600
C	-1.88266300	-0.45646000	1.99075700
C	-2.42392400	-0.06509600	3.21855400
C	-2.39634300	1.27723500	3.58604600
C	-1.81386800	2.19884700	2.72024100
C	-1.25098600	1.75767000	1.51997300
H	-2.89221300	-0.81335800	3.85899700
H	-2.83276200	1.60303300	4.53253400
H	-1.78112000	3.26006100	2.96949400
C	-2.03278900	-1.88056200	1.51471600
C	-0.54475000	2.72653100	0.60617700
H	-3.01359400	-1.96366200	1.01092400
H	-2.01675100	-2.58556400	2.36049400
H	-0.97818400	3.73484200	0.69303600
H	0.51345900	2.77222700	0.91452700
H	-2.33459800	-0.25222900	-1.36468400
C	-1.64753500	-3.63434400	-0.79105000
C	0.53657200	-3.22870800	1.07123800
C	-1.93437500	2.89119100	-2.00187900
C	0.95070900	3.03265700	-1.86750500
H	-2.55503500	-3.18064400	-1.21893100
H	0.14057400	-4.15243800	1.52236200
H	-1.95769800	3.97955400	-1.83142000
H	1.86108000	2.73291600	-1.33099000
C	0.14098900	-0.75626000	-2.41078900
O	0.54541500	-1.10852900	-3.44115000
C	-3.54418900	-0.28975600	-1.04246300
O	-4.00157600	0.83294300	-0.83410900
O	-3.96933400	-1.44743900	-1.00415200
H	-1.84982700	2.69434600	-3.08235500
H	-2.84914000	2.40266400	-1.62570800
H	0.80855400	4.12223800	-1.78692900
H	1.05408400	2.76324000	-2.92973400
H	1.34214200	-3.46937400	0.36348900
H	0.95525400	-2.58601000	1.85905100
H	-0.97482900	-3.96878300	-1.59550700

H	-1.91189900	-4.49384000	-0.15460100
B	1.48929800	-0.12034700	-0.15388900
O	2.47105900	-1.06903700	-0.44358200
O	2.05287200	0.90627700	0.62446200
C	3.77503200	-0.56101500	-0.04955200
C	3.39919300	0.52225800	1.03056300
C	3.29565100	-0.04258700	2.45328000
H	4.28420400	-0.29362400	2.86791500
H	2.83062000	0.71221000	3.10554600
H	2.66848900	-0.94565400	2.48117100
C	4.28322400	1.76816300	1.03556700
H	3.93056000	2.47298200	1.80466000
H	5.32750400	1.50770600	1.27274000
H	4.26806600	2.28669300	0.06770900
C	4.61758200	-1.72590200	0.46695100
H	4.80586100	-2.43723400	-0.35175700
H	5.59330400	-1.37273300	0.83853700
H	4.11300300	-2.27004100	1.27625000
C	4.42439100	0.02981700	-1.30820400
H	5.45284100	0.37402200	-1.11735600
H	4.45813200	-0.74623000	-2.08726200
H	3.83981900	0.87380900	-1.70311500

TS2-3-Bpin

Ru	0.48779300	0.18437800	-0.75742900
P	0.82681000	2.28594200	0.27492400
P	0.47972000	-2.12984500	-1.19471200
N	1.32592200	-0.50175200	1.13913900
C	1.99054900	0.37326400	1.94379900
C	2.56965400	-0.04733500	3.14519700
C	2.51746500	-1.39132600	3.49978000
C	1.87864800	-2.28871700	2.64703600
C	1.28138900	-1.81804900	1.47605500
H	3.08851200	0.67965100	3.77070900
H	2.98212700	-1.73976200	4.42463700
H	1.83301500	-3.35237100	2.88346000
C	2.17009500	1.78899100	1.46647200
C	0.54222400	-2.76303900	0.56281200
H	3.08891600	1.82121500	0.84166400
H	2.28200600	2.48731000	2.31030600
H	0.96197600	-3.77870300	0.62887000
H	-0.51325600	-2.79950500	0.88042700
H	2.57953600	0.34533700	-2.22770500
C	1.51697700	3.70790900	-0.66456400
C	-0.46886900	3.06245000	1.34158000
C	1.93474800	-2.86082200	-2.05249100
C	-0.95872300	-3.03701700	-1.91339100

