

Electronic Supplementary Information

Ligands Effect on Chemoselective Control in One Catalyst Multiple Steps: Ru Catalyzed *anti*-Markovnikov Reductive Hydration of Terminal Alkynes

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1. The mechanism and energy profiles for catalyst D to catalyze hydration.

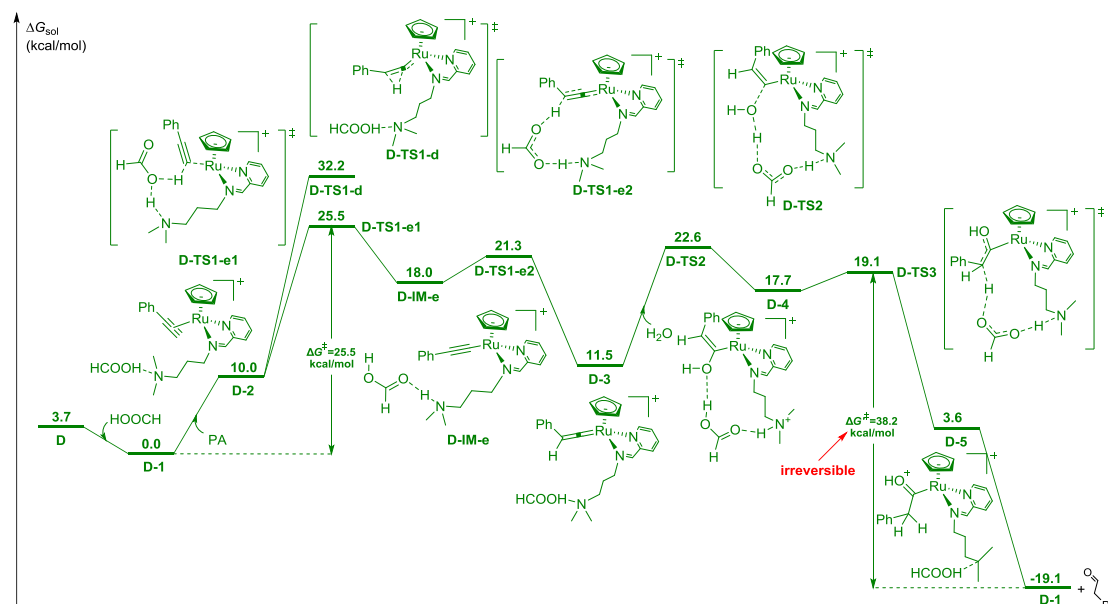


Figure S1. The hydration reaction for catalyst **D**. The free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)/B3LYP-D3/BSI level of theory. Ph = phenyl, PA = phenylacetylene.

The Gibbs free energy barrier of direct 1,2-H shift transition state **D-TS1-d** for catalyst **D** is 32.2kcal/mol, and the Gibbs free energy barrier of formate ion assist deprotonation transition state and protonation transition state is 25.5kcal/mol (**D-TS1-e1**) and 21.3kcal/mol (**D-TS1-e2**). Although the coordinate exchange process is endothermic by 10.0 kcal/mol here, it's mainly caused by formate ion on the amino group in the ligand (without the formic acid, the ligand exchange is endothermic by only 3.8 kcal/mol), the formate ion will also assist protonation and reduce the Gibbs free energy barrier so that the reaction can proceed. For the hydration part, catalyst **D** is almost the same as catalyst **C**, except the position of H₂O for transition state **D-TS2** and **D-TS3**, it's more suitable in this structure.

2. The mechanism and energy profiles for catalyst **D** to catalyze hydrogenation.

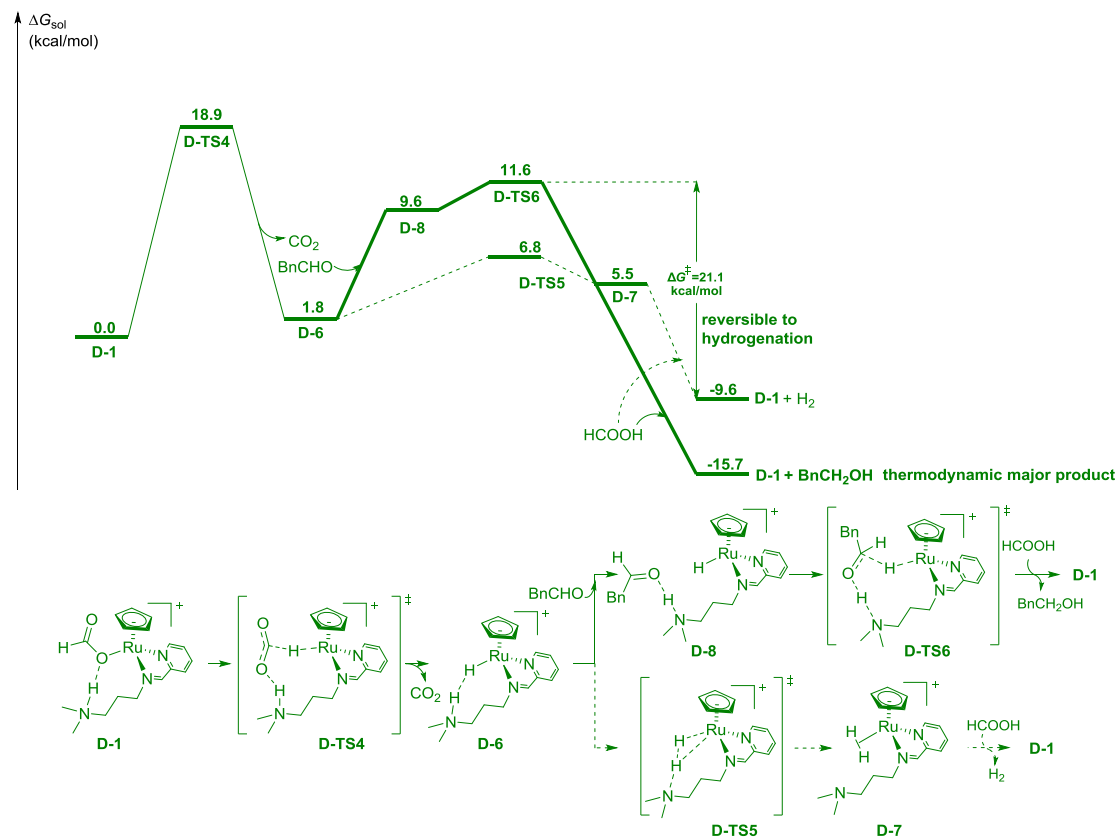


Figure S2. the hydrogenation reaction for catalyst **B** and **C**. The Gibbs energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)/B3LYP-D3/ BSI level of theory. Bn = benzyl, Py = 2-pyridyl. Decarboxylation and hydrogenation: solid lines; Side reaction: dashed lines.

The hydride formation, hydrogenation and side reaction mechanism and Gibbs free energy profiles for catalyst **D** are essentially in agreement with catalyst **C**. The Gibbs free energy barrier of decarboxylation process via transition state **D-TS4** is 18.9 kcal/mol relative to **D-1**, it's 3.3 kcal/mol higher than transition state **C-TS4** may due to structural differences. Hydrogen formation process is reversible to catalyze hydrogenation reaction which the energy barrier is 21.1 kcal/mol.

3. Comparison of the hydration reactions for catalysts A, B, and C

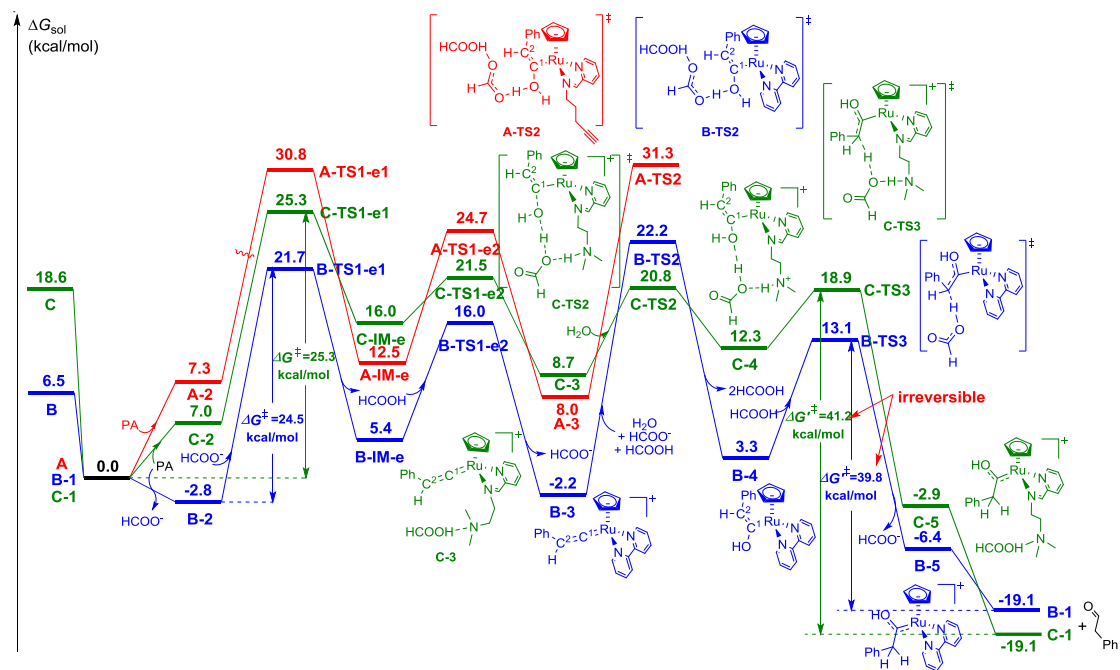


Figure S3. Comparison of the hydration reactions for catalysts A, B, and C. Gibbs free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/BSI level of theory. Ph = phenyl, PA = phenylacetylene.

4. Comparison of pyridine based systems and phosphine ligand systems in hydration.

The reason of higher activity for the current ligand system than previously reported phosphine ligand systems (Dalton Trans., 2014, 43, 11277) can be explained from the following two aspects.

Steric effect: It can be seen roughly from the structure of **C-3** (pyridine based systems) and **P-3** (phosphine ligand systems) given in Figure S3 below. The large steric hindrance groups (phenyl) in phosphine ligand may prevent water to associate the reaction site (the position of HOMO+1 for **C-3**). This may cause the higher activation energy of **P-3** to hydration.

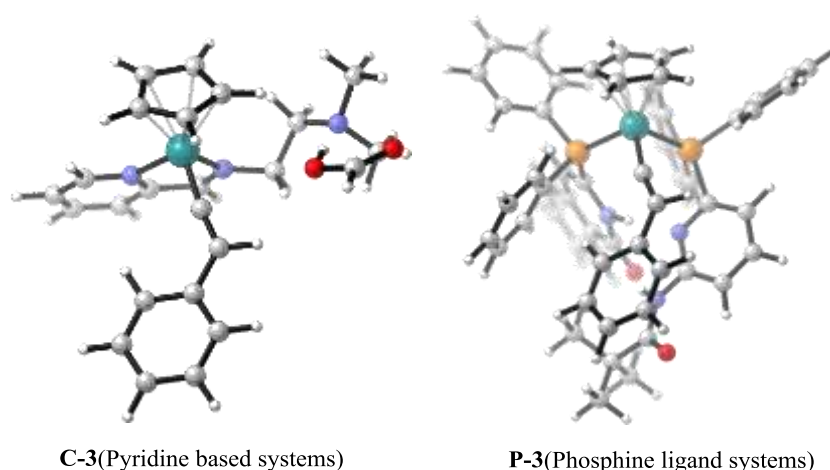
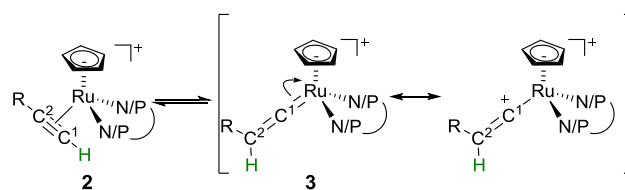


Figure S4. Calculated structures for complexes in pyridine based systems and phosphine ligand systems

Electronic effect: NBO results (shown in Table S1) show the NBO charge of both phosphorous atoms are 1.3 in phosphine ligand systems, this positively charged ligand lead to more negative charge of the ruthenium (-0.836) for complex **P-3**. This also cause it's hard for the charge on C^1 transfer to Ru and water molecule approaches the C^1 , although the positive charge for C^1 in **P-3** is a little higher than that in **B-3**.

Table S1. NBO Charges of Complexes **3** in pyridine based systems and phosphine ligand systems



resonance structure of Fischer type carbene

complex	B-3	P-3
Ru	-0.120	-0.836
C ¹	0.317	0.335
C ²	-0.402	-0.407
N/P	-0.348 and -0.341	1.327 and 1.364

5. Detail mechanisms of complex **5** release aldehyde process.

This process have more than two possible mechanisms, the bifunctional group on **C** will even cause more possibilities in proton transfer, and it is considered to be easy to carry out. For one possible mechanism given in Figure S5 for catalyst **B**, the activation energy is 24.0 kcal/mol.

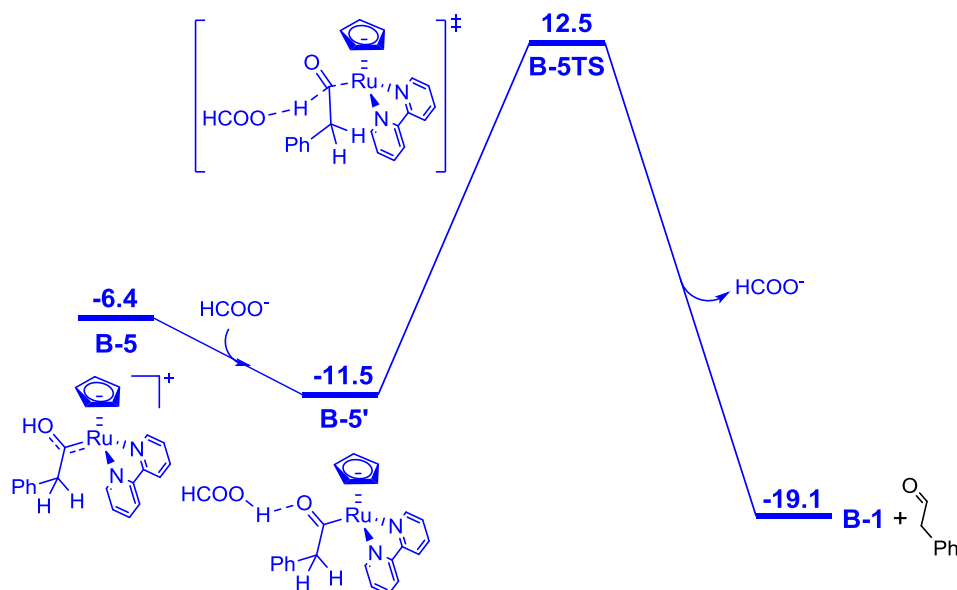


Figure S5. Calculations of a part of hydration reaction for catalysts **B**. Gibbs energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/BSI level of theory. Ph = phenyl.

6. The influence of activation free energy for the formic acid molecule is absent in B-TS2.

The loss of entropy will cause the thermodynamically high energy. For the case of formic acid molecule is absent, we had thought about that at the beginning. The results is shown in Figure S6. The activation free energy of **B-TS2** is 1.1 kcal/mol lower than **B-TS2'** due to the combine effect of loss of entropy and assistance of formic acid.

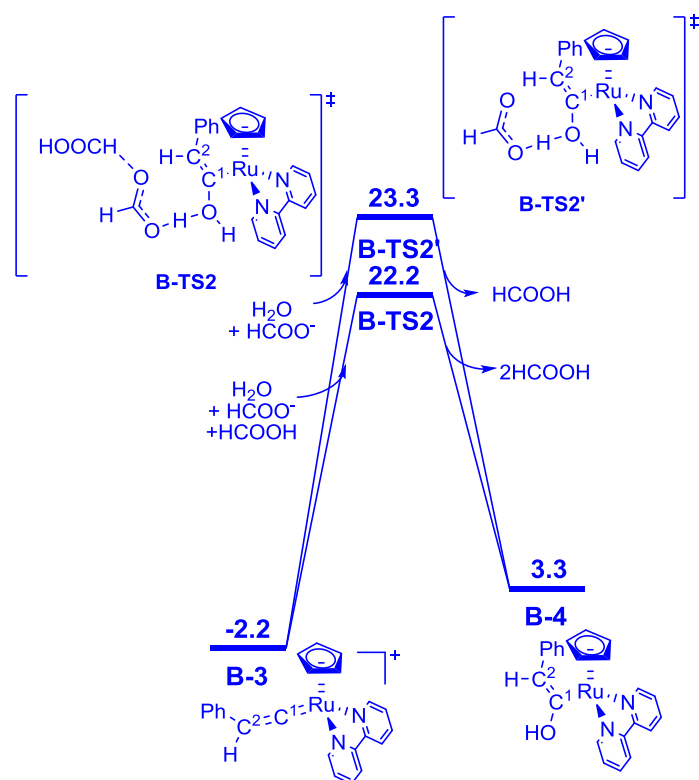


Figure S6. Compare of **B-TS2** and **B-TS2'** in hydration reaction. Gibbs energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)/B3LYP-D3/BSI level of theory. Ph = phenyl.

7. Comparison of dissociation energies for catalyst A and D

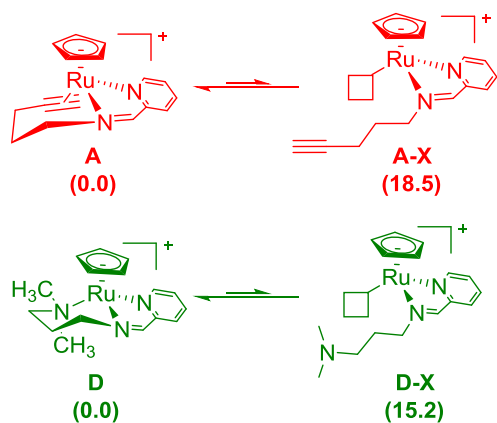


Fig. S7. Comparison of dissociation energies for catalyst **A** and **D**. Gibbs free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/ BSI level of theory

8. LAPS mechanism for catalyst B

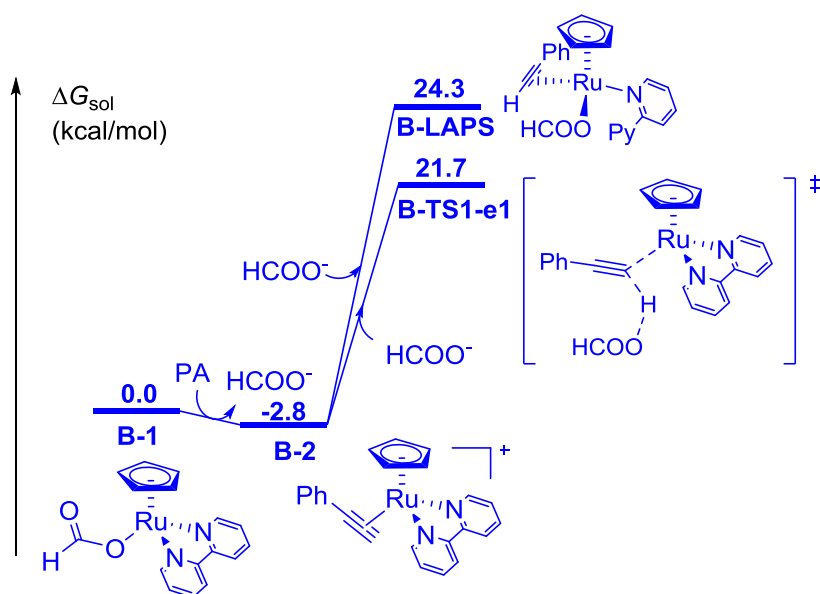


Fig. S8. LAPS mechanism¹ compared with outer-sphere deprotonation mechanism in alkyne-vinylidene transformation for catalyst **B**.

9. Energy profiles of detail hydration reactions for catalyst B

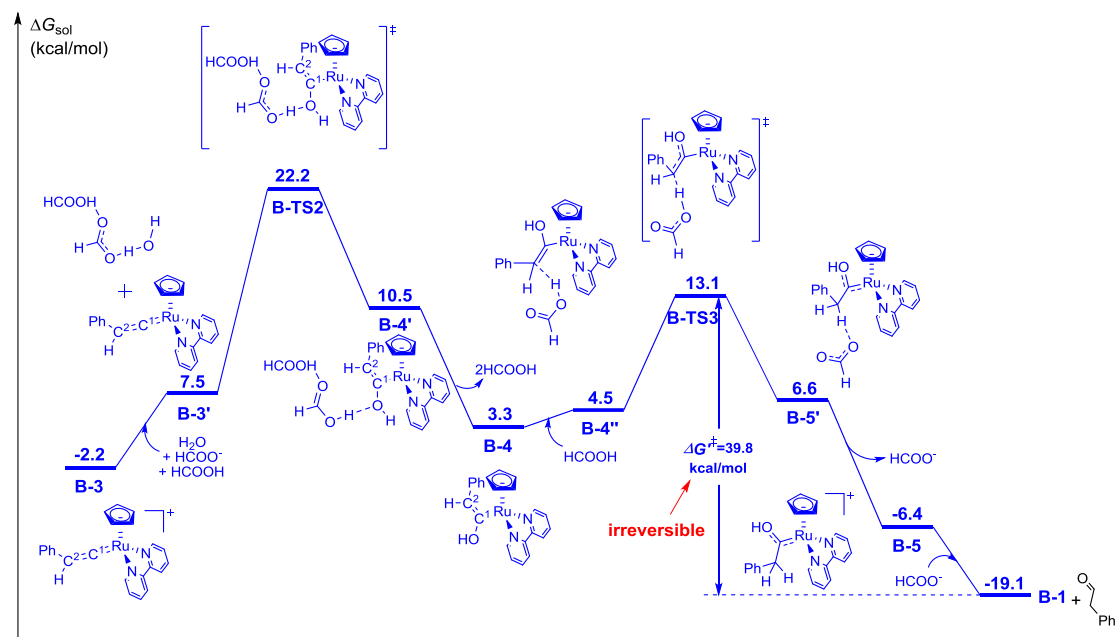


Fig. S9. Energy profiles of detail hydration reactions for catalyst **B**. Gibbs free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/BSI level of theory. Ph = phenyl, PA = phenylacetylene.

10. Energy profiles for key points of hydration of catalyst B that geometry optimizations are done in solvent

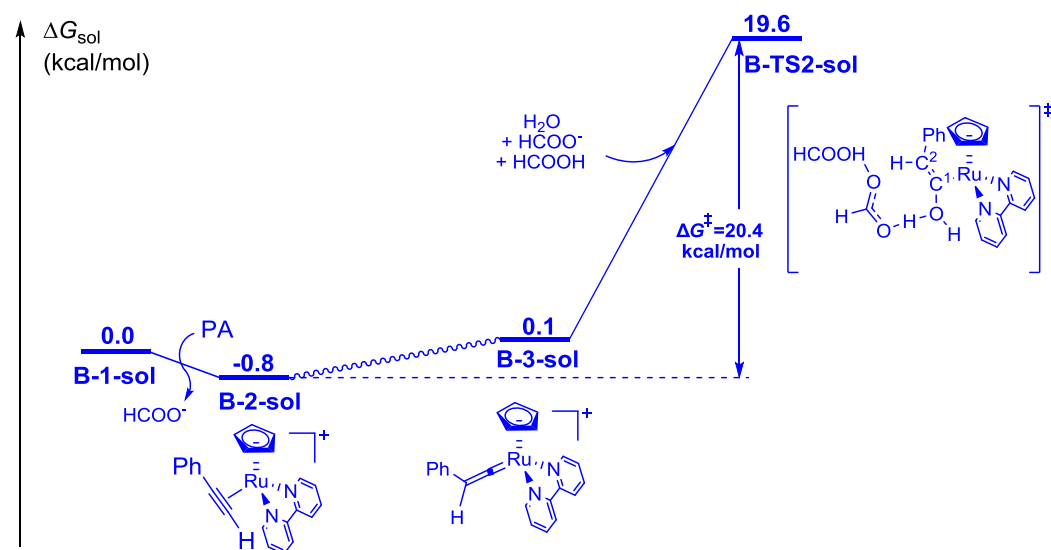


Fig. S10. Energy profiles for key points of hydration of catalyst **B** that geometry optimizations are done in solvent. Gibbs free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/BSI level of theory.

Ph = phenyl, PA = phenylacetylene.

11. Energy profiles of detail hydrogenation reactions for catalyst B

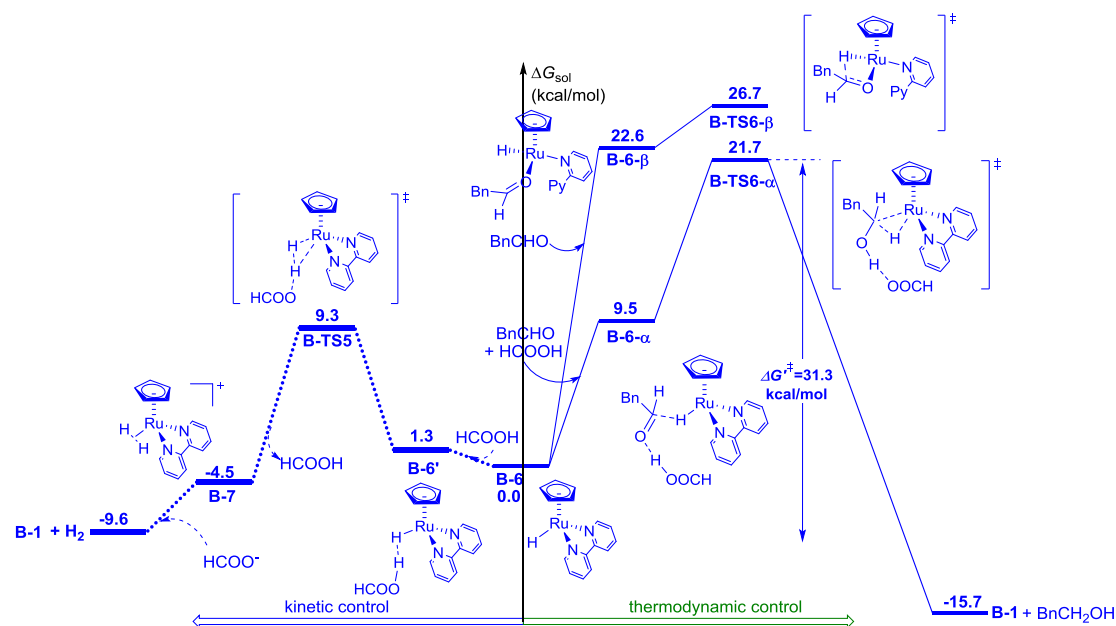


Fig. S11. Energy profiles for detail hydrogenation reactions for catalyst **B**. Gibbs free energies are reported in kcal/mol at the B3LYP-D3/BSII/PCM(H₂O)//B3LYP-D3/BSI level of theory. Ph = phenyl, Bn = benzyl.

12. Structures for transition state B-TS6-α that geometry optimizations are done in solvent

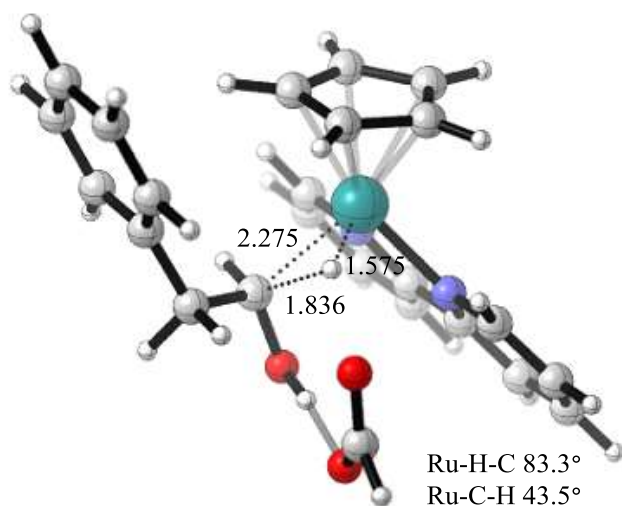


Fig. S12. Calculated structures (in Å and deg) for transition state **B-TS6-α** that geometry optimizations are done in solvent. The color codes for the atoms are ruthenium (green), nitrogen (blue), oxygen (red), carbon (gray), and hydrogen (white).

13. The Cartesian coordinates (xyz) for all optimized structures in gas are presented

CO₂
 0 1
 C 0.000000 0.000000 0.000000
 O 0.000000 0.000000 1.169724
 O 0.000000 0.000000 -1.169724

H₂
 0 1
 H 0.000000 0.000000 0.371396
 H 0.000000 0.000000 -0.371396

H₂O
 0 1
 O 0.000000 0.000000 0.118841
 H 0.000000 -0.760123 -0.475365
 H 0.000000 0.760123 -0.475365

HCOO⁻
 -1 1
 C 0.000047 0.310938 -0.000084
 O -1.142138 -0.208218 0.000054
 H -0.000400 1.465408 0.000058
 O 1.142153 -0.208161 0.000002

HCOOH
 0 1
 C 0.130976 0.362340 -0.000112
 O 1.178878 -0.219708 0.000108
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 O -1.059353 -0.281212 -0.000147
 H -1.779764 0.365910 0.001221

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PhCH₂CH₂OH
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PhCH₂CHO
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A

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A-2*

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A-IM-e

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 H 2.284705 -3.775995 -1.000571
 Ru 0.672287 -1.232462 -0.667257
 C 1.290346 0.448534 1.596730
 C 1.891631 1.566060 -0.462449
 C 0.744651 -0.727311 2.218095
 H 1.008836 1.952050 -0.987443
 C 0.544323 -0.874986 3.598749
 C -0.084785 -2.871466 1.820257
 C 0.025442 -2.063509 4.086729
 H 0.795039 -0.052355 4.261095

C -0.292346 -3.081831 3.174616
 H -0.339636 -3.620551 1.079997
 H -0.138525 -2.201739 5.150432
 H -0.706449 -4.026475 3.509999
 N 1.422293 0.408472 0.301224
 N 0.434526 -1.724885 1.332675
 H 1.572280 1.308102 2.197843
 H 2.563256 1.174924 -1.234159
 C 2.583436 2.686641 0.316593
 H 3.421011 2.285054 0.898586
 H 1.890261 3.155536 1.023070
 C 3.108246 3.770250 -0.649210
 H 3.804859 3.315585 -1.366710
 H 2.272879 4.165850 -1.242402
 C 3.775304 4.869071 0.046554
 C 4.322760 5.764723 0.643203
 H 4.805756 6.560520 1.161364
 C -3.740519 1.692964 0.829642
 C -4.948526 2.378121 0.932589
 C -5.856452 2.378291 -0.130192
 C -5.539461 1.682252 -1.300165
 C -4.332716 0.995663 -1.409892
 C -3.404074 0.985294 -0.345717
 H -3.037052 1.692035 1.657043
 H -5.184285 2.915293 1.847891
 H -6.798274 2.913318 -0.047726
 H -6.237809 1.675002 -2.133249
 H -4.089286 0.456166 -2.320228
 C -2.166773 0.288136 -0.452047
 C -1.101221 -0.315737 -0.548384

A-IM-f

1 1

C -1.529177 -2.909671 1.632066
 C -0.278271 -2.843450 2.367202
 H 0.563944 -3.509607 2.244063
 C -0.378195 -1.767642 3.272274
 H 0.378265 -1.452694 3.978562
 C -2.402686 -1.907491 2.125948
 H -3.402560 -1.704077 1.768215
 C -1.693963 -1.168423 3.104263
 H -2.078229 -0.325309 3.664640
 H -1.767759 -3.635458 0.866151
 Ru -0.447582 -0.915221 1.195435

C -1.704564 0.381055 -1.329171
 C -1.532927 1.785651 0.610380
 C -1.483487 -0.793357 -2.203560
 H -0.544002 2.094100 0.970839
 C -0.215930 -1.348087 -2.425391
 C -2.492621 -2.257619 -3.646345
 C -0.119397 -2.422379 -3.311158
 H 0.658200 -0.937023 -1.934024
 C -1.278754 -2.896915 -3.922558
 H -3.412966 -2.589365 -4.120914
 H 0.845102 -2.872999 -3.523628
 H -1.247616 -3.730173 -4.616645
 N -1.308429 0.510555 -0.115830
 N -2.600158 -1.212432 -2.819972
 H -2.291814 1.173807 -1.791315
 H -2.129254 1.540855 1.497590
 C -2.186571 2.939337 -0.151570
 H -3.194401 2.666241 -0.482319
 H -1.602374 3.189160 -1.044033
 C -2.281876 4.191329 0.748949
 H -2.861730 3.954260 1.651262
 H -1.277956 4.475017 1.092661
 C -2.898525 5.317340 0.052749
 C -3.410265 6.232070 -0.545110
 H -3.862338 7.048479 -1.060993
 C 3.881651 1.428142 -1.075303
 C 5.147910 1.869581 -1.431315
 C 6.271470 1.407659 -0.732677
 C 6.130643 0.500807 0.326095
 C 4.869341 0.052347 0.691557
 C 3.721277 0.509195 -0.006106
 H 3.001496 1.777181 -1.605435
 H 5.268904 2.572322 -2.249318
 H 7.260461 1.756333 -1.014164
 H 7.007653 0.150205 0.860416
 H 4.742860 -0.648947 1.509585
 C 2.441936 0.052417 0.353393
 C 1.316870 -0.341702 0.715565
 H -0.363513 -1.870611 -0.030800

A-IM-f'

1 1

C 3.702853 0.525876 -1.509031
 C 3.496399 -0.891166 -1.588317

H 4.122440 -1.646560 -1.133311
 C 2.326313 -1.119338 -2.351614
 H 1.887426 -2.080266 -2.577798
 C 2.653585 1.172071 -2.251398
 H 2.543439 2.238964 -2.387987
 C 1.798582 0.165386 -2.764813
 H 0.910727 0.318526 -3.360981
 H 4.540375 1.018784 -1.035819
 Ru 1.707531 0.057212 -0.526018
 C 0.116767 1.062159 1.691115
 C -0.214233 2.515796 -0.217779
 C 0.710732 -0.151231 2.246937
 H -0.699220 2.073577 -1.096581
 C 0.443916 -0.603544 3.537767
 C 2.066973 -1.991898 1.809463
 C 1.019116 -1.800245 3.966592
 H -0.208501 -0.028135 4.185920
 C 1.839764 -2.504432 3.088175
 H 2.692468 -2.508090 1.091439
 H 0.825889 -2.175969 4.965711
 H 2.302935 -3.441069 3.377245
 N 0.399487 1.384661 0.481779
 N 1.519526 -0.843063 1.401540
 H -0.574312 1.637939 2.302152
 H 0.612456 3.132269 -0.590134
 C -1.206284 3.362161 0.575996
 H -0.723502 3.795839 1.459234
 H -2.040992 2.743360 0.924099
 C -1.767188 4.505979 -0.297552
 H -0.940775 5.133036 -0.658593
 H -2.248067 4.083786 -1.190244
 C -2.726008 5.331214 0.432149
 C -3.514640 5.997698 1.056540
 H -4.213877 6.596855 1.594280
 C -2.650727 -3.376858 -0.459856
 C -3.917441 -3.955312 -0.463987
 C -5.041586 -3.186745 -0.778072
 C -4.893194 -1.832776 -1.090838
 C -3.629549 -1.247784 -1.089659
 C -2.488915 -2.012247 -0.772252
 H -1.775261 -3.971935 -0.218841
 H -4.029268 -5.008392 -0.223751
 H -6.027666 -3.640979 -0.781465
 H -5.764171 -1.233400 -1.338456

H -3.510735 -0.197119 -1.336786
 C -1.193167 -1.410594 -0.757228
 C -0.083142 -0.898650 -0.754733
 H 2.660169 0.917352 0.446594

A-3

1 1

C 0.240586 -3.385068 -0.927367
 C -0.915206 -2.790172 -1.549504
 H -1.947808 -3.048577 -1.358136
 C -0.446107 -1.907517 -2.569163
 H -1.065314 -1.330489 -3.242094
 C 1.394200 -2.841955 -1.520055
 H 2.415652 -3.074841 -1.248726
 C 0.983008 -1.889852 -2.520584
 H 1.634564 -1.349035 -3.192975
 H 0.222646 -4.103951 -0.118432
 Ru 0.157364 -1.017295 -0.589120
 C 1.624178 0.268951 1.560186
 C 2.828641 0.585946 -0.515631
 C 0.476705 -0.290516 2.249253
 H 2.363276 1.232295 -1.269166
 C 0.246996 -0.149094 3.619871
 C -1.464985 -1.552713 1.990088
 C -0.882247 -0.740015 4.179649
 H 0.946303 0.417713 4.225285
 C -1.749266 -1.454222 3.349407
 H -2.116956 -2.085532 1.308468
 H -1.085448 -0.644637 5.240874
 H -2.641738 -1.927920 3.742435
 N 1.720828 0.053442 0.291059
 N -0.373481 -0.988946 1.445165
 H 2.364292 0.836901 2.117838
 H 3.244172 -0.267240 -1.063578
 C 3.934929 1.333881 0.226018
 H 4.393839 0.688834 0.983972
 H 3.528792 2.211593 0.741233
 C 5.028405 1.802015 -0.759829
 H 5.448189 0.932804 -1.283828
 H 4.578028 2.440169 -1.532088
 C 6.098294 2.531019 -0.084059
 C 6.969342 3.130466 0.497269
 H 7.747579 3.662742 0.995399
 C -1.524716 1.586214 -1.217221

C -0.805272 0.518458 -0.941484
 H -1.016809 2.363006 -1.794481
 C -2.930591 1.827389 -0.842598
 C -3.560732 3.010581 -1.258211
 C -3.662832 0.901592 -0.076871
 C -4.890197 3.261689 -0.918577
 H -3.008163 3.734526 -1.850902
 C -4.988464 1.154963 0.258763
 H -3.183787 -0.016330 0.252176
 C -5.608973 2.336760 -0.160626
 H -5.363607 4.181226 -1.248777
 H -5.543591 0.431190 0.848580
 H -6.643752 2.532282 0.102323

A-T

1 1

C -0.548745 -2.831341 0.461345
 C -1.837504 -2.236983 0.628509
 H -2.394119 -2.179550 1.553827
 C -2.245579 -1.697595 -0.630626
 H -3.191432 -1.217696 -0.840424
 C -0.206542 -2.737121 -0.935375
 H 0.704890 -3.103787 -1.389514
 C -1.235308 -2.043152 -1.598253
 H -1.253476 -1.788127 -2.649774
 H 0.009075 -3.360787 1.221425
 Ru -0.401460 -0.587297 0.092456
 C 0.885202 1.741047 -1.065694
 C -1.476333 1.993757 -1.347645
 C 2.002397 1.030434 -0.471193
 H -2.251128 1.281450 -1.638244
 C 3.326787 1.466385 -0.535132
 C 2.600677 -0.808972 0.828085
 C 4.314178 0.721529 0.106210
 H 3.567832 2.374876 -1.076841
 C 3.942086 -0.431382 0.799519
 H 2.268198 -1.690084 1.363406
 H 5.351640 1.036355 0.071559
 H 4.676041 -1.036148 1.320164
 N -0.288637 1.219200 -0.947996
 N 1.646100 -0.103188 0.200018
 H 1.040765 2.701207 -1.558832
 H -1.223978 2.601964 -2.224804
 C -1.994124 2.930499 -0.227314

H -2.741505 3.573978 -0.706889
H -1.172361 3.583449 0.088915
C -2.653156 2.286390 1.011222
H -3.132609 3.080597 1.590810
H -3.455734 1.612715 0.688613
C -1.686253 1.538049 1.944822
C -1.036597 0.526559 1.428767
H -1.547219 1.869961 2.970904

A-s

O 1

C 0.485075 2.868698 1.550233
C 1.202316 3.043401 0.319770
H 2.275769 3.068450 0.199326
C 0.226034 3.218824 -0.710141
H 0.435560 3.300286 -1.767078
C -0.912371 2.951181 1.276468
H -1.705599 2.864281 2.007368
C -1.075069 3.166314 -0.135698
H -2.007959 3.268953 -0.670888
H 0.927417 2.702878 2.524508
Ru -0.064699 1.164063 0.184254
C -1.249849 -1.411463 0.747373
C -2.891387 0.059914 -0.253246
C 0.101234 -1.575384 1.222252
H -2.685880 0.319684 -1.298561
C 0.622054 -2.772971 1.730490
C 2.136956 -0.489339 1.557283
C 1.938036 -2.809185 2.167361
H -0.011292 -3.653764 1.765771
C 2.706818 -1.641047 2.078427
H 2.708734 0.421140 1.432855
H 2.366206 -3.725636 2.560048
H 3.744723 -1.625563 2.390916
N -1.572974 -0.230950 0.314903
N 0.854936 -0.437850 1.138683
H -1.942547 -2.248393 0.770008
H -3.247388 0.971310 0.241409
C -3.952916 -1.036086 -0.164429
H -4.127855 -1.332305 0.876835
H -3.628213 -1.929095 -0.709629
C -5.279926 -0.539496 -0.777347
H -5.615075 0.361381 -0.245429
H -5.106340 -0.234203 -1.817726

C -6.335880 -1.549326 -0.734263
C -7.193590 -2.398036 -0.687859
H -7.955692 -3.141684 -0.654719
C 0.914224 0.130264 -1.662207
C -0.241760 0.429819 -2.095498
C 2.229596 -0.454778 -1.578474
C 3.380101 0.342742 -1.417245
C 2.391284 -1.854242 -1.596851
C 4.639608 -0.235913 -1.271413
H 3.264647 1.421828 -1.404163
C 3.651624 -2.430711 -1.449113
H 1.510050 -2.476415 -1.714877
C 4.781992 -1.626358 -1.281429
H 5.513526 0.399111 -1.150735
H 3.751750 -3.512916 -1.460469
H 5.763263 -2.077423 -1.163692

A-TS1-a

I 1

C 0.760854 2.696097 1.732494
C 1.052556 3.165322 0.426144
H 2.030463 3.341914 0.004132
C -0.200673 3.380339 -0.247500
H -0.320169 3.736238 -1.260087
C -0.658977 2.583016 1.872779
H -1.188425 2.282554 2.766660
C -1.248962 3.035186 0.638870
H -2.306040 3.109387 0.423811
H 1.489930 2.425558 2.485758
Ru -0.036330 1.149904 0.248924
C -1.323166 -1.391300 0.848730
C -2.955534 0.099610 -0.129738
C 0.028530 -1.596229 1.327405
H -2.826784 0.571693 -1.108341
C 0.481217 -2.789311 1.895868
C 2.111248 -0.595198 1.610432
C 1.799787 -2.870566 2.332410
H -0.196922 -3.631452 1.985030
C 2.624115 -1.752622 2.187172
H 2.726592 0.281570 1.457419
H 2.179505 -3.785175 2.774927
H 3.659302 -1.771755 2.507806
N -1.602216 -0.236063 0.341769
N 0.837746 -0.507960 1.185927

H -2.056550 -2.188352 0.940227
 H -3.322093 0.884885 0.542269
 C -3.969640 -1.040335 -0.210724
 H -4.156265 -1.470348 0.779601
 H -3.589054 -1.843675 -0.852072
 C -5.310242 -0.531269 -0.785123
 H -5.690654 0.287255 -0.159149
 H -5.143469 -0.104444 -1.783185
 C -6.310839 -1.592170 -0.864134
 C -7.120354 -2.485477 -0.917373
 H -7.847957 -3.263076 -0.971239
 C 1.106260 0.499006 -1.532726
 C -0.164697 0.660266 -1.972486
 H -0.845511 -0.164720 -2.159971
 C 2.205654 -0.466711 -1.486286
 C 3.539561 -0.080770 -1.281585
 C 1.891397 -1.834210 -1.573245
 C 4.542037 -1.044666 -1.173855
 H 3.781261 0.974907 -1.209620
 C 2.893843 -2.792412 -1.443959
 H 0.861931 -2.134754 -1.741094
 C 4.221863 -2.402041 -1.246285
 H 5.572732 -0.734519 -1.031605
 H 2.641240 -3.846011 -1.514857
 H 5.002414 -3.151471 -1.160787
 O 1.709929 2.007099 -2.234622
 H 2.236777 1.764528 -3.019245
 H 0.603092 1.863517 -2.509630