H	2.39435200	3.32660100	-1.21020000
H	-0.06610900	3.96139600	1.83467600
H	1.99429400	-3.94733400	-1.88034800
H	-1.87088200	-2.74562100	-1.37534200
C	-0.18076800	0.79896300	-2.36761500
O	-0.60930000	1.18459600	-3.37520100
C	3.34488500	0.44919700	-1.36894700
O	3.62267000	-0.62008300	-0.77410500
O	3.73767000	1.61822300	-1.14891800
H	1.83328500	-2.66688100	-3.13197500
H	2.82560100	-2.32773100	-1.67542000
H	-0.81480900	-4.12708700	-1.84377100
H	-1.06039000	-2.75704000	-2.97302900
H	-1.33569300	3.32905300	0.72143700
H	-0.79923800	2.34482800	2.10675300
H	0.75091600	4.07124000	-1.36666300
H	1.80855300	4.52479900	0.01455200
B	-1.45485600	0.13180800	-0.13809900
O	-2.41174000	1.12016600	-0.36313600
O	-2.03053400	-0.92720700	0.57997600
C	-3.72450900	0.61800700	0.01067600
C	-3.36642000	-0.54013500	1.01815700
C	-3.24285900	-0.07012400	2.47303100
H	-4.22284700	0.18323600	2.90591800
H	-2.79963100	-0.87795700	3.07497000
H	-2.58920500	0.81039900	2.55531700
C	-4.27635900	-1.76502200	0.94859500
H	-3.92990300	-2.52744400	1.66346400
H	-5.31176500	-1.49951800	1.21660100
H	-4.28383200	-2.21630600	-0.05242500
C	-4.53532400	1.76683100	0.60722000
H	-4.71388800	2.53159600	-0.16403100
H	-5.51564000	1.41193600	0.96432200
H	-4.01325800	2.24836400	1.44469700
C	-4.39778100	0.12371900	-1.27653300
H	-5.42990500	-0.21445300	-1.09526400
H	-4.42708100	0.95028900	-2.00187100
H	-3.83404400	-0.70245300	-1.73465100
3-Bpin			
Ru	-0.56863000	-0.16045200	-0.74195500
P	-0.95704300	-2.19035200	0.38167000
P	-0.37635600	2.12674200	-1.23206700
N	-1.29331600	0.64333900	1.16704600
C	-1.95374700	-0.16971700	2.03738200
C	-2.44398700	0.32181500	3.25339300
C	-2.29558000	1.67056600	3.56141000

C	-1.64586700	2.50203000	2.65105800
C	-1.13946200	1.96124300	1.46614500
H	-2.96080400	-0.35630900	3.93350700
H	-2.68610400	2.07213000	4.49906300
H	-1.51246700	3.56486400	2.85685100
C	-2.20887900	-1.59293300	1.62672000
C	-0.35639500	2.82059900	0.50518300
H	-3.14672000	-1.61440400	1.03310800
H	-2.31245000	-2.25117900	2.50338600
H	-0.69100300	3.86885300	0.55016700
H	0.70452700	2.77833200	0.80210800
H	-4.61730700	-0.04744500	-2.03641800
C	-1.75429300	-3.64050300	-0.42725500
C	0.35421500	-2.98876000	1.41581400
C	-1.77616200	2.99353400	-2.06766600
C	1.10403700	2.91438900	-2.00483200
H	-2.66457400	-3.27847400	-0.92441400
H	-0.06416600	-3.84065100	1.97543600
H	-1.68621500	4.08657000	-1.96321200
H	2.00221900	2.55357600	-1.48594800
C	0.03678200	-0.85573100	-2.33712800
O	0.42207200	-1.28858000	-3.34484100
C	-3.79994600	-0.49815600	-1.41144400
O	-2.70904500	0.16928000	-1.45946800
O	-4.05488800	-1.53404300	-0.77751000
H	-1.76941500	2.72252200	-3.13422800
H	-2.71707700	2.62444700	-1.64018300
H	1.05293400	4.01343500	-1.94673000
H	1.15445700	2.61223000	-3.06213600
H	1.17233900	-3.32776700	0.76571000
H	0.76352400	-2.25220800	2.12260500
H	-1.05298900	-4.05569000	-1.16730700
H	-2.00579900	-4.41838800	0.31154400
B	1.41941800	-0.19891300	-0.14268400
O	2.33629100	-1.23313500	-0.37127400
O	2.08240600	0.84230300	0.54388000
C	3.67901500	-0.79173200	-0.04614200
C	3.41072500	0.40443900	0.94326100
C	3.32261300	-0.02375600	2.41433400
H	4.30603800	-0.30966700	2.81892800
H	2.93754900	0.81822900	3.00986900
H	2.63453200	-0.87167300	2.54366900
C	4.37399000	1.58399900	0.81326400
H	4.08441200	2.38021800	1.51690400
H	5.40471900	1.27925700	1.05726400
H	4.37058500	2.00877400	-0.19941800

C	4.44976000	-1.96785200	0.55233900
H	4.56016200	-2.75873000	-0.20541100
H	5.45984900	-1.65976000	0.86822900
H	3.93116800	-2.40142500	1.41780600
C	4.34262300	-0.35924200	-1.36137900
H	5.39394300	-0.06556000	-1.21450200
H	4.31367600	-1.20230300	-2.06771300
H	3.80594600	0.48144200	-1.82548300