A-TS1-b

1 1

C -0.899254 2.114112 -2.314961
 C -1.071970 2.853355 -1.118028
 H -2.010418 3.121506 -0.657001
 C 0.235746 3.195421 -0.614534
 H 0.446685 3.751034 0.287880
 C 0.504332 1.951043 -2.548749
 H 0.955481 1.459716 -3.400070
 C 1.197294 2.651641 -1.496657
 H 2.269671 2.745998 -1.393439
 H -1.691324 1.705280 -2.929112
 Ru 0.032185 0.910228 -0.619068
 C 1.350758 -1.686691 -0.674774
 C 2.986683 0.001707 -0.119724

C -0.013443 -2.013198 -1.036050
 H 2.858525 0.704987 0.708304
 C -0.457598 -3.311439 -1.299479
 C -2.118237 -1.131679 -1.486530
 C -1.783963 -3.508639 -1.670139
 H 0.234864 -4.142177 -1.212875
 C -2.623004 -2.396647 -1.769976
 H -2.746025 -0.252010 -1.526615
 H -2.156856 -4.505484 -1.879443
 H -3.663405 -2.500333 -2.055567
 N 1.630083 -0.440621 -0.480603
 N -0.839846 -0.931721 -1.118609
 H 2.091347 -2.477876 -0.590002
 H 3.355000 0.586972 -0.970907
 C 3.993808 -1.084908 0.255480
 H 4.191215 -1.751134 -0.591658
 H 3.597815 -1.700189 1.071862
 C 5.330324 -0.456926 0.707783
 H 5.738050 0.164836 -0.100594
 H 5.150534 0.218001 1.555363
 C 6.310059 -1.471070 1.089120
 C 7.099437 -2.328975 1.400872
 H 7.809475 -3.074222 1.679034
 C -1.055256 0.704211 1.347121
 C 0.251163 0.720983 1.652665
 H 0.745935 -0.219918 1.884682
 C -2.214929 -0.193560 1.473274
 C -3.513995 0.181725 1.088378
 C -1.995399 -1.508057 1.922200
 C -4.566473 -0.730728 1.161470
 H -3.692948 1.186097 0.719417
 C -3.046263 -2.420973 1.975192
 H -0.998031 -1.808523 2.225612
 C -4.336269 -2.036344 1.599035
 H -5.565694 -0.421272 0.870205
 H -2.860337 -3.431594 2.325879
 H -5.155303 -2.746616 1.653434
 O -1.770194 2.312865 1.711699
 H -2.377719 2.147266 2.451236
 H 0.617903 2.143915 2.208885
 O 0.382840 3.179427 2.467761
 H 0.540651 3.303896 3.413958
 H -0.915385 2.843711 2.111380

A-TS1-c

O 1

C 0.838435 -3.555211 -0.163043
 C 1.301520 -3.051081 1.106792
 H 2.321738 -3.058169 1.465591
 C 0.168527 -2.567566 1.809098
 H 0.184484 -2.078288 2.773603
 C -0.579485 -3.388900 -0.205169
 H -1.221018 -3.661757 -1.033150
 C -1.007119 -2.760942 1.005638
 H -2.017327 -2.466647 1.261152
 H 1.450090 -4.012655 -0.929268
 Ru 0.379485 -1.348899 -0.096037
 C 0.146444 0.271394 -2.479472
 C -2.035762 -0.507409 -1.874673
 C 1.558459 0.335995 -2.205537
 H -2.446990 -1.189905 -1.131882
 C 2.472179 1.114067 -2.929057
 C 3.244882 -0.410078 -0.779388
 C 3.807749 1.115450 -2.553589
 H 2.117467 1.712542 -3.762049
 C 4.198492 0.337423 -1.456521
 H 3.498167 -0.999977 0.092055
 H 4.533190 1.715429 -3.093154
 H 5.228380 0.318248 -1.118567
 N -0.576160 -0.445749 -1.668444
 N 1.946302 -0.427796 -1.139055
 H -0.283389 0.802719 -3.327251
 H -2.235392 -0.909697 -2.877569
 C -2.702974 0.865198 -1.708253
 H -2.352323 1.559394 -2.480891
 H -2.421107 1.281100 -0.739017
 C -4.237033 0.737119 -1.772446
 H -4.534702 0.258344 -2.716204
 H -4.551304 0.079762 -0.953263
 C -4.901340 2.032962 -1.652769
 C -5.425843 3.116384 -1.551747
 H -5.903226 4.062866 -1.448145
 C 2.549507 0.809205 2.226458
 C 3.717530 1.541295 2.433338
 C 3.917552 2.752610 1.766210
 C 2.932442 3.232357 0.899834
 C 1.756143 2.510392 0.701309
 C 1.550396 1.288590 1.362985

H 2.398339 -0.140464 2.730400
 H 4.475010 1.163803 3.114791
 H 4.831363 3.318497 1.922134
 H 3.078329 4.174327 0.378319
 H 0.990117 2.878799 0.026043
 C 0.365121 0.494207 1.083831
 C -0.890019 0.477985 1.263210
 H -1.897434 0.055190 1.174274
 O -1.644509 1.956249 2.513624
 H -1.837804 2.685004 1.908481
 H -2.556059 1.497626 2.651861
 O -3.538581 -0.644081 1.034221
 C -4.243352 -0.122043 1.946977
 O -3.926653 0.804375 2.736696
 H -5.273700 -0.528474 2.069386

A-TS1-d

I 1

C 0.943836 -3.259046 -1.436895
 C -0.352556 -2.911680 -1.946138
 H -1.275092 -3.449731 -1.781141
 C -0.173580 -1.776975 -2.802125
 H -0.959401 -1.270795 -3.346743
 C 1.897898 -2.348106 -1.958857
 H 2.960954 -2.360873 -1.758610
 C 1.203034 -1.410926 -2.803418
 H 1.650092 -0.617681 -3.386116
 H 1.157918 -4.072105 -0.755114
 Ru 0.385352 -1.170830 -0.703929
 C 1.656479 0.226809 1.518297
 C 2.439445 1.177397 -0.560239
 C 0.840261 -0.764490 2.193081
 H 1.730136 1.743113 -1.176566
 C 0.762693 -0.891217 3.583157
 C -0.627960 -2.544713 1.886235
 C -0.034768 -1.893212 4.126948
 H 1.325070 -0.211908 4.215352
 C -0.739584 -2.733578 3.260955
 H -1.168765 -3.164096 1.180483
 H -0.108260 -2.018021 5.202028
 H -1.373089 -3.527659 3.640164
 N 1.634668 0.230876 0.225269
 N 0.151175 -1.587581 1.352674
 H 2.260382 0.915492 2.103816

H	3.022689	0.568730	-1.260666
C	3.357828	2.129793	0.203825
H	4.069324	1.567113	0.818682
H	2.777540	2.770722	0.877302
C	4.146768	3.026149	-0.776060
H	4.737770	2.396522	-1.454778
H	3.444930	3.586199	-1.408942
C	5.029981	3.958706	-0.080603
C	5.751932	4.719320	0.516471
H	6.396392	5.396612	1.029124
C	-2.272002	0.708201	-0.412312
C	-1.201820	0.052416	-0.545016
H	-1.114150	1.193190	-0.972735
C	-3.494255	1.435980	-0.280454
C	-3.751037	2.176125	0.892249
C	-4.451383	1.402248	-1.315829
C	-4.950345	2.868049	1.023284
H	-3.009782	2.195268	1.684628
C	-5.646595	2.099224	-1.173460
H	-4.247738	0.828384	-2.213992
C	-5.895413	2.830535	-0.007346
H	-5.151250	3.436622	1.925451
H	-6.385302	2.073480	-1.967877
H	-6.829892	3.372838	0.099035

A-TS1-e1

0 1

C	0.500325	3.119625	1.623303
C	1.175404	3.278524	0.362185
H	2.238091	3.408447	0.211926
C	0.176904	3.255204	-0.652978
H	0.365988	3.281762	-1.717390
C	-0.904968	3.016582	1.363916
H	-1.676708	2.904167	2.114430
C	-1.112971	3.102028	-0.054427
H	-2.052617	3.037007	-0.584238
H	0.967363	3.106129	2.599522
Ru	0.102686	1.284853	0.433611
C	-0.661581	-1.357162	1.349890
C	-2.651429	-0.091441	0.810544
C	0.769012	-1.361046	1.546482
H	-2.807325	0.519191	-0.079061
C	1.496437	-2.469167	2.000544
C	2.700977	-0.062499	1.464255

C	2.864599	-2.348342	2.198199
H	0.977562	-3.404025	2.187488
C	3.474848	-1.117494	1.926271
H	3.138874	0.894847	1.210419
H	3.450658	-3.192258	2.546774
H	4.542851	-0.979581	2.050504
N	-1.195824	-0.242970	0.955124
N	1.368834	-0.162548	1.278597
H	-1.242720	-2.251692	1.559897
H	-2.982865	0.507948	1.669236
C	-3.476179	-1.375345	0.709420
H	-3.436531	-1.949532	1.642380
H	-3.072918	-2.012420	-0.086155
C	-4.949413	-1.044150	0.382657
H	-5.331339	-0.312703	1.108698
H	-5.000802	-0.572075	-0.606737
C	-5.798342	-2.233618	0.405995
C	-6.479262	-3.230670	0.437412
H	-7.091455	-4.102152	0.447986
C	2.683106	-2.100546	-1.483374
C	3.957265	-2.658549	-1.417684
C	5.088857	-1.842991	-1.507792
C	4.939596	-0.462754	-1.671754
C	3.667563	0.100196	-1.742446
C	2.517357	-0.710417	-1.644154
H	1.800221	-2.725746	-1.401053
H	4.069605	-3.731744	-1.292065
H	6.081526	-2.280875	-1.454516
H	5.816663	0.173767	-1.748362
H	3.541423	1.171030	-1.867840
C	1.214551	-0.128130	-1.643685
C	0.062901	0.341768	-1.646702
H	-1.424116	0.766764	-2.078383
O	-2.453757	0.970375	-2.219400
C	-3.039937	-0.090021	-2.748441
O	-4.242740	-0.255833	-2.808222
H	-2.322429	-0.845010	-3.133238

A-TS1-e2

0 1

C	-0.442824	-3.873832	-0.683264
C	-0.039893	-3.214118	-1.886440
H	-0.689069	-2.943491	-2.707829
C	1.356916	-2.934784	-1.802363

H 1.960686 -2.467913 -2.567679
 C 0.736487 -4.060912 0.121031
 H 0.770645 -4.531052 1.095050
 C 1.829340 -3.485234 -0.557869
 H 2.846435 -3.435571 -0.191115
 H -1.432992 -4.248540 -0.463086
 Ru 0.258298 -1.756938 -0.198085
 C 1.103748 0.539015 1.359627
 C 2.617325 0.252720 -0.491515
 C -0.085492 0.090889 2.056934
 H 2.144655 0.671702 -1.386635
 C -0.692845 0.825461 3.077796
 C -1.693593 -1.582743 2.206579
 C -1.828462 0.309006 3.689045
 H -0.290455 1.800205 3.327577
 C -2.325930 -0.924311 3.255217
 H -2.074207 -2.514256 1.804380
 H -2.329984 0.860391 4.477560
 H -3.211931 -1.362049 3.701863
 N 1.507846 -0.177727 0.366631
 N -0.593160 -1.091506 1.610632
 H 1.579680 1.462148 1.663947
 H 3.159311 -0.651831 -0.786214
 C 3.579113 1.279792 0.103746
 H 4.020757 0.900583 1.032810
 H 3.050269 2.206757 0.338554
 C 4.696452 1.609021 -0.908267
 H 5.212089 0.686347 -1.208979
 H 4.241097 2.022229 -1.817831
 C 5.672965 2.557706 -0.376672
 C 6.469649 3.339643 0.083467
 H 7.171868 4.035206 0.480863
 C -1.351479 0.751661 -1.172487
 C -0.822832 -0.400046 -0.964100
 C -2.710628 1.297477 -1.196849
 C -2.958725 2.558906 -0.627631
 C -3.780066 0.578403 -1.759029
 C -4.252202 3.079604 -0.620935
 H -2.139391 3.096001 -0.160382
 C -5.069322 1.108153 -1.750825
 H -3.584814 -0.388735 -2.213616
 C -5.311212 2.362033 -1.183361
 H -4.433625 4.052895 -0.172678
 H -5.885861 0.543033 -2.192717

H -6.315723 2.775994 -1.181176
 H -0.429778 1.535165 -1.225383
 O 0.642331 2.590823 -1.258118
 C 0.634647 3.320967 -0.209120
 O 0.066957 3.098754 0.878127
 H 1.231313 4.261229 -0.308727

A-T-TS1-d

1 1
 C -0.141875 -2.943457 0.352777
 C -1.469657 -2.566934 0.700078
 H -1.911639 -2.658688 1.683275
 C -2.112302 -2.010417 -0.456970
 H -3.139782 -1.681685 -0.522081
 C 0.042376 -2.641679 -1.044984
 H 0.937860 -2.822389 -1.624382
 C -1.165636 -2.070565 -1.532462
 H -1.334063 -1.727155 -2.544896
 H 0.573518 -3.423331 1.006063
 Ru -0.357736 -0.721675 0.086999
 C 0.684045 1.812731 -0.990091
 C -1.683010 1.900118 -1.261623
 C 1.868560 1.184047 -0.435845
 H -2.473764 1.153229 -1.352677
 C 3.148912 1.737282 -0.524776
 C 2.658007 -0.609539 0.817435
 C 4.214939 1.073305 0.075078
 H 3.294255 2.670491 -1.059110
 C 3.959910 -0.117930 0.758898
 H 2.419942 -1.524056 1.346972
 H 5.220583 1.475472 0.016605
 H 4.757258 -0.665389 1.249197
 N -0.440100 1.183674 -0.890120
 N 1.622860 0.014617 0.225707
 H 0.755747 2.809547 -1.429272
 H -1.539696 2.359152 -2.246507
 C -2.095500 3.014038 -0.259950
 H -2.791159 3.687029 -0.772920
 H -1.212024 3.613030 -0.011292
 C -2.776103 2.537323 1.050265
 H -2.938327 3.370366 1.741556
 H -3.776921 2.132849 0.837850
 C -2.051669 1.415472 1.663890
 C -1.207410 0.491054 1.497723

H -0.622234 1.368074 2.047915

A-TS2

O 1

C -0.638284 -2.466785 -1.662814

C -0.846560 -1.193353 -2.250597

H -1.774219 -0.644250 -2.183052

C 0.374518 -0.774597 -2.876939

H 0.526753 0.132704 -3.445002

C 0.705537 -2.881119 -1.976985

H 1.172718 -3.811239 -1.680964

C 1.318708 -1.845167 -2.721130

H 2.338763 -1.846302 -3.085281

H -1.397773 -2.995071 -1.104365

Ru 0.748249 -0.955356 -0.638774

C 2.972237 -0.449170 1.157418

C 2.159933 -1.375739 1.913691

C 2.482464 -1.825383 3.197230

C 0.208158 -2.652881 1.878577

C 1.633560 -2.730594 3.824342

H 3.382223 -1.460839 3.682275

C 0.482609 -3.147109 3.151277

H -0.710559 -2.887259 1.352304

H 1.857618 -3.097415 4.820836

H -0.217288 -3.837840 3.608132

N 2.561183 -0.141094 -0.031131

N 1.036929 -1.790911 1.262796

C -0.109033 0.630748 -0.049501

C -0.469851 1.895930 -0.206434

C -1.522010 2.716227 0.433610

H 0.108731 2.377191 -1.001585

C -2.859892 2.285403 0.440375

C -1.207988 3.963763 0.994878

C -3.856582 3.073314 1.018476

H -3.135868 1.349675 -0.032538

C -2.204630 4.749064 1.574519

H -0.177634 4.309744 0.984702

C -3.529518 4.304114 1.592019

H -4.879831 2.715126 0.984010

H -1.946143 5.709318 2.012710

H -4.304028 4.920406 2.039865

O -1.120337 0.157464 1.868997

H -1.751860 0.869010 2.044149

H -1.679824 -0.629323 1.601525

O -5.591134 0.836415 -0.363023

O -2.498040 -1.898219 0.966492

C -5.957376 0.451753 -1.465059

C -3.442936 -1.484775 0.239651

O -5.507299 -0.579082 -2.135320

H -6.753793 0.974239 -2.027555

O -3.631672 -1.793071 -0.971088

H -4.165183 -0.773314 0.688593

H -4.745740 -1.080845 -1.615480

H 3.884315 -0.047482 1.592063

C 3.260370 0.831164 -0.873103

H 2.583584 1.691083 -0.958418

H 3.316621 0.388300 -1.873426

C 4.645260 1.290988 -0.417092

H 4.585609 1.801149 0.550517

H 5.311380 0.429587 -0.292152

C 5.259993 2.260859 -1.448915

H 4.589101 3.119206 -1.589081

H 5.328855 1.763015 -2.425583

C 6.582918 2.736719 -1.050092

C 7.674060 3.115856 -0.699424

H 8.637639 3.457678 -0.399106

B

1 1

C -2.666238 -1.237966 -0.744898

C -3.210747 -0.507688 0.337752

H -3.647764 -0.933301 1.231610

C -3.064382 0.904181 0.064973

H -3.425827 1.714039 0.683005

C -2.138586 -0.292839 -1.702196

H -1.694344 -0.528519 -2.659445

C -2.420919 1.021647 -1.200173

H -2.155620 1.948611 -1.692995

H -2.644623 -2.315577 -0.837012

Ru -1.035982 -0.014064 0.162647

C 1.842768 0.756510 -0.121668

C 0.491496 2.654338 0.032752

C 2.982486 1.557150 -0.247429

C 1.863676 -0.718203 -0.121732

C 1.585656 3.503029 -0.091361

H -0.514914 3.039312 0.148442

C 2.855560 2.943117 -0.236290

H 3.960950 1.105509 -0.355882

C 3.026878 -1.484585 -0.243284
 H 1.438255 4.577001 -0.075362
 H 3.732351 3.573791 -0.337996
 C 0.568252 -2.653742 0.028233
 C 2.940599 -2.873892 -0.233074
 H 3.992214 -1.004416 -0.346843
 C 1.687374 -3.470420 -0.093318
 H -0.425916 -3.068911 0.141812
 H 3.836022 -3.478491 -0.330963
 H 1.571063 -4.548206 -0.078152
 N 0.606070 1.311377 0.012394
 N 0.642636 -1.308393 0.008531
 O -0.622643 -0.015770 2.402260
 H -0.070553 -0.751176 2.702354
 H -0.191135 0.790593 2.716683

B-1

O 1
 C -2.606554 -1.751974 -0.016531
 C -3.088528 -0.417720 0.214956
 H -3.503685 -0.042783 1.140047
 C -2.835398 0.372162 -0.933851
 H -3.082219 1.418676 -1.042506
 C -2.041691 -1.765412 -1.337179
 H -1.586494 -2.620094 -1.822504
 C -2.178789 -0.464949 -1.909105
 H -1.868118 -0.169998 -2.902365
 H -2.694254 -2.591877 0.658120
 Ru -0.875684 -0.338621 -0.094239
 C 1.791095 0.932278 -0.323087
 C 0.094713 2.510777 -0.609645
 C 2.766756 1.932486 -0.419599
 C 2.079966 -0.487056 -0.087150
 C 1.015730 3.543008 -0.728422
 H -0.971756 2.687997 -0.606162
 C 2.378590 3.248742 -0.634534
 H 3.816453 1.683677 -0.317724
 C 3.369167 -1.020621 0.038545
 H 0.665127 4.559013 -0.871619
 H 3.123588 4.034223 -0.712031
 C 1.145803 -2.601545 0.229810
 C 3.534058 -2.381566 0.258405
 H 4.234894 -0.372810 -0.032866
 C 2.395734 -3.188637 0.356086

H 0.232947 -3.178288 0.317533
 H 4.527604 -2.806385 0.357977
 H 2.472338 -4.255356 0.536362
 N 0.467888 1.227551 -0.440317
 N 0.977135 -1.282944 0.001181
 O -0.459006 0.138139 1.932697
 C -0.981161 1.225888 2.400814
 O -1.701545 2.041981 1.823971
 H -0.704047 1.384974 3.467788

B-2

I 1
 C 0.544440 -2.463605 1.747537
 C 0.299458 -3.147989 0.528870
 H -0.623065 -3.628891 0.235943
 C 1.516808 -3.112596 -0.239578
 H 1.658992 -3.552456 -1.217106
 C 1.898116 -1.985941 1.747124
 H 2.396817 -1.472289 2.557330
 C 2.495985 -2.414108 0.512772
 H 3.518184 -2.232705 0.207699
 H -0.173809 -2.312720 2.543072
 Ru 0.807377 -0.973452 0.070518
 C 1.428742 1.937982 0.060203
 C 3.082175 0.732772 -1.062630
 C 2.109952 3.135103 -0.186180
 C 0.158262 1.843270 0.790853
 C 3.806949 1.886154 -1.333133
 H 3.417787 -0.239686 -1.401388
 C 3.311662 3.111963 -0.884714
 H 1.705897 4.075963 0.166789
 C -0.542405 2.940505 1.302473
 H 4.736343 1.818858 -1.887162
 H 3.850341 4.033232 -1.079256
 C -1.478101 0.385899 1.595351
 C -1.737476 2.736232 1.983693
 H -0.159469 3.944573 1.167512
 C -2.213798 1.433754 2.133329
 H -1.829421 -0.635578 1.654224
 H -2.289629 3.579325 2.385104
 H -3.145504 1.225081 2.645938
 N 1.925255 0.747387 -0.372329
 N -0.314474 0.576887 0.944018
 C -3.949865 1.241709 -1.246279

C -4.827593 0.276660 -0.745055
 C -4.384527 -1.034694 -0.546173
 C -3.066940 -1.380053 -0.836152
 C -2.178431 -0.413534 -1.344399
 C -2.632504 0.903351 -1.547284
 H -4.294037 2.258622 -1.407847
 H -5.854640 0.542983 -0.515456
 H -5.067465 -1.787881 -0.165506
 H -2.714614 -2.394022 -0.676237
 H -1.945672 1.648043 -1.936340
 C -0.805196 -0.737831 -1.599730
 C 0.331240 -0.920046 -2.077733
 H 1.011221 -1.038234 -2.900900

B-IM-e

0 1

C -2.984831 -2.220440 -0.706707
 C -1.744567 -2.795716 -1.159022
 H -1.454482 -2.977157 -2.184640
 C -1.000346 -3.162085 0.001234
 H -0.009681 -3.594682 0.001134
 C -2.984451 -2.219901 0.709511
 H -3.777270 -1.844099 1.343395
 C -1.743955 -2.794840 1.161613
 H -1.453329 -2.975505 2.187214
 H -3.777982 -1.845118 -1.340459
 Ru -1.210046 -0.909365 0.000456
 C -1.080243 1.947297 0.730209
 C -1.234370 0.609399 2.637677
 C -0.974728 3.096253 1.525877
 C -1.080591 1.946698 -0.731701
 C -1.147394 1.710558 3.474033
 H -1.313316 -0.398767 3.025287
 C -1.011219 2.983780 2.907950
 H -0.860913 4.068616 1.061128
 C -0.975599 3.095013 -1.528364
 H -1.173097 1.569991 4.549079
 H -0.928507 3.865605 3.534746
 C -1.235492 0.607217 -2.637998
 C -1.012733 2.981399 -2.910325
 H -0.861722 4.067775 -1.064470
 C -1.149023 1.707695 -3.475299
 H -1.314526 -0.401275 -3.024741
 H -0.930437 3.862720 -3.537885

H -1.175209 1.566244 -4.550217
 N -1.213021 0.710567 1.291585
 N -1.213520 0.709498 -1.291997
 C 4.012150 0.831662 0.001622
 C 5.396425 0.983027 0.001519
 C 6.232678 -0.137141 -0.000324
 C 5.663761 -1.414010 -0.002072
 C 4.280159 -1.572261 -0.001987
 C 3.420315 -0.451351 -0.000129
 H 3.363787 1.702974 0.003072
 H 5.826845 1.981475 0.002894
 H 7.312364 -0.016831 -0.000398
 H 6.303600 -2.292980 -0.003514
 H 3.841389 -2.565498 -0.003353
 C 2.005105 -0.605618 -0.000013
 C 0.783997 -0.743619 0.000125

B-3

1 1

C -1.305681 -2.316955 -2.031621
 C 0.037634 -2.580181 -1.576077
 H 0.939226 -2.496289 -2.167369
 C -0.053912 -3.135676 -0.261421
 H 0.775819 -3.477446 0.342003
 C -2.193901 -2.646404 -0.995593
 H -3.269086 -2.524319 -1.020451
 C -1.427940 -3.123828 0.128999
 H -1.828057 -3.518538 1.052787
 H -1.577238 -1.901433 -2.993177
 Ru -0.684110 -0.984685 -0.137455
 C -2.141506 1.556696 0.359199
 C -2.934113 -0.138344 1.760824
 C -3.056676 2.461051 0.907056
 C -1.171516 1.894012 -0.693208
 C -3.866741 0.713086 2.340178
 H -2.835398 -1.171277 2.070648
 C -3.929313 2.037220 1.903821
 H -3.087119 3.486395 0.559919
 C -1.037009 3.163540 -1.264012
 H -4.522541 0.340987 3.118945
 H -4.643467 2.730154 2.335935
 C 0.556071 1.074706 -2.036241
 C -0.077213 3.376238 -2.248039
 H -1.671691 3.979188 -0.940506

C 0.735943 2.312604 -2.640668
 H 1.172774 0.223000 -2.292273
 H 0.038287 4.357446 -2.696034
 H 1.504146 2.434330 -3.395601
 N -2.096612 0.266649 0.788060
 N -0.379924 0.863345 -1.093150
 C 5.306754 0.856251 1.654283
 C 5.660897 0.553518 0.338681
 C 4.726962 -0.056552 -0.504997
 C 3.450467 -0.355555 -0.038372
 C 3.080007 -0.040667 1.281820
 C 4.026772 0.561694 2.124378
 H 6.028574 1.320199 2.319598
 H 6.658526 0.779483 -0.024473
 H 5.002639 -0.312248 -1.524211
 H 2.736517 -0.858053 -0.685577
 H 3.757773 0.802487 3.149213
 C 1.722523 -0.321125 1.793995
 C 0.673682 -0.594532 1.047101
 H 1.563773 -0.282670 2.873725

B-4

0 1

C 2.323944 -2.650133 0.535213
 C 1.442377 -2.957571 -0.546877
 H 0.530027 -3.533612 -0.472895
 C 1.931807 -2.329493 -1.724944
 H 1.490505 -2.401912 -2.709667
 C 3.396572 -1.852648 -0.002239
 H 4.237282 -1.464578 0.558440
 C 3.162440 -1.662699 -1.384782
 H 3.787597 -1.098396 -2.064284
 H 2.265075 -3.046546 1.540620
 Ru 1.387001 -0.697031 -0.209014
 C 0.545205 2.095490 -0.536581
 C 0.662175 1.019862 -2.608643
 C 0.035681 3.249510 -1.150084
 C 0.833622 1.970466 0.886820
 C 0.173216 2.134655 -3.267714
 H 0.901543 0.104487 -3.135473
 C -0.155446 3.275562 -2.522298
 H -0.214539 4.115513 -0.548659
 C 0.630855 2.983685 1.834867
 H 0.040584 2.105177 -4.343664

H -0.555082 4.160368 -3.006571
 C 1.716291 0.574648 2.541847
 C 0.986047 2.775923 3.158302
 H 0.191310 3.926348 1.530756
 C 1.549910 1.543182 3.515839
 H 2.135687 -0.397963 2.772319
 H 0.828611 3.551903 3.899948
 H 1.847309 1.332880 4.537354
 N 0.852730 0.982518 -1.269880
 N 1.370505 0.763389 1.247195
 C -0.597724 -0.919262 0.303202
 C -1.689078 -0.515981 -0.399146
 O -0.788606 -1.546635 1.520804
 C -3.114954 -0.615026 -0.084401
 H -1.479796 -0.033463 -1.348535
 H 0.094054 -1.746483 1.856214
 C -3.653016 -1.247914 1.059451
 C -4.034124 -0.032968 -0.987055
 C -5.029300 -1.287537 1.276092
 H -2.981830 -1.707136 1.772513
 C -5.407873 -0.075157 -0.767234
 H -3.650259 0.461757 -1.877195
 C -5.919529 -0.704520 0.370551
 H -5.411361 -1.783079 2.165717
 H -6.082193 0.384208 -1.486220
 H -6.990973 -0.740833 0.547126

B-5

1 1

C -3.247632 -1.730432 0.092647
 C -2.245019 -2.747154 0.122492
 H -2.119686 -3.533547 -0.613350
 C -1.515613 -2.631236 1.345606
 H -0.732678 -3.294250 1.687225
 C -3.190925 -1.041633 1.357831
 H -3.823405 -0.214777 1.653614
 C -2.143458 -1.587802 2.116307
 H -1.829537 -1.253809 3.096663
 H -3.997788 -1.596478 -0.674668
 Ru -1.178693 -0.747387 0.093803
 C 0.407609 1.601277 0.958664
 C 1.399140 -0.382032 1.692547
 C 1.372184 2.355888 1.632606
 C -0.671923 2.172837 0.139758

C 2.386546 0.312792 2.379119
 H 1.379122 -1.463149 1.660588
 C 2.367990 1.707363 2.354939
 H 1.347774 3.437924 1.591599
 C -0.854020 3.541581 -0.083638
 H 3.157254 -0.235226 2.907683
 H 3.124088 2.281151 2.880078
 C -2.512592 1.678131 -1.214439
 C -1.900173 3.973642 -0.891991
 H -0.184443 4.262664 0.368962
 C -2.744504 3.024047 -1.470070
 H -3.132153 0.900148 -1.643232
 H -2.051265 5.032754 -1.071750
 H -3.567743 3.314272 -2.112864
 N 0.422524 0.242412 1.009450
 N -1.507018 1.256017 -0.423972
 C -0.140196 -1.046219 -1.520054
 C 0.906656 -0.131562 -2.122915
 O -0.213055 -2.140551 -2.281106
 C 2.267573 -0.325919 -1.463149
 H 0.593712 0.908291 -2.003514
 H -0.856464 -2.755942 -1.899668
 C 2.770155 -1.607927 -1.199449
 C 3.040157 0.788008 -1.115730
 C 4.014861 -1.767974 -0.588240
 H 2.191709 -2.481937 -1.481967
 C 4.288726 0.628773 -0.513061
 H 2.662860 1.786784 -1.319105
 C 4.777265 -0.650550 -0.240242
 H 4.393491 -2.767043 -0.393460
 H 4.878862 1.503898 -0.257162
 H 5.748573 -0.776327 0.228282
 H 0.979258 -0.338345 -3.198001

B-5'

O 1

C 0.620576 -1.839047 2.044168
 C 1.688740 -1.170604 1.388794
 H 2.339215 -1.608448 0.645784
 C 1.724849 0.186734 1.845131
 H 2.445602 0.935136 1.547897
 C 0.018794 -0.912395 2.968699
 H -0.812836 -1.119427 3.629190
 C 0.692013 0.326662 2.833318

H 0.453779 1.235638 3.372251
 H 0.344273 -2.874230 1.900686
 Ru -0.263071 -0.143525 0.773530
 C -2.481548 1.538160 -0.216117
 C -0.691247 2.853566 0.521647
 C -3.201310 2.690310 -0.561021
 C -2.969385 0.169884 -0.381277
 C -1.363458 4.023201 0.210273
 H 0.313803 2.858450 0.925521
 C -2.646507 3.944307 -0.348504
 H -4.191736 2.599078 -0.991707
 C -4.196546 -0.174427 -0.961315
 H -0.885183 4.979496 0.392806
 H -3.195323 4.842066 -0.612767
 C -2.450560 -2.090377 -0.069653
 C -4.552347 -1.511550 -1.079936
 H -4.861193 0.600346 -1.325833
 C -3.658042 -2.486542 -0.625490
 H -1.711278 -2.809665 0.258939
 H -5.499825 -1.790732 -1.529090
 H -3.882842 -3.543925 -0.712032
 N -1.224695 1.624216 0.321063
 N -2.107421 -0.791077 0.070726
 C 0.315683 -0.343095 -1.167995
 C 0.901922 0.843398 -1.959490
 O 0.302710 -1.423862 -1.776951
 C 2.284798 1.163468 -1.430399
 H 0.252149 1.718098 -1.864480
 C 3.252055 0.149876 -1.350922
 C 2.607291 2.442281 -0.962419
 C 4.507487 0.413169 -0.803600
 H 3.004421 -0.855809 -1.680688
 C 3.866624 2.709015 -0.419033
 H 1.863967 3.233625 -1.021861
 C 4.819668 1.692130 -0.333121
 H 5.239606 -0.386455 -0.735816
 H 4.101221 3.708238 -0.061488
 H 5.796974 1.893810 0.096124
 H 0.949036 0.551560 -3.015575
 H 0.318602 -2.800435 -1.069009
 O 0.375332 -3.737748 -0.666251
 C 1.644475 -4.107448 -0.561624
 O 2.621807 -3.439420 -0.836253
 H 1.714530 -5.139092 -0.171748

B-6

O 1

C -2.793950 1.149498 0.617595
C -3.067071 0.721107 -0.713341
H -3.275981 1.359554 -1.559901
C -3.067001 -0.721366 -0.713137
H -3.275875 -1.360078 -1.559505
C -2.661169 0.000206 1.455742
H -2.468120 0.000371 2.519609
C -2.793843 -1.149337 0.617934
H -2.731615 -2.178830 0.948122
H -2.731824 2.179095 0.947479
Ru -0.983953 0.000023 -0.219972
C 1.862324 -0.726015 0.010417
C 0.511111 -2.636360 -0.006533
C 3.012995 -1.528759 0.060228
C 1.862350 0.725969 0.010416
C 1.610489 -3.470822 0.060309
H -0.498471 -3.026038 -0.052740
C 2.897088 -2.908303 0.088039
H 3.992088 -1.063571 0.078441
C 3.013051 1.528669 0.060233
H 1.464821 -4.545582 0.081892
H 3.780128 -3.537474 0.128066
C 0.511209 2.636364 -0.006536
C 2.897197 2.908217 0.088042
H 3.992126 1.063443 0.078452
C 1.610619 3.470784 0.060308
H -0.498358 3.026080 -0.052743
H 3.780261 3.537355 0.128071
H 1.464991 4.545550 0.081889
N 0.607844 -1.282639 -0.031720
N 0.607890 1.282639 -0.031723
H -0.642756 0.000009 -1.782547

B-7

I 1

C 2.520373 -1.157093 0.884862
C 3.192829 -0.723161 -0.283651
H 3.652446 -1.356978 -1.029609
C 3.192628 0.723836 -0.283213
H 3.652151 1.358260 -1.028710
C 2.061336 -0.000388 1.607401

H 1.568300 -0.000753 2.569592
C 2.520081 1.156862 0.885603
H 2.353552 2.186438 1.174528
H 2.354228 -2.186895 1.173195
Ru 1.051674 0.000078 -0.363724
C -1.816656 0.736190 0.040109
C -0.505180 2.650635 -0.215524
C -2.959163 1.521724 0.222307
C -1.816591 -0.736322 0.040109
C -1.603220 3.484453 -0.039096
H 0.483892 3.049140 -0.405075
C -2.853406 2.908493 0.186933
H -3.922877 1.056590 0.388539
C -2.959030 -1.521948 0.222309
H -1.473483 4.559813 -0.082424
H -3.732690 3.527957 0.328208
C -0.504963 -2.650647 -0.215578
C -2.853161 -2.908710 0.186920
H -3.922781 -1.056893 0.388547
C -1.602933 -3.484560 -0.039142
H 0.484127 -3.049075 -0.405191
H -3.732394 -3.528247 0.328199
H -1.473103 -4.559908 -0.082498
N -0.600817 1.308741 -0.169139
N -0.600698 -1.308764 -0.169152
H 0.883626 -0.420631 -2.073886
H 0.884299 0.421711 -2.073635

B-TS1-d

I 1

C -2.308876 2.465772 1.195840
C -0.942711 2.863795 1.409770
H -0.438899 2.951884 2.361939
C -0.409214 3.230796 0.134663
H 0.598082 3.580909 -0.047264
C -2.597913 2.571452 -0.186043
H -3.543453 2.332792 -0.654890
C -1.413066 3.035460 -0.860708
H -1.324111 3.273319 -1.911616
H -2.997120 2.127969 1.959726
Ru -0.906414 1.042716 0.080588
C -1.789121 -1.686801 -0.744926
C -1.736601 -0.249702 -2.583319
C -2.238752 -2.734958 -1.555615

C -1.551547 -1.803672 0.702732
 C -2.190072 -1.247430 -3.437199
 H -1.516472 0.748948 -2.940846
 C -2.445128 -2.516050 -2.913230
 H -2.429088 -3.712428 -1.129645
 C -1.736567 -2.979183 1.439000
 H -2.335625 -1.029307 -4.489180
 H -2.797432 -3.320049 -3.550661
 C -0.881247 -0.667454 2.628007
 C -1.491754 -2.978934 2.807851
 H -2.070515 -3.885553 0.948843
 C -1.055802 -1.799609 3.414331
 H -0.531633 0.268669 3.045901
 H -1.635683 -3.882770 3.390307
 H -0.848702 -1.752399 4.477468
 N -1.543549 -0.453339 -1.265589
 N -1.130363 -0.659241 1.305022
 C 5.456319 -1.653332 -0.182021
 C 6.380599 -0.606804 -0.267131
 C 5.945986 0.720819 -0.337170
 C 4.585291 1.008946 -0.324008
 C 3.647712 -0.041347 -0.237904
 C 4.093220 -1.377626 -0.167727
 H 5.801299 -2.680705 -0.126316
 H 7.443733 -0.826658 -0.277888
 H 6.668805 1.527651 -0.401082
 H 4.235062 2.034722 -0.375408
 H 3.365400 -2.179703 -0.099641
 C 2.249631 0.248865 -0.206231
 C 1.018437 0.526750 -0.177277
 H 1.422990 0.352733 -1.311766

B-TS1-e1

0 1

C -0.899878 2.748206 1.888860
 C -0.323248 3.268775 0.676195
 H 0.637304 3.755254 0.575994
 C -1.272537 3.055018 -0.365796
 H -1.113807 3.276842 -1.412261
 C -2.196339 2.229770 1.574960
 H -2.879988 1.774097 2.279950
 C -2.438133 2.424983 0.171648
 H -3.312768 2.129669 -0.389498
 H -0.442787 2.762554 2.869849

Ru -0.693427 1.058663 0.459803
 C 0.848434 -1.320533 1.367899
 C 1.928228 -2.103104 1.797247
 C 2.180997 0.593101 1.423502
 C 3.156801 -1.506637 2.045593
 H 1.803455 -3.170957 1.932838
 C 3.283734 -0.127658 1.853976
 H 2.236453 1.657657 1.234239
 H 4.002094 -2.103025 2.372549
 H 4.226669 0.382083 2.015322
 N 0.979349 0.024195 1.189512
 C 2.766930 -1.248049 -1.639118
 C 4.145704 -1.431664 -1.574383
 C 5.005942 -0.331186 -1.627993
 C 4.478302 0.957209 -1.754283
 C 3.100025 1.146254 -1.821778
 C 2.219642 0.045620 -1.760101
 H 2.092001 -2.095978 -1.585009
 H 4.552050 -2.434643 -1.477805
 H 6.081193 -0.476848 -1.575910
 H 5.143645 1.814818 -1.802145
 H 2.681434 2.143342 -1.915968
 C 0.806541 0.241105 -1.745386
 C -0.428498 0.376783 -1.708201
 H -2.036257 0.349842 -2.060714
 O -3.074757 0.231942 -2.135595
 C -3.347243 -0.998261 -2.541373
 O -4.449883 -1.505823 -2.506374
 H -2.454011 -1.546116 -2.908785
 N -1.408309 -0.890961 0.752704
 C -0.493536 -1.841681 1.087585
 C -2.676934 -1.264382 0.494517
 C -0.848999 -3.194806 1.148749
 C -3.089229 -2.589367 0.536794
 H -3.351257 -0.472594 0.199054
 C -2.155939 -3.574961 0.867964
 H -0.105736 -3.942500 1.399734
 H -4.113114 -2.831676 0.277930
 H -2.440534 -4.621795 0.897058

B-TS1-e2

0 1

C -2.494421 -0.549436 -2.782809
 C -1.462877 0.355567 -3.227489

H -1.614284 1.340550 -3.648009
 C -0.218163 -0.328843 -3.122473
 H 0.751930 0.074513 -3.377062
 C -1.871722 -1.749462 -2.373494
 H -2.373817 -2.607338 -1.944485
 C -0.452242 -1.623108 -2.553411
 H 0.306086 -2.353616 -2.301517
 H -3.555218 -0.338572 -2.749228
 Ru -0.990810 -0.058626 -1.021224
 C -1.790448 -0.300615 1.825807
 C -0.675451 -2.218401 1.080285
 C -1.908142 -0.841727 3.109174
 C -2.256412 1.035182 1.434662
 C -0.746818 -2.800011 2.342671
 H -0.140217 -2.707812 0.276309
 C -1.382488 -2.104958 3.370386
 H -2.386060 -0.274977 3.899701
 C -2.927730 1.920208 2.287109
 H -0.259295 -3.757228 2.483645
 H -1.451932 -2.527697 4.367718
 C -2.363251 2.592140 -0.303716
 C -3.325765 3.164733 1.815793
 H -3.135532 1.632802 3.310753
 C -3.037167 3.507788 0.492056
 H -2.100138 2.812109 -1.331287
 H -3.847141 3.857378 2.468387
 H -3.321319 4.470094 0.081029
 N -1.191346 -1.002400 0.825722
 N -1.985312 1.378112 0.143580
 C 3.232851 2.394666 0.213034
 C 4.416597 3.083491 0.462735
 C 5.632919 2.396366 0.532254
 C 5.653334 1.011814 0.348781
 C 4.470986 0.317209 0.099057
 C 3.242707 0.998594 0.026836
 H 2.286693 2.926526 0.162469
 H 4.392338 4.160846 0.604428
 H 6.554877 2.936417 0.727980
 H 6.593733 0.469970 0.400448
 H 4.481793 -0.758765 -0.049402
 C 2.025251 0.248215 -0.234332
 C 0.774418 0.397108 -0.479645
 H 2.101582 -0.979025 -0.302759
 O 2.016724 -2.409624 -0.446272

C 2.356890 -3.150232 0.555216
 O 1.716521 -4.102266 1.011098
 H 3.325088 -2.869201 1.040090

B-TS2

O 1
 C 0.069063 -2.800254 -0.803373
 C -0.589635 -1.921920 -1.703074
 H -1.616548 -1.604822 -1.595271
 C 0.342922 -1.524071 -2.716966
 H 0.131289 -0.898369 -3.573144
 C 1.407532 -3.009433 -1.294764
 H 2.164613 -3.634175 -0.839381
 C 1.569731 -2.227530 -2.461477
 H 2.478468 -2.142170 -3.044842
 H -0.411402 -3.235702 0.061041
 Ru 1.089739 -0.755890 -0.711570
 C 3.374801 0.880064 0.239439
 C 2.993431 1.228715 -2.038281
 C 4.417138 1.815147 0.222435
 C 2.944987 0.135042 1.428354
 C 4.020578 2.158176 -2.118594
 H 2.386414 0.970140 -2.897633
 C 4.747062 2.459076 -0.963238
 H 4.960148 2.039278 1.132599
 C 3.547080 0.245176 2.685538
 H 4.236875 2.639803 -3.065688
 H 5.551532 3.186860 -0.986619
 C 1.420910 -1.436055 2.248534
 C 3.068708 -0.522623 3.741371
 H 4.378617 0.923029 2.837025
 C 1.988601 -1.375813 3.516604
 H 0.531623 -2.022194 2.043278
 H 3.525368 -0.448066 4.723108
 H 1.567567 -1.979712 4.312489
 N 2.676520 0.592997 -0.893205
 N 1.896430 -0.705939 1.222025
 C -0.081749 0.722992 -0.446824
 C -0.779082 1.747240 -0.918682
 C -1.930556 2.497015 -0.370732
 H -0.441907 2.027485 -1.921292
 C -3.089923 1.817797 0.042825
 C -1.907894 3.899056 -0.304946
 C -4.190914 2.521538 0.532998

H -3.151438 0.739101 -0.045315
 C -3.008074 4.601551 0.187448
 H -1.019790 4.434131 -0.631037
 C -4.149765 3.915381 0.611652
 H -5.073551 1.960091 0.820509
 H -2.973806 5.686499 0.240170
 H -5.006280 4.466550 0.989703
 O -0.656764 0.755733 1.631190
 H -1.426630 1.337032 1.708552
 H -1.006029 -0.174723 1.793899
 O -5.328151 -0.434796 0.284644
 O -1.497002 -1.702862 1.865875
 C -5.677197 -1.286513 -0.521183
 C -2.596569 -1.830160 1.257761
 O -5.048723 -2.393043 -0.830380
 H -6.617151 -1.190657 -1.096491
 O -2.848195 -2.682867 0.361796
 H -3.411257 -1.123849 1.514778
 H -4.152331 -2.500692 -0.295045

B-TS2'

0 1

C -1.148222 -3.321503 -1.310354
 C -0.152664 -3.574938 -0.321251
 H 0.897966 -3.747455 -0.510096
 C -0.770558 -3.508309 0.967455
 H -0.287483 -3.700720 1.915788
 C -2.405981 -3.168132 -0.623729
 H -3.358073 -2.952182 -1.091401
 C -2.178321 -3.284603 0.759226
 H -2.924124 -3.179560 1.536244
 H -0.999170 -3.339589 -2.381128
 Ru -0.853808 -1.460887 -0.008606
 C -1.574701 1.198853 1.068824
 C -0.867843 -0.218328 2.784263
 C -1.638568 2.283432 1.951576
 C -1.928335 1.275060 -0.356314
 C -0.958486 0.800105 3.720340
 H -0.532241 -1.213991 3.048370
 C -1.337113 2.075675 3.290257
 H -1.807456 3.281554 1.556044
 C -2.455494 2.414601 -0.978407
 H -0.706043 0.600837 4.756178
 H -1.367212 2.907041 3.987092

C -2.076372 0.070064 -2.356965
 C -2.803617 2.351810 -2.319373
 H -2.478926 3.354974 -0.438514
 C -2.623512 1.154975 -3.022823
 H -1.878543 -0.871793 -2.853771
 H -3.191808 3.233297 -2.819143
 H -2.880464 1.067458 -4.072776
 N -1.178269 -0.027758 1.487148
 N -1.737310 0.126607 -1.050654
 C 0.929682 -0.863496 -0.008882
 C 2.163282 -0.855560 0.468983
 O 1.170750 0.922144 -1.684869
 C 3.498060 -0.394865 0.061921
 H 2.140743 -1.360575 1.443348
 H 0.327367 0.838460 -2.140950
 C 3.848463 -0.079613 -1.262984
 C 4.496153 -0.326114 1.051991
 C 5.149856 0.309567 -1.571474
 H 3.085937 -0.108904 -2.028231
 C 5.796162 0.064476 0.738252
 H 4.244272 -0.574200 2.080496
 C 6.130187 0.385260 -0.578482
 H 5.400145 0.556356 -2.599738
 H 6.546795 0.117242 1.522060
 H 7.142517 0.689760 -0.828610
 C 0.140286 4.123420 -0.176370
 O -0.903035 4.703126 0.204885
 H 0.951535 4.768365 -0.599323
 O 0.385024 2.878772 -0.135028
 H 1.034883 1.717352 -1.092708

B-TS3

0 1

C -1.555974 -3.015085 -1.489322
 C -0.646934 -3.417328 -0.459947
 H 0.378227 -3.730479 -0.608431
 C -1.307057 -3.309157 0.797502
 H -0.887890 -3.577624 1.757608
 C -2.812714 -2.713199 -0.846651
 H -3.709514 -2.374302 -1.349490
 C -2.668313 -2.901883 0.542475
 H -3.431307 -2.734863 1.290927
 H -1.381269 -3.069479 -2.555784
 Ru -1.152917 -1.235030 -0.127871

C -1.499250 1.414836 1.156366
 C -1.011445 -0.208715 2.756379
 C -1.599104 2.392959 2.151807
 C -1.689156 1.679976 -0.274877
 C -1.099847 0.712551 3.787795
 H -0.766103 -1.248147 2.937297
 C -1.403590 2.042304 3.478274
 H -1.804493 3.419503 1.877793
 C -1.824252 2.959537 -0.821617
 H -0.925881 0.393760 4.809610
 H -1.469605 2.792618 4.259256
 C -1.906344 0.714349 -2.386736
 C -2.025641 3.098713 -2.188889
 H -1.667154 3.831190 -0.203229
 C -2.092451 1.953650 -2.984550
 H -1.915180 -0.204412 -2.962758
 H -2.101653 4.087452 -2.627923
 H -2.253627 2.014571 -4.055354
 N -1.221458 0.122997 1.465371
 N -1.697218 0.571423 -1.063595
 C 0.752153 -0.730967 -0.477022
 C 1.746071 -0.275547 0.450764
 O 1.176329 -0.789058 -1.750206
 C 3.215517 -0.388258 0.167383
 H 1.488009 -0.552145 1.474008
 H 0.405055 -1.027137 -2.287050
 C 3.806799 0.222497 -0.950955
 C 4.048071 -1.075385 1.063270
 C 5.180752 0.131900 -1.170972
 H 3.182543 0.770742 -1.647673
 C 5.423993 -1.163937 0.847005
 H 3.609528 -1.544149 1.941442
 C 5.996986 -0.562201 -0.274569
 H 5.617014 0.613493 -2.042088
 H 6.047485 -1.702833 1.555654
 H 7.067814 -0.627975 -0.445489
 C 1.369817 3.180207 -0.270224
 O 0.747935 4.216352 -0.517110
 H 2.327911 2.977300 -0.807518
 O 1.013362 2.267513 0.571276
 H 1.459610 0.963934 0.455279

B-5TS

0 1

C 1.228562 3.180523 0.884964
 C 0.014207 3.329128 0.174446
 H -0.102019 3.754302 -0.811210
 C -1.036676 2.702474 0.934633
 H -2.080425 2.653184 0.662400
 C 0.944772 2.475127 2.114542
 H 1.657187 2.217964 2.886647
 C -0.449930 2.200488 2.134406
 H -0.970070 1.653182 2.910577
 H 2.195424 3.552810 0.573677
 Ru 0.471504 1.111369 0.351369
 C 1.011800 -1.739565 0.968035
 C -1.194855 -1.179564 1.479676
 C 0.808289 -3.041507 1.430859
 C 2.297679 -1.229178 0.476496
 C -1.454108 -2.453890 1.967357
 H -1.961804 -0.417394 1.448866
 C -0.435473 -3.406191 1.933693
 H 1.613723 -3.763827 1.389888
 C 3.465211 -1.993897 0.378868
 H -2.445517 -2.688417 2.336882
 H -0.606661 -4.416519 2.290999
 C 3.411125 0.640195 -0.359148
 C 4.627338 -1.407338 -0.099626
 H 3.452438 -3.042451 0.647636
 C 4.599624 -0.063710 -0.482986
 H 3.322987 1.671867 -0.673181
 H 5.537774 -1.990900 -0.190834
 H 5.476811 0.429767 -0.885808
 N 0.006165 -0.823663 0.986787
 N 2.291197 0.083195 0.136735
 C -0.674716 0.843672 -1.551091
 C -1.472622 -0.439174 -1.817699
 O -0.985502 1.871566 -2.134742
 C -2.837201 -0.465116 -1.156532
 H -0.880396 -1.310756 -1.533619
 C -3.591934 0.697248 -0.941561
 C -3.377389 -1.692511 -0.743000
 C -4.830745 0.635793 -0.298288
 H -3.203030 1.647939 -1.289142
 C -4.618934 -1.758067 -0.109647
 H -2.805079 -2.601895 -0.906292
 C -5.347851 -0.589796 0.126599
 H -5.396446 1.549562 -0.136017

H -5.015467 -2.720960 0.202222
H -6.311747 -0.635653 0.625670
H -1.597794 -0.476522 -2.907403
H 0.644652 0.555872 -1.484411
O 1.486274 0.018487 -2.657533
C 1.649261 -1.249287 -2.694419
O 1.249070 -2.104456 -1.883682
H 2.236411 -1.598025 -3.578231

B-TS4

O 1
C -2.941389 -1.048987 -0.444904
C -3.197788 -0.098117 0.581443
H -3.432332 -0.345610 1.608095
C -2.980585 1.226501 0.070687
H -3.134658 2.151231 0.608659
C -2.504161 -0.317987 -1.608128
H -2.236758 -0.740611 -2.567613
C -2.538731 1.084504 -1.288414
H -2.286700 1.890958 -1.965559
H -3.029753 -2.121738 -0.348570
Ru -1.083417 0.089962 -0.028185
C 1.800494 0.804002 -0.332534
C 0.502049 2.723711 -0.079800
C 2.968647 1.575655 -0.345269
C 1.777845 -0.660292 -0.474996
C 1.620637 3.543579 -0.085031
H -0.497679 3.124322 0.039196
C 2.881413 2.954852 -0.219655
H 3.935714 1.097402 -0.438176
C 2.921828 -1.454932 -0.599509
H 1.503855 4.616227 0.022125
H 3.780186 3.563073 -0.221006
C 0.412841 -2.545971 -0.563800
C 2.785461 -2.831795 -0.715955
H 3.906343 -1.004534 -0.580866
C 1.506133 -3.390592 -0.698757
H -0.598380 -2.926775 -0.504332
H 3.664205 -3.462397 -0.805798
H 1.354067 -4.461620 -0.769689
N 0.579763 1.385740 -0.209800
N 0.539271 -1.211638 -0.477150
O -0.634480 -1.390063 2.281954
C 0.169868 -0.423084 2.259926

O 1.403905 -0.360223 2.367852
H -0.353787 0.599030 2.042046

B-TS5

O 1
C 1.467807 -2.571194 0.617642
C 2.481282 -1.595960 0.356222
H 3.147432 -1.563290 -0.499383
C 2.370291 -0.545128 1.318476
H 2.978681 0.347081 1.331648
C 0.725282 -2.112171 1.762136
H -0.123721 -2.612166 2.211422
C 1.283708 -0.879261 2.199508
H 0.929156 -0.286354 3.032564
H 1.321203 -3.500242 0.084952
Ru 0.511756 -0.606557 0.095043
C -2.362358 0.140176 -0.228001
C -3.743566 -0.000070 -0.407347
C -2.041813 -2.119092 -0.718016
C -4.272153 -1.240565 -0.744228
H -4.397561 0.854767 -0.283872
C -3.402805 -2.321566 -0.906427
H -1.321393 -2.919109 -0.839623
H -5.341472 -1.361333 -0.883917
H -3.767099 -3.305902 -1.178721
N -1.525328 -0.923169 -0.374738
H 0.732351 -0.380291 -1.638365
C 3.634122 1.005500 -1.579124
O 3.468672 -0.100883 -2.137685
H 4.658691 1.462586 -1.648695
O 2.781510 1.683445 -0.931517
H 1.347364 0.123944 -1.348356
C -1.691835 1.408308 0.100289
C -2.348461 2.634078 0.239660
C 0.389230 2.430221 0.429840
C -1.602225 3.779926 0.501798
H -3.425231 2.695926 0.135476
C -0.214830 3.676161 0.584895
H 1.466310 2.294228 0.387668
H -2.097165 4.738975 0.617920
H 0.407871 4.547930 0.752166
N -0.340989 1.316752 0.228296

B-TS6- α

O 1
 C -1.833022 -0.457521 1.781542
 C -1.324485 -1.718613 1.343227
 H -1.785703 -2.373177 0.619273
 C -0.077324 -1.974118 2.005091
 H 0.548101 -2.841616 1.834915
 C -0.894123 0.051925 2.741080
 H -0.967371 1.009426 3.242857
 C 0.165284 -0.875687 2.895133
 H 1.029004 -0.753831 3.535120
 H -2.767281 -0.004554 1.485555
 Ru 0.136587 -0.194990 0.660882
 C 2.680936 1.093939 -0.168408
 C 2.936231 -1.218128 0.084995
 C 4.012937 1.227158 -0.568819
 C 1.736076 2.212268 -0.067263
 C 4.270762 -1.140260 -0.304737
 H 2.456421 -2.175900 0.301773
 C 4.820947 0.096876 -0.635950
 H 4.410086 2.199597 -0.834664
 C 2.051207 3.550771 -0.334714
 H 4.853668 -2.053321 -0.355930
 H 5.856689 0.182285 -0.949288
 C -0.471903 2.805446 0.424715
 C 1.071822 4.527368 -0.204942
 H 3.053067 3.821983 -0.644870
 C -0.216758 4.148070 0.182685
 H -1.458518 2.445740 0.692380
 H 1.305472 5.567040 -0.410369
 H -1.014559 4.875158 0.286135
 N 2.162109 -0.119111 0.163679
 N 0.480989 1.858288 0.316642
 C -3.830837 -1.199042 -0.875526
 C -2.896830 -0.288515 -1.386163
 C -3.169436 1.080979 -1.238281
 C -4.309373 1.522596 -0.566186
 C -5.217275 0.599521 -0.038268
 C -4.978467 -0.765254 -0.207497
 H -3.649644 -2.264069 -0.996352
 H -2.479447 1.811449 -1.651438
 H -4.496025 2.588561 -0.461429
 H -6.105013 0.941181 0.486120
 H -5.681215 -1.494353 0.186110
 C -1.641037 -0.772199 -2.072634

H -1.535749 -1.855540 -1.978531
 H -1.707416 -0.556441 -3.149880
 C -0.341588 -0.094084 -1.603724
 H 0.178409 -1.292340 -0.506207
 H -0.467240 0.987475 -1.637401
 O 0.737547 -0.382232 -2.440864
 H 0.897608 -1.347045 -2.337085
 O 0.551382 -2.853913 -1.485796
 C 0.971199 -3.882024 -0.864910
 O 1.611548 -3.931964 0.205755
 H 0.721690 -4.856364 -1.353268

B-TS6-β

O 1
 C -0.753122 -1.451725 -2.447474
 C 0.019717 -2.543071 -1.938993
 H 0.991093 -2.851780 -2.302079
 C -0.699949 -3.146883 -0.858278
 H -0.384292 -4.003915 -0.278940
 C -1.980451 -1.407057 -1.683905
 H -2.775330 -0.682836 -1.805896
 C -1.950398 -2.445500 -0.725802
 H -2.706661 -2.631815 0.024717
 H -0.499710 -0.820147 -3.287399
 Ru -0.201039 -1.033051 -0.335454
 C -2.726707 1.109540 0.465365
 C -4.994272 0.753024 0.373273
 C -2.599770 0.333483 1.625521
 C -1.556322 1.804276 -0.144728
 C -4.970954 -0.052319 1.512446
 H -5.929423 0.942994 -0.150406
 C -3.746800 -0.255036 2.152031
 H -1.625299 0.176340 2.072224
 C -1.713502 3.143236 -0.532634
 H -5.886875 -0.498627 1.887027
 H -3.681138 -0.865460 3.047907
 C 0.654437 1.843414 -0.843542
 C -0.643216 3.843713 -1.071239
 H -2.685575 3.602411 -0.399940
 C 0.574646 3.177745 -1.216676
 H 1.571424 1.284995 -0.974686
 H -0.753203 4.882615 -1.366972
 H 1.450470 3.669704 -1.626285
 N -3.904639 1.333316 -0.144319

N -0.382574 1.145238 -0.323708
 H 1.427766 -0.790911 -0.216422
 O 0.040451 -1.051610 1.794466
 C 1.272967 -1.060615 1.355498
 H 1.796086 -2.030972 1.340569
 C 2.165812 0.103870 1.809539
 H 1.587214 1.026268 1.716718
 H 2.326276 -0.059419 2.885126
 C 3.492368 0.220405 1.098908
 C 4.377367 -0.867171 1.037131
 C 3.874937 1.419571 0.481450
 C 5.593788 -0.764592 0.361722
 H 4.115697 -1.800828 1.527821
 C 5.094002 1.528836 -0.190658
 H 3.211020 2.278528 0.536468
 C 5.956367 0.433852 -0.257793
 H 6.262766 -1.619952 0.324076
 H 5.369869 2.469812 -0.659003
 H 6.904751 0.514283 -0.781169

C

1 1

C 1.804229 -2.009410 -1.413661
 C 2.356628 -2.495451 -0.180273
 H 3.400695 -2.508548 0.099322
 C 1.267383 -3.041332 0.572731
 H 1.345775 -3.469787 1.564792
 C 0.395405 -2.259713 -1.411354
 H -0.287368 -2.028840 -2.218154
 C 0.061173 -2.915205 -0.171801
 H -0.914256 -3.274099 0.125398
 H 2.355827 -1.536884 -2.216153
 Ru 0.871595 -0.859168 0.199075
 C -0.521609 1.694592 -0.013889
 C -2.157964 -0.071626 0.183532
 C 0.876101 2.083773 -0.137912
 H -2.228421 -0.874952 -0.554710
 C 1.297464 3.408322 -0.269392
 C 3.064050 1.306729 -0.285122
 C 2.656602 3.673994 -0.422193
 H 0.565690 4.209272 -0.254130
 C 3.552681 2.603672 -0.432968
 H 3.726495 0.448519 -0.282465
 H 3.010089 4.693642 -0.532687

H 4.618250 2.762741 -0.555186
 N -0.784898 0.435739 0.088536
 N 1.754063 1.041444 -0.143948
 H -1.289848 2.464254 -0.037668
 H -2.259637 -0.553198 1.162066
 C -3.298832 0.936933 0.002257
 H -3.238954 1.687330 0.798833
 H -3.186914 1.475444 -0.960328
 C -4.948603 -0.459248 -1.105752
 H -5.885297 -0.999118 -0.944086
 H -5.082949 0.212011 -1.974425
 H -4.187874 -1.201041 -1.365304
 C -5.650489 1.180959 0.509525
 H -5.403645 1.651122 1.466270
 H -5.832899 1.977959 -0.234383
 H -6.581878 0.623304 0.640747
 N -4.584775 0.259384 0.115001
 O 0.939914 -0.133910 2.363073
 H 0.426469 -0.708940 2.946371
 H 1.845092 -0.153405 2.702515

C-1

1 1

C -1.041315 2.869715 0.170619
 C 0.248174 2.860521 0.752156
 H 0.449939 2.921698 1.812969
 C 1.228550 2.679395 -0.288386
 H 2.302375 2.723307 -0.168624
 C -0.889163 2.678203 -1.251790
 H -1.683665 2.665134 -1.985158
 C 0.510466 2.574943 -1.523962
 H 0.949966 2.445058 -2.504938
 H -1.972625 2.989392 0.706160
 Ru -0.101603 0.877996 -0.232877
 C -0.340767 -1.763626 -1.447589
 C 1.844660 -0.962662 -1.917887
 C -1.625883 -1.602505 -0.804658
 H 1.967178 -1.970811 -2.333172
 C -2.625614 -2.580214 -0.805922
 C -2.894543 -0.201360 0.551683
 C -3.805854 -2.332779 -0.111526
 H -2.468768 -3.511921 -1.339755
 C -3.935834 -1.127109 0.582305
 H -2.933638 0.722097 1.113630

H -4.603759 -3.067623 -0.100000
H -4.830349 -0.901111 1.151782
N 0.506938 -0.782560 -1.357646
N -1.769256 -0.414913 -0.150580
H -0.103739 -2.688861 -1.975332
H 1.981726 -0.252211 -2.740242
C 2.935094 -0.649383 -0.887174
H 3.915700 -0.915717 -1.295736
H 2.916018 0.416302 -0.656605
C 3.828346 -0.918903 1.389733
H 3.645405 -1.391134 2.355939
H 4.813298 -1.207034 1.015996
H 3.770009 0.164107 1.503884
C 2.721944 -2.839550 0.310100
H 1.854203 -3.127112 -0.281554
H 3.637650 -3.204001 -0.161513
H 2.625095 -3.270461 1.307455
N 2.767881 -1.355874 0.431686
O 0.641908 -0.325425 1.409865
C 0.059662 -0.251199 2.591359
O -0.888028 0.454306 2.874775
H 0.534356 -0.921640 3.337118
H 1.826621 -1.007820 0.888569

C-1'

1 1
C -0.930806 2.944059 -0.016714
C 0.214874 2.790340 0.796122
H 0.252807 2.939362 1.867103
C 1.311395 2.345797 -0.024091
H 2.328216 2.214817 0.312358
C -0.573443 2.586740 -1.367266
H -1.217683 2.633301 -2.234296
C 0.812758 2.236967 -1.361630
H 1.383459 1.959708 -2.239404
H -1.906157 3.270365 0.317933
Ru -0.291852 0.781452 -0.096859
C -0.832136 -1.903747 -1.060123
C 1.359004 -1.377108 -1.765171
C -2.099959 -1.525579 -0.482783
H 1.144910 -2.129209 -2.535116
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C 2.445255 -1.989415 -0.873161
H 1.998684 -2.756277 -0.234838
H 3.190649 -2.471208 -1.515407
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H 4.394197 0.669339 0.040999
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H 3.173304 0.639341 -1.242840
C 4.148955 -1.825305 0.880704
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H 4.901282 -2.301395 0.247288
H 4.619172 -1.136649 1.581829
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C 0.781399 -0.442118 2.487290
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H 0.581870 -0.738776 3.532409
H 2.491997 -0.620932 0.787969

C-2

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C -1.073254 0.019299 2.667488
H -1.381443 -0.918867 3.108555
C -1.850649 0.853408 1.790331
H -2.847849 0.669124 1.424979
H 0.974058 0.309832 3.517134
Ru 0.032395 0.206832 0.706342
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C -1.800731 -1.637157 -1.120666
C 1.716273 -2.112299 -0.059875
H -1.985191 -0.699907 -1.651074

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 C 2.957776 -0.624446 1.228259
 C 4.026178 -2.606854 0.377581
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C-2*
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 C 2.264598 -1.776036 0.598835
 H 3.218497 -1.480577 0.174447
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 H 0.577069 -2.985462 1.273183
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 C 2.102390 -1.360725 1.476404
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C-IM-e

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C-3

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Ru -0.113084 -0.941907 -0.674185
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C-5

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 C 1.480793 0.170609 1.952517
 C 2.742245 -1.521827 0.836262
 C 0.223727 0.860127 2.165957
 H 3.510144 -1.216593 1.556835
 C 0.071081 1.966736 3.003835
 C -2.026728 0.932249 1.549460
 C -1.183351 2.561982 3.111132
 H 0.927504 2.349076 3.548879
 C -2.243889 2.036696 2.369975
 H -2.816819 0.511891 0.938805
 H -1.330188 3.423988 3.753250
 H -3.233437 2.477163 2.408903
 N 1.498066 -0.778755 1.072680
 N -0.820919 0.344435 1.454537
 H 2.369990 0.465616 2.506237
 H 2.522428 -2.578364 1.013080
 C -3.746172 0.063305 -1.770236
 C -4.856260 0.735555 -1.253528
 C -4.756525 2.084076 -0.901829
 C -3.546091 2.756787 -1.086879
 C -2.437024 2.081753 -1.599208
 C -2.522856 0.724165 -1.938833
 H -3.838083 -0.978130 -2.064918
 H -5.799539 0.209950 -1.138503
 H -5.620174 2.609795 -0.506134
 H -3.465176 3.810458 -0.836427
 H -1.495804 2.605589 -1.730407
 C -1.291182 -0.034938 -2.424434
 C -0.297204 -0.054193 -1.270246
 O 0.442815 1.035066 -1.386838

H 1.065069 1.230918 -0.646026
 C 3.240248 -1.373826 -0.604758
 H 3.968423 -2.169733 -0.815159
 H 2.385848 -1.518438 -1.271499
 N 3.838630 -0.049771 -0.890097
 C 3.802204 0.249716 -2.341291
 H 4.231758 1.240089 -2.499465
 H 4.365347 -0.494481 -2.918152
 H 2.761728 0.261526 -2.675132
 C 5.220296 0.073826 -0.373099
 H 5.901810 -0.611477 -0.893019
 H 5.547553 1.104999 -0.517170
 H 5.241877 -0.150732 0.695796
 H 3.119194 1.044918 -0.302555
 C 3.081372 3.052572 -0.294186
 O 4.141948 3.151307 -0.871081
 H 2.464444 3.918410 -0.000386
 O 2.518228 1.895667 0.074038
 H -0.837176 0.475763 -3.281505
 H -1.572600 -1.041582 -2.727413

C-6

1 1
 C 0.133825 2.755569 1.059380
 C 0.272439 2.954832 -0.357068
 H 1.144354 3.349497 -0.860848
 C -0.950284 2.596000 -0.978658
 H -1.162572 2.659369 -2.036844
 C -1.176440 2.253859 1.295363
 H -1.591842 2.012778 2.265632
 C -1.861007 2.147119 0.042125
 H -2.910102 1.924345 -0.095256
 H 0.884603 2.961203 1.809763
 Ru -0.087165 0.727628 -0.026192
 C 0.858392 -1.805755 1.049386
 C -1.428729 -1.586455 1.642654
 C 2.025745 -1.291215 0.399491
 H -1.318837 -2.657957 1.849214
 C 3.262670 -1.953551 0.352760
 C 2.869055 0.489493 -0.846550
 C 4.325536 -1.354311 -0.303774
 H 3.367662 -2.920278 0.834595
 C 4.119323 -0.107502 -0.912988
 H 2.668943 1.441979 -1.320677

H 5.294581 -1.839394 -0.348917
 H 4.921432 0.397482 -1.439705
 N -0.217053 -1.056547 1.013567
 N 1.826969 -0.072591 -0.195412
 H 0.870499 -2.776697 1.543151
 H -1.586326 -1.083701 2.603119
 C -2.680334 -1.322813 0.790629
 H -3.502498 -1.973896 1.100589
 H -2.984865 -0.281888 0.894702
 C -3.595108 -1.060996 -1.496809
 H -3.342552 -1.164919 -2.552671
 H -4.475165 -1.662583 -1.261243
 H -3.782949 -0.011105 -1.272739
 C -2.024258 -2.912872 -1.038212
 H -1.117865 -3.172388 -0.494361
 H -2.829839 -3.607895 -0.792025
 H -1.816957 -2.947235 -2.108304
 N -2.436105 -1.524601 -0.678564
 H -1.611486 -0.859184 -0.890316
 H -0.404602 -0.035401 -1.437917

C-7

1 1
 C 0.339339 2.519179 1.296745
 C 0.910161 2.894271 0.032774
 H 1.958792 3.090262 -0.150103
 C -0.119734 2.926606 -0.939691
 H -0.005625 3.182565 -1.983904
 C -1.078654 2.372635 1.094745
 H -1.802235 2.113303 1.856372
 C -1.363089 2.600516 -0.274132
 H -2.339480 2.565925 -0.737759
 H 0.861169 2.462552 2.241923
 Ru 0.018822 0.829157 -0.112032
 C 0.527053 -1.780484 1.092880
 C -1.708385 -1.169878 1.637960
 C 1.788011 -1.491622 0.433932
 H -1.728796 -2.198277 2.016407
 C 2.886035 -2.353762 0.448571
 C 2.928326 0.048575 -0.883764
 C 4.046212 -1.979954 -0.225252
 H 2.821888 -3.296767 0.981251
 C 4.064120 -0.758900 -0.901380
 H 2.898434 0.995687 -1.408966

H 4.916418 -2.627554 -0.226951
H 4.943613 -0.428635 -1.442699
N -0.405178 -0.892200 1.028122
N 1.809921 -0.298079 -0.224316
H 0.385364 -2.729882 1.610584
H -1.825511 -0.499479 2.496352
C -2.866573 -0.910458 0.661737
H -3.794241 -1.266269 1.147248
H -2.967723 0.170032 0.524840
C -3.661730 -1.016043 -1.607888
H -3.451462 -1.422887 -2.600766
H -4.691112 -1.300054 -1.330061
H -3.611866 0.075804 -1.671342
C -2.619444 -2.963064 -0.630253
H -1.790531 -3.315235 -0.009550
H -3.552916 -3.410221 -0.246073
H -2.452531 -3.339544 -1.642762
N -2.658735 -1.500803 -0.657267
H -0.944068 -0.204127 -1.246734
H -0.307704 0.111754 -1.695565

C-8

1 1

C 2.579105 -2.831620 -0.995366
C 1.581174 -2.466239 -1.961413
H 0.686995 -3.022708 -2.204673
C 2.028522 -1.276977 -2.605813
H 1.502127 -0.755395 -3.393430
C 3.622232 -1.864964 -1.044794
H 4.522573 -1.873138 -0.444625
C 3.280864 -0.886762 -2.037650
H 3.909419 -0.073653 -2.374642
H 2.547488 -3.698015 -0.347999
Ru 1.679364 -0.812956 -0.397064
C 1.382805 0.505383 2.171847
C 3.147662 1.557569 0.960535
C 0.371329 -0.495713 2.221405
H 3.201313 2.172969 1.867411
C -0.510972 -0.696652 3.300606
C -0.601277 -2.269050 1.043218
C -1.438411 -1.720028 3.240175
H -0.441439 -0.046737 4.167072
C -1.476919 -2.523577 2.083150
H -0.615477 -2.855563 0.132639

H -2.120419 -1.902762 4.063516
H -2.184658 -3.340490 1.994017
N 2.126904 0.520013 1.083021
N 0.325920 -1.277192 1.087278
H 1.531175 1.211155 2.986481
H 4.125714 1.085196 0.824945
C 2.886810 2.409225 -0.283646
H 3.590032 3.243742 -0.353085
H 2.971999 1.774066 -1.164719
C 1.086926 3.381715 -1.687064
H 0.064639 3.757985 -1.649506
H 1.765476 4.154735 -2.051674
H 1.129251 2.496750 -2.322616
C 1.298032 4.094526 0.672327
H 1.585940 3.755125 1.666407
H 1.914041 4.943699 0.371883
H 0.242570 4.361239 0.680952
N 1.492065 2.977462 -0.304250
H 0.808395 2.233036 -0.036879
H 0.642107 0.254445 -1.019025

C -4.118178 -0.876014 -0.335180
C -4.050171 0.486973 -0.017590
C -4.886053 1.386702 -0.689647
C -5.786537 0.929758 -1.653338
C -5.850752 -0.430297 -1.962945
C -5.013903 -1.332823 -1.302646
H -3.474220 -1.579849 0.186441
H -4.839849 2.446073 -0.449836
H -6.438459 1.634886 -2.160066
H -6.552432 -0.785810 -2.711200
H -5.064995 -2.392407 -1.535132
C -3.036993 0.990894 0.992319
H -3.334243 1.932828 1.461205
H -2.891296 0.246311 1.788454
C -1.691406 1.162742 0.341488
O -0.969468 2.138094 0.505891
H -1.357609 0.337022 -0.310810

C-TS1-d

1 1

C -0.555140 -1.863451 2.769831
C 0.266364 -0.733012 3.074396
H 1.216558 -0.747376 3.588824
C -0.459903 0.435572 2.654469

H -0.120156 1.458090 2.749380
 C -1.757431 -1.407673 2.163845
 H -2.580576 -2.034934 1.849836
 C -1.694769 0.029476 2.082947
 H -2.451202 0.699386 1.697351
 H -0.298432 -2.899187 2.952680
 Ru 0.017257 -0.807017 0.834134
 C -0.128640 -1.708482 -1.943502
 C -1.768391 -0.005696 -1.654989
 C 0.899250 -2.564217 -1.390056
 H -1.632090 0.983117 -1.210469
 C 1.597064 -3.525415 -2.128693
 C 2.076285 -3.104578 0.544093
 C 2.556223 -4.302856 -1.489208
 H 1.379546 -3.651791 -3.184214
 C 2.796194 -4.087009 -0.128872
 H 2.244975 -2.895737 1.593914
 H 3.108349 -5.059869 -2.035820
 H 3.535405 -4.669075 0.410112
 N -0.704860 -0.871756 -1.140947
 N 1.136509 -2.356824 -0.062518
 H -0.395653 -1.776890 -2.998473
 H -1.685559 0.087271 -2.743942
 C -3.150695 -0.555399 -1.249554
 H -3.447411 -1.364853 -1.937643
 H -3.060646 -0.991535 -0.252189
 C -5.397221 0.052519 -0.530658
 H -6.051359 0.916863 -0.399620
 H -5.915958 -0.718145 -1.119446
 H -5.160725 -0.356782 0.455907
 C -4.452890 1.121792 -2.489282
 H -3.538900 1.524775 -2.933085
 H -4.900655 0.400464 -3.189175
 H -5.140335 1.953775 -2.325656
 N -4.157317 0.507851 -1.183291
 C 3.946022 3.021771 0.771871
 C 5.032650 3.857817 0.538061
 C 5.718616 3.789544 -0.679022
 C 5.321889 2.883839 -1.668451
 C 4.236142 2.043329 -1.446896
 C 3.540968 2.106524 -0.221852
 H 3.406672 3.062995 1.712585
 H 5.347012 4.561798 1.301645
 H 6.566203 4.444238 -0.856822

H 5.860102 2.835773 -2.609481
 H 3.918668 1.335265 -2.205515
 C 2.434777 1.235210 0.021005
 C 1.459005 0.477013 0.274585
 H 1.120600 1.530904 -0.244307
 H -3.609219 1.697137 -0.248632
 O -3.263661 2.459442 0.359873
 C -4.212200 3.396026 0.406342
 O -5.275046 3.344716 -0.177905
 H -3.910190 4.239066 1.049442

C-TS1-e1

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 C 1.501822 -2.271111 -2.202997
 C 0.537886 -1.403044 -2.829403
 H -0.350969 -1.709451 -3.362929
 C 0.995453 -0.068485 -2.676087
 H 0.478235 0.816195 -3.021440
 C 2.539980 -1.453024 -1.675888
 H 3.425760 -1.826207 -1.177960
 C 2.232935 -0.080154 -1.954759
 H 2.842149 0.789220 -1.760321
 H 1.461651 -3.351237 -2.167422
 Ru 0.570517 -0.919450 -0.635575
 C 0.041872 -1.722800 2.130787
 C 1.857802 -0.242125 2.270094
 C -1.020232 -2.368054 1.402446
 H 1.441131 0.769696 2.306232
 C -2.020775 -3.137444 2.008944
 C -1.976439 -2.658894 -0.694625
 C -3.019408 -3.689769 1.217683
 H -2.003457 -3.286550 3.083675
 C -2.993308 -3.441113 -0.158822
 H -1.939883 -2.429650 -1.751607
 H -3.805534 -4.293752 1.657821
 H -3.756208 -3.843278 -0.816152
 N 0.919616 -1.035823 1.462837
 N -0.989486 -2.137483 0.059185
 H 0.069423 -1.791296 3.218696
 H 1.883367 -0.622743 3.297167
 C 3.284496 -0.208045 1.697984
 H 4.031994 -0.459071 2.455026
 H 3.356955 -0.926266 0.882385
 C 4.807204 1.102685 0.213490

H 4.870186 2.075558 -0.274150
H 5.713301 0.887590 0.783610
H 4.650328 0.325234 -0.532741
C 3.855124 2.180750 2.197090
H 2.995461 2.206838 2.865661
H 4.761508 1.943754 2.757651
H 3.943324 3.141593 1.689485
N 3.637214 1.141474 1.141412
C -3.667150 2.475507 -1.156413
C -4.922782 3.064758 -1.053486
C -5.631827 2.998878 0.150394
C -5.082330 2.343313 1.257231
C -3.825069 1.756053 1.165601
C -3.099730 1.812456 -0.045348
H -3.110050 2.518777 -2.086829
H -5.352401 3.575057 -1.909860
H -6.612265 3.459181 0.226224
H -5.635635 2.295739 2.190019
H -3.386981 1.248323 2.019083
C -1.824444 1.202832 -0.146506
C -0.691255 0.704452 -0.235793
H 0.307830 1.527154 0.010468
H 2.772508 1.491724 0.621693
O 1.370905 2.212920 0.280277
C 1.740523 3.188055 -0.520149
O 2.908429 3.531490 -0.652615
H 0.917352 3.677167 -1.072316

C-TS1-e2

1 1

C 2.562933 1.503540 -2.217455
C 1.864800 0.395352 -2.818594
H 2.314783 -0.448697 -3.322838
C 0.472114 0.665021 -2.726343
H -0.320237 0.025332 -3.088816
C 1.600814 2.423585 -1.745446
H 1.825495 3.360788 -1.251984
C 0.291059 1.901026 -2.028262
H -0.659845 2.384537 -1.860134
H 3.636574 1.610811 -2.137644
Ru 1.259339 0.380036 -0.631646
C 1.875904 0.173525 2.218128
C -0.046953 1.535546 2.034019
C 2.837189 -0.720250 1.620259

H -0.923112 0.909807 1.829497
C 3.781927 -1.451149 2.349654
C 3.554946 -1.666381 -0.380719
C 4.642176 -2.306513 1.672666
H 3.826380 -1.341991 3.428276
C 4.522127 -2.413055 0.282832
H 3.421732 -1.735832 -1.453021
H 5.386118 -2.883886 2.210809
H 5.166378 -3.073630 -0.286709
N 1.078813 0.822303 1.425502
N 2.726158 -0.822241 0.263729
H 1.806448 0.256367 3.302710
H 0.075817 1.592959 3.121379
C -0.255512 2.937893 1.433826
H 0.020715 3.735112 2.129266
H 0.351409 3.029618 0.534777
C -1.864535 4.337465 0.133925
H -2.882873 4.300118 -0.254031
H -1.692081 5.251068 0.706432
H -1.154233 4.279780 -0.691185
C -2.635899 3.202412 2.172088
H -2.506957 2.315357 2.792517
H -2.443942 4.102188 2.759993
H -3.644704 3.208438 1.758619
N -1.681730 3.149011 1.020758
C -1.816193 -3.860283 -0.568424
C -2.694611 -4.937107 -0.482189
C -3.972221 -4.765390 0.059284
C -4.367392 -3.507082 0.518248
C -3.492992 -2.425249 0.434485
C -2.206345 -2.587677 -0.109714
H -0.825602 -3.989004 -0.993461
H -2.383392 -5.913940 -0.840312
H -4.654510 -5.607397 0.122332
H -5.357391 -3.368320 0.942258
H -3.796575 -1.450072 0.803207
C -1.302491 -1.460305 -0.201978
C -0.184290 -0.900645 -0.346341
H -1.892959 -0.215619 -0.213163
H -1.967703 2.278872 0.466056
O -2.479069 0.902592 -0.121414
C -3.690503 1.139757 -0.590046
O -4.230765 2.230404 -0.491513
H -4.176993 0.273968 -1.072315

C-TS2

1 1

C 3.736881 -1.933847 -0.581564
C 2.780718 -2.818602 0.037678
H 2.864080 -3.272503 1.015290
C 1.769008 -3.088309 -0.926693
H 0.913572 -3.732619 -0.778075
C 3.297735 -1.640332 -1.887355
H 3.797628 -0.990162 -2.593261
C 2.048260 -2.324750 -2.105857
H 1.491854 -2.357777 -3.032357
H 4.628200 -1.538733 -0.111294
Ru 1.630584 -0.900234 -0.400547
C 1.426451 2.012840 -0.440005
C 0.684667 1.235544 -2.557544
C 1.916110 1.750354 0.898913
H 0.927925 2.251325 -2.890411
C 2.131813 2.746012 1.854318
C 2.601257 0.087583 2.378854
C 2.602132 2.381644 3.111597
H 1.915513 3.779692 1.607965
C 2.845908 1.029471 3.374289
H 2.756526 -0.971840 2.544389
H 2.773518 3.132414 3.875596
H 3.214159 0.701992 4.340079
N 1.211356 0.999103 -1.210492
N 2.139413 0.434791 1.162765
H 1.251980 3.037383 -0.762102
H 1.183257 0.539053 -3.235650
C -2.840569 -1.964652 1.831305
C -4.103369 -2.163706 2.384078
C -5.226115 -2.316397 1.565802
C -5.077607 -2.280910 0.178388
C -3.815616 -2.087805 -0.379684
C -2.681617 -1.908576 0.436285
H -1.977867 -1.838270 2.469280
H -4.211346 -2.204452 3.463855
H -6.206176 -2.471303 2.006268
H -5.939838 -2.411921 -0.468435
H -3.703881 -2.076751 -1.461847
C -1.387831 -1.717660 -0.237750
C -0.199790 -1.186268 0.009980
H -1.359366 -2.114779 -1.261555

O -0.776847 0.061872 1.941791
H 0.031578 0.163801 2.454590
C -0.819782 0.960148 -2.646568
H -1.123737 0.961085 -3.699008
H -1.022794 -0.021879 -2.222769
N -1.676213 1.940255 -1.912191
C -3.067177 1.414274 -1.743583
H -3.630517 2.156633 -1.178028
H -3.522227 1.245098 -2.723005
H -3.025430 0.482529 -1.177950
C -1.705481 3.288499 -2.550592
H -2.189564 3.223558 -3.528624
H -2.252165 3.951176 -1.879243
H -0.688211 3.662812 -2.671786
H -1.329286 2.091371 -0.840101
C -1.901158 3.229680 1.000608
O -2.703193 3.868982 0.328470
H -1.830709 3.385545 2.095895
O -1.069162 2.329383 0.540993
H -0.899585 0.921473 1.466343

C-TS3

1 1

C 3.629467 -1.262185 -1.682787
C 2.718136 -2.350423 -1.441293
H 2.918478 -3.236594 -0.854836
C 1.560143 -2.119425 -2.247937
H 0.692368 -2.763245 -2.303785
C 3.023389 -0.367035 -2.596274
H 3.466442 0.543862 -2.977365
C 1.721619 -0.884793 -2.936928
H 1.033933 -0.466422 -3.659355
H 4.609311 -1.146811 -1.238064
Ru 1.703496 -0.466720 -0.689612
C 1.308103 2.012198 0.788261
C 0.856811 2.471957 -1.497505
C 1.840064 1.130387 1.791150
H 1.051296 3.503716 -1.182049
C 1.992274 1.472339 3.141413
C 2.881852 -0.925757 2.142864
C 2.609303 0.577461 4.004394
H 1.624374 2.431076 3.491750
C 3.074938 -0.639046 3.488090
H 3.238831 -1.852455 1.704652

H 2.736690 0.818335 5.054164
 H 3.584841 -1.358540 4.119072
 N 1.188526 1.533083 -0.419754
 N 2.259931 -0.076192 1.296189
 H 1.085011 3.049843 1.031271
 H 1.533461 2.261251 -2.329766
 C -2.909294 -2.139436 1.236958
 C -4.161588 -2.701930 1.485018
 C -5.130897 -2.751914 0.480601
 C -4.836636 -2.234869 -0.782211
 C -3.584859 -1.673598 -1.032394
 C -2.596617 -1.621744 -0.033505
 H -2.166860 -2.107400 2.025497
 H -4.382018 -3.100754 2.470966
 H -6.104380 -3.188684 0.680158
 H -5.579593 -2.271226 -1.573605
 H -3.360364 -1.287212 -2.025194
 C -1.316831 -0.921759 -0.336149
 C -0.020055 -1.243874 0.093606
 H -1.313708 -0.419140 -1.301220
 O 0.036457 -2.129795 1.102354
 H 0.955293 -2.232832 1.383949
 C -0.560843 2.324921 -2.047840
 H -0.676312 2.953583 -2.936147
 H -0.726650 1.284511 -2.331374
 N -1.650521 2.697803 -1.082494
 C -2.994007 2.275193 -1.598882
 H -3.742412 2.558133 -0.860103
 H -3.183861 2.766143 -2.555391
 H -3.003443 1.191302 -1.717842
 C -1.673482 4.142699 -0.698145
 H -1.939869 4.747896 -1.567111
 H -2.408528 4.247432 0.100582
 H -0.694188 4.440325 -0.325700
 H -1.511365 2.146737 -0.170613
 C -2.731885 1.465999 1.704786
 O -3.354957 2.501691 1.556600
 H -3.091900 0.633154 2.331027
 O -1.556161 1.242861 1.114853
 H -1.381597 0.176619 0.559588

C-TS4

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C -0.926538 2.984357 -0.909715

C -1.228784 2.930654 0.495631
 H -2.215704 2.970929 0.936065
 C -0.007676 2.845134 1.208135
 H 0.091281 2.786386 2.283590
 C 0.493157 2.926805 -1.045487
 H 1.035798 2.963430 -1.981673
 C 1.076673 2.836898 0.256787
 H 2.130902 2.879647 0.493480
 H -1.642182 3.080842 -1.714486
 Ru -0.187040 1.002121 -0.079211
 C -0.233056 -1.485917 -1.596935
 C 1.862530 -0.434629 -1.983921
 C -1.530401 -1.483450 -0.977959
 H 2.044159 -1.346452 -2.566267
 C -2.463237 -2.520439 -1.101973
 C -2.955951 -0.283049 0.420507
 C -3.683157 -2.411004 -0.447751
 H -2.219470 -3.391555 -1.701302
 C -3.929854 -1.269923 0.324693
 H -3.099084 0.598111 1.032495
 H -4.426706 -3.196517 -0.528513
 H -4.865661 -1.145982 0.857964
 N 0.536315 -0.455699 -1.368109
 N -1.775550 -0.367344 -0.224507
 H 0.079601 -2.315027 -2.231080
 H 1.917185 0.411668 -2.676704
 C 2.944756 -0.214235 -0.928244
 H 3.944023 -0.261275 -1.369919
 H 2.790077 0.759960 -0.465459
 C 3.619399 -0.740898 1.399406
 H 3.512671 -1.485138 2.188502
 H 4.671696 -0.595780 1.149422
 H 3.166597 0.197606 1.720402
 C 3.334102 -2.591460 -0.218218
 H 2.760206 -2.919322 -1.084165
 H 4.397800 -2.563826 -0.460640
 H 3.148916 -3.273143 0.612007
 N 2.882713 -1.224274 0.187353
 H 1.891318 -1.338177 0.510727
 H 0.375662 0.142549 1.247376
 C -0.012398 -1.133280 2.048146
 O 0.708938 -1.992781 1.575263
 O -0.824070 -0.814025 2.851196

C-TS5

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C 0.199833 2.650830 1.125452
 C 0.402137 2.930204 -0.271106
 H 1.324282 3.274923 -0.719715
 C -0.811267 2.686532 -0.959833
 H -0.976443 2.815602 -2.020555
 C -1.163694 2.249072 1.283498
 H -1.634522 1.979461 2.220272
 C -1.795056 2.256044 0.007213
 H -2.840202 2.065167 -0.191611
 H 0.924909 2.781218 1.916556
 Ru -0.121492 0.743700 -0.046355
 C 0.823194 -1.751921 1.135894
 C -1.486378 -1.532402 1.660394
 C 1.998374 -1.270148 0.447754
 H -1.379116 -2.597203 1.898565
 C 3.230159 -1.932860 0.449766
 C 2.819137 0.391847 -0.956887
 C 4.288622 -1.391066 -0.270703
 H 3.342542 -2.853615 1.012823
 C 4.073677 -0.209696 -0.986962
 H 2.611993 1.297609 -1.513061
 H 5.257907 -1.877700 -0.281116
 H 4.866998 0.245234 -1.569623
 N -0.243070 -1.015289 1.086717
 N 1.793030 -0.110577 -0.244361
 H 0.837096 -2.716538 1.644357
 H -1.685954 -1.003359 2.598528
 C -2.690524 -1.291358 0.730297
 H -3.532174 -1.906655 1.076618
 H -2.986541 -0.242583 0.797486
 C -3.510433 -1.103394 -1.558856
 H -3.230634 -1.249249 -2.604507
 H -4.433831 -1.658759 -1.353543
 H -3.685205 -0.038120 -1.391182
 C -2.019024 -2.947503 -0.982994
 H -1.141119 -3.222804 -0.397167
 H -2.837032 -3.643860 -0.757740
 H -1.761328 -3.033220 -2.040846
 N -2.402695 -1.553824 -0.695759
 H -1.306199 -0.653877 -0.988139
 H -0.573182 -0.131720 -1.440517

C-TS6

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C 3.444719 -1.811954 -1.317702
 C 2.340211 -1.826667 -2.234496
 H 1.769570 -2.691820 -2.541473
 C 2.183389 -0.496181 -2.728319
 H 1.433908 -0.175124 -3.439395
 C 3.957534 -0.483105 -1.254845
 H 4.803800 -0.159282 -0.663349
 C 3.171488 0.341783 -2.128314
 H 3.348013 1.384069 -2.356379
 H 3.833458 -2.665395 -0.777961
 Ru 1.811344 -0.478333 -0.496021
 C 1.071498 0.414585 2.152109
 C 2.317320 2.151752 1.102875
 C 0.556056 -0.923782 2.122544
 H 2.319066 2.583289 2.111491
 C -0.208268 -1.505243 3.145096
 C 0.467226 -2.889795 0.867212
 C -0.629543 -2.818673 3.011999
 H -0.460348 -0.916917 4.021231
 C -0.276069 -3.524032 1.850809
 H 0.743129 -3.392747 -0.051715
 H -1.219826 -3.292918 3.788630
 H -0.577600 -4.555829 1.708757
 N 1.754143 0.803943 1.104541
 N 0.883039 -1.608740 0.981512
 H 0.925920 1.048757 3.024908
 H 3.359495 2.087513 0.776906
 C 1.602325 3.062543 0.104112
 H 2.099011 4.037237 0.053691
 H 1.635405 2.583390 -0.876465
 C -0.527432 3.990420 -0.722579
 H -1.595405 4.052377 -0.508790
 H -0.113239 4.993003 -0.852232
 H -0.373468 3.406492 -1.630743
 C -0.068423 4.049112 1.688962
 H 0.345532 3.483165 2.521944
 H 0.409206 5.030094 1.630661
 H -1.141934 4.165411 1.843083
 N 0.150372 3.301373 0.416979
 H -0.385235 2.340097 0.531181
 H 0.279932 -0.017482 -0.884525
 C -4.122389 -0.862846 -1.879756

C -3.511715 -0.566066 -0.655758
 C -4.276098 0.017666 0.364650
 C -5.630683 0.282585 0.168808
 C -6.235914 -0.025386 -1.053069
 C -5.479348 -0.597760 -2.076782
 H -3.538673 -1.315910 -2.677334
 H -3.799214 0.264271 1.309294
 H -6.216250 0.725896 0.968928
 H -7.291709 0.177703 -1.204400
 H -5.944347 -0.841864 -3.027228
 C -2.031425 -0.835391 -0.437137
 H -1.860478 -1.349401 0.511800
 H -1.624487 -1.447548 -1.245357
 C -1.318480 0.496204 -0.395997
 O -1.236787 1.145610 0.679021
 H -1.256806 1.026596 -1.360165

D

1 1

C 0.611905 2.745759 0.248277
 C 1.770979 2.160676 0.806041
 H 2.068817 2.216728 1.843816
 C 2.507523 1.515650 -0.260042
 H 3.471937 1.035248 -0.172595
 C 0.592899 2.464555 -1.164756
 H -0.143930 2.809120 -1.876887
 C 1.785361 1.727620 -1.465573
 H 2.074810 1.372725 -2.446359
 H -0.137718 3.306429 0.791075
 Ru 0.489933 0.520407 -0.102690
 C -1.228312 -1.380086 -1.482566
 C 1.072761 -1.887857 -1.917614
 C -2.184556 -0.618001 -0.701931
 H 0.640472 -2.780317 -2.387813
 C -3.566609 -0.818435 -0.741378
 C -2.400168 1.005968 0.950245
 C -4.382815 -0.061768 0.094985
 H -3.982943 -1.555930 -1.419765
 C -3.785398 0.862815 0.955488
 H -1.900748 1.704215 1.611283
 H -5.459627 -0.191497 0.081361
 H -4.380900 1.468043 1.630019
 N 0.014612 -1.038050 -1.380131
 N -1.601676 0.292332 0.134907

H -1.549365 -2.233786 -2.080007
 H 1.618174 -1.326545 -2.681873
 C 2.025033 -2.285888 -0.763870
 H 2.542850 -3.207358 -1.048659
 H 2.791351 -1.518088 -0.630548
 C 1.279172 -2.510759 0.555660
 H 0.328134 -3.013911 0.359016
 H 1.855344 -3.174090 1.212988
 N 0.978307 -1.240834 1.308839
 C 2.171715 -0.884588 2.122483
 H 1.968794 0.026486 2.684097
 H 2.413402 -1.691920 2.827398
 H 3.029091 -0.713282 1.472888
 C -0.145023 -1.505805 2.243167
 H 0.100456 -2.327595 2.929798
 H -0.351541 -0.604968 2.823344
 H -1.039411 -1.770865 1.678797

D-1

1 1

C -1.589336 2.640109 0.728255
 C -0.246420 2.777934 1.151343
 H 0.088627 2.709455 2.177772
 C 0.598073 2.941890 -0.003010
 H 1.658142 3.153951 0.001415
 C -1.605570 2.706635 -0.713397
 H -2.481579 2.665277 -1.346396
 C -0.259499 2.904161 -1.151591
 H 0.053790 3.015448 -2.181926
 H -2.443012 2.501370 1.376435
 Ru -0.402322 0.943028 -0.138525
 C -0.298811 -1.426231 -1.830639
 C 1.515251 -0.007436 -2.444242
 C -1.477437 -1.675161 -1.027813
 H 1.657045 -0.769613 -3.222730
 C -2.240605 -2.844679 -1.101409
 C -2.851771 -0.799172 0.634274
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 H -1.955275 -3.632188 -1.791425
 C -3.663511 -1.931282 0.601503
 H -3.023316 0.007439 1.334256
 H -3.972377 -3.863326 -0.319162
 H -4.518031 -1.991963 1.266042
 N 0.333653 -0.308089 -1.636368

N -1.790320 -0.656657 -0.176864
 H 0.013930 -2.146058 -2.588274
 H 1.339997 0.950633 -2.941557
 C 2.777159 0.109914 -1.575465
 H 3.602365 0.435835 -2.215039
 H 2.602302 0.905126 -0.845101
 O -0.904913 -0.072307 2.885219
 C 0.131461 -0.542134 2.461828
 O 0.641603 -0.355210 1.259307
 H 0.766041 -1.204795 3.089623
 H 1.951741 -0.811713 0.870936
 C 3.051767 -2.548752 1.198346
 H 2.908530 -2.489225 2.278297
 H 2.257742 -3.158697 0.765067
 H 4.026263 -2.992082 0.980657
 C 3.932899 -0.257120 1.300591
 H 3.683573 -0.212821 2.361639
 H 4.952847 -0.627886 1.172832
 H 3.846376 0.742144 0.876160
 N 2.972526 -1.174825 0.621939
 C 3.157612 -1.206798 -0.870927
 H 4.201008 -1.479977 -1.055216
 H 2.533588 -2.028402 -1.233422

D-1*

1 1

C 1.567967 2.698031 -0.933774
 C 0.143239 2.825428 -0.838337
 H -0.544957 2.864009 -1.672040
 C -0.236112 2.812891 0.529766
 H -1.239594 2.933920 0.912001
 C 2.070085 2.600734 0.409103
 H 3.109238 2.496552 0.693847
 C 0.966300 2.663227 1.311797
 H 1.030496 2.642415 2.391588
 H 2.153277 2.723649 -1.841967
 Ru 0.767255 0.854652 0.035244
 C 0.635002 -1.709868 1.406776
 C -1.126688 -0.352751 2.268267
 C 1.833554 -1.842456 0.606052
 H -1.271797 -1.222717 2.924224
 C 2.588825 -3.016537 0.519001
 C 3.305262 -0.714431 -0.798783
 C 3.746459 -3.017267 -0.251774

H 2.263945 -3.905720 1.049523
 C 4.109680 -1.844432 -0.920088
 H 3.540667 0.209515 -1.313689
 H 4.354263 -3.912074 -0.334138
 H 5.004053 -1.800291 -1.531482
 N 0.013211 -0.570235 1.371357
 N 2.194429 -0.699332 -0.044267
 H 0.312950 -2.528830 2.051648
 H -0.872492 0.500762 2.903558
 C -2.417846 -0.022818 1.505891
 H -3.153704 0.345651 2.227413
 H -2.193999 0.770494 0.788055
 O -0.000353 -0.314903 -1.605326
 C -1.162363 -0.221837 -2.087544
 O -2.121851 0.472567 -1.652257
 H -1.327140 -0.837655 -2.994860
 H -3.280550 -0.227261 -1.012529
 C -4.305821 -2.033764 -1.171228
 H -4.922762 -1.701675 -2.007140
 H -3.409907 -2.523393 -1.556156
 H -4.870147 -2.728898 -0.545765
 C -5.078264 -0.061982 0.095005
 H -5.691988 0.189531 -0.770736
 H -5.660646 -0.657263 0.802487
 H -4.738900 0.857624 0.569092
 N -3.897345 -0.846246 -0.366812
 C -2.959590 -1.235769 0.747583
 H -3.487625 -1.935503 1.403918
 H -2.134463 -1.766550 0.264848

D-2

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C 0.304970 1.864714 2.183150
 C -0.925799 2.018246 1.460875
 H -1.193498 2.854433 0.830475
 C -1.732466 0.872533 1.682776
 H -2.716597 0.725169 1.275140
 C 0.239178 0.608791 2.855128
 H 1.019548 0.180643 3.471593
 C -1.007271 -0.017699 2.548989
 H -1.354760 -0.963555 2.941442
 H 1.112427 2.580899 2.236178
 Ru 0.158897 0.215549 0.630255
 C 0.525838 -2.273967 -0.839271

C -1.639636 -1.525578 -1.411967
 C 1.793547 -2.122060 -0.162450
 H -2.054750 -0.529381 -1.549779
 C 2.872510 -2.998807 -0.311209
 C 3.031580 -0.731412 1.233357
 C 4.063599 -2.719141 0.350055
 H 2.768209 -3.874522 -0.943183
 C 4.142038 -1.562769 1.130660
 H 3.064274 0.188185 1.803275
 H 4.917664 -3.380727 0.252823
 H 5.055253 -1.295823 1.649961
 N -0.395234 -1.389412 -0.625364
 N 1.869654 -1.004887 0.612420
 H 0.377230 -3.101096 -1.534477
 H -1.370984 -1.906698 -2.403651
 C -2.675150 -2.479217 -0.784019
 H -3.282861 -2.885128 -1.598338
 H -2.152206 -3.338370 -0.348588
 C 3.451371 0.483836 -1.992637
 C 4.844297 0.481388 -2.013787
 C 5.562720 1.356597 -1.194533
 C 4.882358 2.239362 -0.350327
 C 3.490151 2.242058 -0.315151
 C 2.760347 1.366246 -1.141276
 H 2.888431 -0.190234 -2.630038
 H 5.370291 -0.199265 -2.676177
 H 6.648004 1.355739 -1.218311
 H 5.438085 2.927203 0.279514
 H 2.955836 2.920894 0.342066
 C 1.328993 1.325986 -1.075622
 C 0.097485 1.360633 -1.251586
 C -3.590319 -1.888103 0.291350
 H -2.988093 -1.556347 1.141991
 H -4.247181 -2.693417 0.659422
 N -4.411091 -0.738742 -0.152076
 H -3.646848 0.610148 -0.689062
 C -5.269541 -0.275109 0.959886
 H -6.016887 -1.033158 1.235290
 H -4.657719 -0.064951 1.841767
 H -5.776480 0.641354 0.652714
 C -5.263090 -1.061006 -1.316416
 H -5.879287 -0.189028 -1.540517
 H -4.647365 -1.270683 -2.193796
 H -5.911154 -1.927568 -1.119219

H -0.827375 1.629615 -1.729229
 O -3.206803 1.467656 -1.071784
 C -4.154938 2.360905 -1.372614
 O -5.344455 2.207149 -1.202608
 H -3.712563 3.275801 -1.800422

D-2*

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 C -0.586090 -2.485211 1.829480
 C -1.063265 -3.040989 0.608761
 H -2.085207 -3.307465 0.380566
 C 0.076374 -3.232246 -0.243488
 H 0.049129 -3.630844 -1.248627
 C 0.830337 -2.319524 1.740654
 H 1.477875 -1.951686 2.524712
 C 1.240382 -2.798412 0.446130
 H 2.252870 -2.845093 0.069820
 H -1.196411 -2.208013 2.679672
 Ru -0.108939 -1.008624 0.167725
 C 0.844215 1.733246 0.275082
 C 2.613928 0.394028 -0.582997
 C -0.472489 1.841341 0.864968
 H 2.590749 -0.397894 -1.335492
 C -1.053275 3.042319 1.282415
 C -2.347129 0.630560 1.533284
 C -2.321962 3.015816 1.852472
 H -0.509688 3.972581 1.155381
 C -2.976436 1.788091 1.979960
 H -2.836697 -0.333784 1.580306
 H -2.795418 3.932768 2.186746
 H -3.969195 1.721011 2.409681
 N 1.252928 0.552379 -0.058723
 N -1.115055 0.645381 0.993428
 H 1.468047 2.616959 0.140352
 H 2.948982 1.313716 -1.073136
 C 3.603145 0.033978 0.534449
 H 3.567039 0.812934 1.304297
 H 3.299658 -0.897174 1.022310
 C -3.882749 -0.851943 -1.149323
 C -5.175579 -0.360085 -0.991099
 C -5.437186 1.001071 -1.177298
 C -4.401324 1.869324 -1.532500
 C -3.106341 1.384566 -1.701298
 C -2.835510 0.016271 -1.511175

H -3.671057 -1.905755 -1.001720
H -5.980929 -1.037324 -0.724066
H -6.445971 1.381715 -1.051152
H -4.603973 2.925039 -1.684164
H -2.297269 2.053091 -1.976883
C -1.491065 -0.466429 -1.635301
C -0.335611 -0.762793 -1.998801
H 0.414237 -0.919432 -2.752321
C 5.025089 -0.128194 -0.020712
H 5.034760 -0.987532 -0.702488
H 5.708878 -0.379775 0.812878
N 5.475981 1.040647 -0.774433
C 6.640041 0.726993 -1.601932
H 6.912776 1.602567 -2.198170
H 7.524360 0.427780 -1.010421
H 6.398369 -0.088059 -2.291037
C 5.745821 2.188458 0.088443
H 6.535488 1.989236 0.836477
H 6.063125 3.038128 -0.522505
H 4.841857 2.491493 0.626123

D-IM-e

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C 0.615168 -0.676058 2.745205
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C 0.401618 -1.882770 2.006327
H -0.558692 -2.352231 1.858832
C 2.684329 -1.507604 2.145216
H 3.754284 -1.620872 2.033675
C 1.699320 -2.396450 1.653437
H 1.908389 -3.310150 1.112081
H 2.479490 0.396193 3.339935
Ru 1.367828 -0.330363 0.648661
C 1.921916 0.131682 -2.178171
C 0.079866 -1.322577 -2.147483
C 2.871609 0.991931 -1.522935
H -0.853947 -0.967913 -1.701740
C 3.776324 1.816745 -2.203130
C 3.599720 1.784389 0.538220
C 4.623856 2.636497 -1.470722
H 3.798209 1.805375 -3.288013
C 4.527912 2.617148 -0.074094
H 3.483395 1.760884 1.613984

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H 5.160370 3.248678 0.539961
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H 1.824139 0.163153 -3.263550
H 0.066869 -0.998535 -3.195115
C 0.174961 -2.863588 -2.144848
H -0.253076 -3.228654 -3.083933
H 1.230221 -3.154986 -2.167486
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C -3.518480 4.201247 -1.171158
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C -2.113426 2.741731 0.177404
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H -3.731926 4.676877 -2.123920
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H -1.708493 0.096189 0.393105
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H -3.915888 0.499157 0.606077

D-3

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 H -2.188510 -2.667630 1.703556
 H 1.335929 -0.784141 3.458090
 Ru 0.143687 -0.819558 0.687842
 C 0.413720 -1.828570 -2.026040
 C -1.570720 -0.539043 -2.029284
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 H -1.717959 0.445742 -1.586296
 C 2.589981 -3.083058 -2.035445
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 H 2.907001 -1.987524 1.622942
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 H 4.719794 -3.357284 0.593569
 N -0.437522 -1.161881 -1.317541
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 C 3.589935 1.826048 0.022065
 C 4.862827 2.385976 -0.010572
 C 5.029511 3.743552 -0.305098
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 H -5.713436 0.295013 -2.144795
 H 0.253455 2.698302 -0.473456
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 C -2.967056 3.203640 0.261138
 O -4.158401 3.405394 0.164429
 H -2.236410 3.986593 0.525254

D-2'

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 C 0.607693 -2.953411 -0.009854
 H 0.537222 -3.537251 -0.917479
 C 1.736379 -2.201954 0.409019
 H 2.682938 -2.140329 -0.109936
 C 0.070610 -1.954485 1.993543
 H -0.472530 -1.634332 2.873774
 C 1.403135 -1.560841 1.654299
 H 2.058774 -0.948065 2.257317
 H -1.401091 -3.281982 0.951217
 Ru 0.031239 -0.754938 0.062308
 C 0.479111 2.062960 -0.486345
 C 2.298126 0.833837 -1.423381
 C -0.718280 2.093543 0.324853
 H 2.281954 -0.092837 -2.003265
 C -1.424889 3.256688 0.644618
 C -2.201611 0.781208 1.551658
 C -2.550669 3.160610 1.456208
 H -1.086816 4.212084 0.257400
 C -2.941847 1.901052 1.916989
 H -2.495258 -0.214514 1.858299
 H -3.115931 4.047485 1.721981
 H -3.816643 1.777754 2.544909
 N 1.029639 0.909772 -0.688588
 N -1.104118 0.866088 0.778413

H	0.905366	2.983486	-0.885070
H	2.373181	1.672099	-2.127650
C	3.492254	0.838600	-0.461797
H	3.547300	1.813326	0.036009
H	3.323856	0.094218	0.320983
C	-3.663440	0.692693	-1.516074
C	-4.979588	0.989244	-1.169248
C	-5.745764	0.061734	-0.458195
C	-5.191810	-1.169585	-0.093934
C	-3.874477	-1.471292	-0.429258
C	-3.098136	-0.543136	-1.148498
H	-3.063122	1.408482	-2.068110
H	-5.409811	1.942991	-1.458814
H	-6.772436	0.294286	-0.193083
H	-5.788815	-1.894953	0.450071
H	-3.438625	-2.423788	-0.145869
C	-1.726990	-0.816673	-1.468135
C	-0.620032	-0.977615	-2.020335
C	4.814287	0.532108	-1.205017
H	4.982175	1.300962	-1.970389
H	4.701757	-0.421776	-1.739528
N	6.006777	0.443988	-0.380869
C	6.007380	-0.669327	0.555228
H	5.295161	-0.556892	1.395647
H	5.768276	-1.598986	0.026929
H	7.005862	-0.780362	0.988980
C	6.409804	1.700624	0.234670
H	7.412255	1.591449	0.659868
H	6.452004	2.488216	-0.524591
H	5.740762	2.040800	1.047309
H	-0.005761	-1.150289	-2.885005

D-3'

1 1

C	-0.080326	-1.723647	2.239098
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C	1.184490	-2.628865	0.527039
H	1.497776	-3.245857	-0.303784
C	1.246676	-1.161682	2.309253
H	1.583794	-0.422058	3.023298
C	2.013662	-1.713617	1.262806
H	3.015236	-1.411140	0.973574
H	-0.888437	-1.542575	2.934854

Ru	0.174185	-0.600279	0.276413
C	1.098884	1.801816	-1.047041
C	2.275762	-0.091137	-1.981551
C	0.117442	2.317766	-0.114298
H	2.524991	-1.063336	-1.560372
C	-0.220762	3.669208	-0.004888
C	-1.384161	1.740162	1.571453
C	-1.174759	4.052148	0.932998
H	0.258553	4.396136	-0.651992
C	-1.764050	3.069688	1.732532
H	-1.828922	0.946069	2.157934
H	-1.458576	5.093901	1.037007
H	-2.517058	3.322167	2.470442
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H	1.629855	2.482920	-1.708988
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C	3.562742	0.699918	-2.240622
H	4.145339	0.120090	-2.964029
H	3.354526	1.651928	-2.742169
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C	-6.088076	-0.460587	-1.544763
C	-4.785919	-0.677029	-1.996122
C	-3.727631	-0.800377	-1.082777
H	-3.197396	-0.847887	1.007974
H	-5.508534	-0.443370	1.805813
H	-7.367396	-0.201148	0.171793
H	-6.896448	-0.368919	-2.263824
H	-4.586765	-0.746979	-3.061997
C	-2.351984	-1.000133	-1.582976
C	-1.258872	-0.839802	-0.866480
C	4.391525	0.981691	-0.978954
H	3.842297	1.683738	-0.340498
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H	5.435865	-0.712046	1.724789
C	5.534412	-1.166621	-0.868703
H	5.728866	-2.022344	-0.216312
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D-4

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H 0.794896 0.330049 -3.507615
C 2.440456 2.495314 -1.547671
H 2.589212 3.385476 -0.950074
C 1.224751 2.112373 -2.207141
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Ru 1.702637 0.481325 -0.679689
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C 0.587548 2.049627 1.951972
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C 0.328972 -0.657327 2.781462
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C 0.654663 -2.639765 1.652561
H 0.482528 -3.531921 1.065415
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D-6

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 Ru 0.018554 0.840287 -0.020682
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D-7

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C 0.101525 2.870933 -1.238861
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H -2.136140 2.626798 -1.065973
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H 0.964560 2.863286 2.010159
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H -1.703144 2.568836 1.582481
H 2.160339 3.069508 -0.402257
Ru 0.113312 0.915728 -0.104418
C 0.550556 -1.506515 1.458976
C -1.535712 -0.586712 2.147241
C 1.759625 -1.429049 0.659726
H -1.490352 -1.437510 2.839799
C 2.783019 -2.378500 0.704198
C 2.910672 -0.163932 -0.917348
C 3.910547 -2.192925 -0.091579
H 2.687759 -3.240711 1.355875
C 3.972816 -1.065541 -0.913163
H 2.914401 0.714173 -1.552273
H 4.723109 -2.911315 -0.073791
H 4.831021 -0.880281 -1.549401
N -0.318636 -0.560941 1.329145
N 1.823500 -0.330140 -0.144808
H 0.405277 -2.333824 2.154350
H -1.535045 0.329965 2.745588
C -2.828296 -0.661118 1.321528
H -3.654418 -0.689157 2.040301
H -2.944492 0.258949 0.741611
H -0.289211 0.027584 -1.541072
H -0.903966 -0.290989 -1.030937
C -1.815803 -2.826336 -1.580217
H -1.353310 -2.560849 -2.536206

H -1.047986 -3.281291 -0.946446
H -2.595996 -3.580036 -1.777385
C -3.287653 -0.926697 -1.809067
H -2.792928 -0.639892 -2.742262
H -4.161947 -1.551028 -2.056416
H -3.646259 -0.013659 -1.325738
N -2.334110 -1.618299 -0.938358
C -2.904678 -1.884257 0.392152
H -3.948597 -2.227687 0.305188
H -2.349245 -2.714895 0.843076

D-8

1 1

C 3.850818 -1.733598 -0.889331
C 3.033496 -1.534345 -2.051442
H 2.572337 -2.305029 -2.653038
C 3.003352 -0.132775 -2.313744
H 2.470553 0.342724 -3.125870
C 4.312795 -0.459513 -0.445367
H 4.960315 -0.281398 0.403283
C 3.780479 0.541402 -1.323296
H 3.987642 1.601947 -1.288751
H 4.087336 -2.687017 -0.435548
Ru 2.027821 -0.500092 -0.284725
C 0.638952 -0.100691 2.223204
C 2.063998 1.782023 1.783480
C 0.167584 -1.384373 1.813861
H 1.923593 1.988042 2.854089
C -0.747671 -2.177503 2.531810
C 0.379903 -3.046139 0.176839
C -1.076473 -3.434407 2.060331
H -1.171997 -1.791680 3.453364
C -0.495595 -3.875272 0.854983
H 0.839383 -3.344373 -0.758093
H -1.768644 -4.068077 2.604332
H -0.724062 -4.854443 0.448949
N 1.529209 0.465763 1.429835
N 0.731295 -1.816386 0.632151
H 0.324847 0.353009 3.161485
H 3.136850 1.766580 1.583276
C 1.412340 2.884195 0.926196
H 2.038498 3.781194 0.956179
H 1.389751 2.512750 -0.104406
H 0.783909 0.169479 -1.058751

C -0.003645 3.202568 1.413558
 H 0.003868 3.907209 2.251626
 H -0.504295 2.287941 1.742106
 N -0.888867 3.778562 0.339330
 C -0.330646 5.010386 -0.291846
 C -2.276970 4.005290 0.844656
 H -0.982012 3.007368 -0.410279
 H -1.019775 5.350787 -1.065594
 H -0.211635 5.786213 0.468114
 H 0.632322 4.780960 -0.745354
 H -2.667505 3.065902 1.238348
 H -2.263833 4.764486 1.629347
 H -2.904453 4.335491 0.016029
 O -1.303419 1.825502 -1.354303
 C -1.270171 0.669212 -0.910976
 C -1.780357 -0.505734 -1.694792
 H -1.060412 0.476938 0.154605
 C -3.205663 -0.729599 -1.206268
 H -1.157638 -1.379574 -1.492831
 H -1.747426 -0.266536 -2.760586
 C -4.236658 0.117145 -1.637475
 C -3.489779 -1.736365 -0.275773
 C -5.536957 -0.059087 -1.165320
 H -4.015205 0.907647 -2.349885
 C -4.791087 -1.910171 0.198971
 H -2.694470 -2.392045 0.063913
 C -5.816819 -1.073652 -0.245274
 H -6.332966 0.589976 -1.518114
 H -5.004331 -2.702580 0.910453
 H -6.830128 -1.213415 0.118795

D-TS1-d

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 C -1.872804 -2.337779 -2.423057
 H -2.947739 -2.314116 -2.530394
 C -0.941107 -1.382452 -2.959875
 H -1.202149 -0.481241 -3.498089
 C 0.280074 -3.062788 -1.947227
 H 1.103420 -3.672184 -1.601092
 C 0.378281 -1.814796 -2.659686
 H 1.290487 -1.313865 -2.953455
 H -1.499404 -4.239898 -1.298983
 Ru -0.718901 -1.402985 -0.716067

C 0.540832 -0.873270 1.859626
 C 2.017087 -0.085063 0.167408
 C -0.683005 -1.544783 2.244686
 H 1.785741 0.538718 -0.699638
 C -1.059967 -1.787335 3.569257
 C -2.615840 -2.564642 1.442078
 C -2.253979 -2.454790 3.820240
 H -0.417810 -1.454832 4.378211
 C -3.042655 -2.849868 2.735669
 H -3.205868 -2.837731 0.575218
 H -2.567840 -2.661806 4.837782
 H -3.981957 -3.370765 2.884247
 N 0.771346 -0.732233 0.594131
 N -1.455133 -1.933812 1.189358
 H 1.233183 -0.505706 2.617585
 H 2.379327 0.579662 0.957162
 C 3.085001 -1.125651 -0.198538
 H 3.386880 -1.664656 0.706169
 H 2.645343 -1.870434 -0.868126
 C -3.810617 3.078930 -1.516406
 C -4.612288 4.212416 -1.433006
 C -4.819992 4.832597 -0.196625
 C -4.229344 4.320802 0.963567
 C -3.427092 3.186965 0.893314
 C -3.212953 2.557492 -0.350170
 H -3.641592 2.587835 -2.469168
 H -5.075033 4.614344 -2.328434
 H -5.445252 5.718124 -0.136844
 H -4.396370 4.807120 1.919132
 H -2.964094 2.778290 1.785649
 C -2.399116 1.386112 -0.428976
 C -1.684806 0.351003 -0.526521
 H -1.037932 1.380008 -0.633716
 C 4.296584 -0.512538 -0.909684
 H 3.978502 -0.138650 -1.890466
 H 5.039346 -1.306843 -1.094742
 N 4.915215 0.620834 -0.198806
 C 5.982991 1.226584 -1.018372
 H 6.360605 2.109789 -0.499751
 H 6.809980 0.523236 -1.196897
 H 5.570463 1.535920 -1.982952
 C 5.446064 0.249738 1.124331
 H 6.226139 -0.523354 1.051890
 H 5.858882 1.146057 1.590444

H 4.642832 -0.124790 1.764343
H 3.935592 1.916658 0.055410
O 3.348703 2.742841 0.241245
C 4.073924 3.644642 0.897507
O 5.233505 3.514575 1.235127
H 3.480940 4.550883 1.107082

D-TS1-e1

1 1

C -0.195353 -1.935706 2.770741
C -0.764259 -0.636450 2.792073
H -0.318230 0.239073 3.243493
C -2.010018 -0.664713 2.082122
H -2.681915 0.173160 1.984538
C -1.092483 -2.796956 2.042523
H -0.959910 -3.855551 1.865599
C -2.205085 -2.012099 1.629772
H -3.052573 -2.391098 1.073630
H 0.727576 -2.230092 3.250701
Ru -0.326465 -1.177302 0.656447
C 0.166292 -1.611613 -2.190884
C -1.726920 -0.228923 -2.122796
C 1.290560 -2.267334 -1.569800
H -1.559392 0.786135 -1.755222
C 2.310296 -2.904118 -2.286720
C 2.358228 -2.686831 0.450139
C 3.377486 -3.459498 -1.592271
H 2.254201 -2.950854 -3.369447
C 3.398883 -3.342499 -0.198431
H 2.353922 -2.558982 1.524847
H 4.180140 -3.963787 -2.119515
H 4.217028 -3.748614 0.386031
N -0.736752 -1.068106 -1.432964
N 1.305437 -2.168664 -0.210833
H 0.123791 -1.536814 -3.278078
H -1.495130 -0.220889 -3.194670
C -3.204716 -0.651041 -1.976576
H -3.709442 -0.391803 -2.912683
H -3.262259 -1.741978 -1.901278
C 3.591205 2.212386 -1.077401
C 4.746104 2.978825 -1.190647
C 5.295279 3.590052 -0.058608
C 4.689200 3.431205 1.191890
C 3.537474 2.661292 1.316041

C 2.970813 2.041123 0.180214
H 3.153690 1.737095 -1.949733
H 5.219112 3.105528 -2.159558
H 6.195074 4.190636 -0.151140
H 5.118227 3.907483 2.067945
H 3.061423 2.529149 2.282384
C 1.797316 1.254469 0.299313
C 0.742961 0.607636 0.402532
C -4.014095 -0.079465 -0.808090
H -3.696520 -0.518561 0.133827
H -5.075876 -0.304379 -0.950559
N -3.892914 1.408827 -0.619174
H -2.886906 1.618799 -0.316071
C -4.745152 1.890622 0.514029
H -5.797709 1.821365 0.232329
H -4.558494 1.270258 1.391148
H -4.458259 2.921839 0.721633
C -4.163277 2.222668 -1.843261
H -3.980208 3.265645 -1.584964
H -3.481674 1.928708 -2.639887
H -5.196534 2.067488 -2.160998
H -0.340731 1.342972 0.313209
O -1.443299 2.025783 0.183183
C -1.401863 3.338757 0.276589
O -2.374666 4.055257 0.091304
H -0.407908 3.745901 0.538751

D-TS1-e2

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C -3.048901 -1.586026 -1.925676
C -3.785077 -0.381361 -1.816533
H -4.749050 -0.262091 -1.341409
C -3.015118 0.658371 -2.450647
H -3.314000 1.690861 -2.570346
C -1.826534 -1.322926 -2.632732
H -1.095263 -2.052501 -2.950348
C -1.832299 0.069060 -2.975614
H -1.060579 0.589282 -3.526563
H -3.359367 -2.546979 -1.535601
Ru -1.758482 -0.093454 -0.721226
C -1.421899 -0.524622 2.139341
C -0.952213 -2.617057 1.183128
C -1.874614 0.846127 2.077566
H -0.285594 -2.705508 2.049778

C -1.995522 1.672179 3.199460
 C -2.607393 2.543071 0.666453
 C -2.454213 2.974119 3.031500
 H -1.730281 1.287944 4.178909
 C -2.766954 3.412566 1.741690
 H -2.814364 2.853048 -0.350253
 H -2.562405 3.636702 3.883534
 H -3.124768 4.420321 1.562511
 N -1.338091 -1.200419 1.037739
 N -2.180941 1.277843 0.822147
 H -1.160512 -0.959936 3.103130
 H -1.864269 -3.175098 1.426606
 C -0.329188 -3.298818 -0.039486
 H -0.205379 -4.355254 0.223696
 H -1.044826 -3.276246 -0.864555
 C 2.892990 1.539785 -2.230838
 C 4.131040 2.039703 -2.626967
 C 4.994333 2.612773 -1.688298
 C 4.607263 2.689417 -0.348737
 C 3.369050 2.192075 0.054170
 C 2.494035 1.610716 -0.880510
 H 2.222285 1.090758 -2.957367
 H 4.423678 1.982666 -3.671232
 H 5.959272 2.999779 -2.000234
 H 5.269503 3.140132 0.384204
 H 3.065091 2.274181 1.092663
 C 1.225852 1.045959 -0.465974
 C 0.052221 0.632309 -0.667048
 C 0.978372 -2.740873 -0.604457
 H 0.805197 -1.759250 -1.047931
 H 1.362412 -3.416459 -1.375263
 N 2.080849 -2.536385 0.398545
 H 1.766614 -1.754062 1.046461
 C 3.308553 -1.991119 -0.268337
 H 3.719898 -2.749236 -0.937452
 H 3.039137 -1.095746 -0.828812
 H 4.024934 -1.732799 0.510987
 C 2.422876 -3.729035 1.228543
 H 3.147035 -3.406233 1.976229
 H 1.531065 -4.098858 1.732297
 H 2.835213 -4.510316 0.586644
 H 1.248262 0.444128 0.772028
 O 1.479633 -0.319879 1.763561
 C 2.532151 -0.165023 2.552944

O 3.286074 -1.077153 2.848116
 H 2.673054 0.859488 2.941586

D-TS2

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 C 3.811198 -1.480531 -1.353397
 C 3.042318 -2.578565 -0.820805
 H 3.323581 -3.221503 0.001435
 C 1.903683 -2.741454 -1.659648
 H 1.133087 -3.489681 -1.535083
 C 3.136775 -0.963108 -2.477858
 H 3.461215 -0.126438 -3.082549
 C 1.923462 -1.719260 -2.661809
 H 1.222028 -1.611362 -3.477665
 H 4.736729 -1.098821 -0.942008
 Ru 1.709153 -0.739381 -0.637053
 C 1.280699 2.071594 0.020759
 C 0.343052 1.750276 -2.125600
 C 1.992943 1.580039 1.182765
 H 0.139489 2.820161 -1.994025
 C 2.289847 2.368757 2.297498
 C 3.037206 -0.272647 2.135324
 C 2.986444 1.800522 3.359778
 H 1.967198 3.404194 2.319755
 C 3.370649 0.458723 3.272492
 H 3.298185 -1.319303 2.031974
 H 3.226493 2.387883 4.239632
 H 3.917253 -0.023064 4.075411
 N 1.020509 1.235379 -0.928014
 N 2.356166 0.269920 1.108327
 H 0.963953 3.111178 -0.025847
 H 1.049369 1.645710 -2.956208
 C -2.492425 -2.560653 1.796680
 C -3.714968 -2.892131 2.377538
 C -4.886692 -2.910562 1.616819
 C -4.827761 -2.604933 0.255774
 C -3.607157 -2.277005 -0.330059
 C -2.423701 -2.231405 0.432303
 H -1.591586 -2.543120 2.392950
 H -3.750880 -3.144974 3.433089
 H -5.834168 -3.172432 2.077722
 H -5.728282 -2.632299 -0.350755
 H -3.566051 -2.058123 -1.395120
 C -1.183825 -1.873634 -0.273782

C -0.019794 -1.290151 -0.027928
 H -1.214543 -2.080831 -1.351121
 O -0.392377 -0.618270 2.086864
 H 0.488631 -0.457843 2.439840
 C -0.936263 0.988140 -2.486488
 H -1.254577 1.319357 -3.480832
 H -0.686716 -0.072152 -2.581414
 C -2.090672 1.058912 -1.488527
 H -2.905874 0.420030 -1.843065
 H -1.775570 0.701509 -0.509225
 N -2.671672 2.423167 -1.234160
 C -3.905045 2.282024 -0.399143
 H -4.240301 3.277295 -0.104231
 H -4.684275 1.776338 -0.974255
 H -3.645945 1.706423 0.489228
 C -2.940606 3.226974 -2.453927
 H -3.619063 2.685722 -3.118716
 H -3.395880 4.172207 -2.154907
 H -2.006442 3.438153 -2.973805
 H -1.977723 2.989414 -0.570388
 O -1.426126 1.772444 1.524382
 H -0.806503 0.274034 1.983555
 C -1.201466 3.004306 1.504334
 O -1.283698 3.756682 0.481218
 H -0.890385 3.503618 2.445645

D-TS3

1 1

C 2.826107 -1.161712 2.582337
 C 2.448171 0.198862 2.866898
 H 3.124301 1.024377 3.044678
 C 1.033005 0.243227 2.992572
 H 0.445831 1.120526 3.228811
 C 1.640510 -1.927496 2.492391
 H 1.590714 -2.986364 2.275334
 C 0.515589 -1.065310 2.735308
 H -0.515883 -1.367124 2.849585
 H 3.835001 -1.526652 2.445899
 Ru 1.539384 -0.291115 0.837862
 C 1.822468 -1.010377 -1.974604
 C -0.121508 -2.107354 -1.241426
 C 2.901726 -0.079533 -1.775024
 H -0.896878 -1.384838 -1.496194
 C 3.796679 0.305485 -2.781121

C 3.968277 1.296933 -0.226254
 C 4.806277 1.210742 -2.483807
 H 3.685494 -0.108204 -3.778111
 C 4.891158 1.710682 -1.177903
 H 4.001850 1.663971 0.792985
 H 5.512224 1.524520 -3.244971
 H 5.663728 2.417805 -0.896724
 N 1.075739 -1.308339 -0.952054
 N 2.978934 0.415697 -0.501699
 H 1.628569 -1.414074 -2.967707
 H 0.045693 -2.723907 -2.134354
 C -2.260096 3.132618 -0.424103
 C -3.285361 4.066007 -0.273341
 C -4.301581 3.860092 0.662755
 C -4.282666 2.710825 1.454898
 C -3.253647 1.780143 1.308494
 C -2.225212 1.975912 0.371704
 H -1.485954 3.290387 -1.165955
 H -3.294872 4.955791 -0.896343
 H -5.099947 4.587545 0.773208
 H -5.063924 2.542522 2.190881
 H -3.232371 0.898377 1.946083
 C -1.171817 0.926503 0.217154
 C 0.219294 1.146912 0.281133
 H -1.442628 -0.031161 0.654291
 O 0.614258 2.392550 -0.023789
 H 1.580528 2.423124 -0.016184
 C -0.603938 -2.986270 -0.089362
 H 0.087359 -3.820402 0.071011
 H -0.603060 -2.404967 0.833175
 C -1.985841 -3.583799 -0.366504
 H -2.006358 -4.059426 -1.351196
 H -2.241252 -4.344219 0.377280
 N -3.114790 -2.577063 -0.361812
 C -3.418713 -2.039074 0.998091
 H -4.100515 -1.194820 0.889762
 H -3.873132 -2.825080 1.604932
 H -2.501649 -1.691170 1.468135
 C -4.349521 -3.156044 -0.983641
 H -4.655413 -4.044243 -0.427194
 H -5.134440 -2.400585 -0.960984
 H -4.131140 -3.407101 -2.021239
 H -2.889346 -1.743921 -0.999054
 O -1.388153 0.728839 -2.399165

H -1.212194 0.700822 -1.186460
 C -2.475570 0.165403 -2.774041
 O -3.110689 -0.716233 -2.160129
 H -2.858490 0.504003 -3.751317

D-TS4

1 1

C -0.269989 2.651389 1.174274
 C 0.894071 2.610335 0.317695
 H 1.918342 2.515847 0.651208
 C 0.453462 2.777358 -1.022732
 H 1.087422 2.811385 -1.899696
 C -1.405974 2.841033 0.340551
 H -2.431882 2.906241 0.679554
 C -0.974631 2.927934 -1.019847
 H -1.603552 3.103322 -1.881283
 H -0.275216 2.594329 2.253568
 Ru -0.429331 0.864303 -0.191030
 C -0.976608 -1.476846 -1.834767
 C 1.023154 -0.440691 -2.633268
 C -2.056208 -1.505740 -0.880032
 H 1.041039 -1.316468 -3.295783
 C -3.035934 -2.504157 -0.824722
 C -2.953982 -0.435443 0.987181
 C -4.007031 -2.442303 0.167239
 H -3.021115 -3.309457 -1.552006
 C -3.958495 -1.391357 1.089938
 H -2.866390 0.376979 1.697357
 H -4.782085 -3.198672 0.229688
 H -4.689260 -1.310904 1.886874
 N -0.125589 -0.496195 -1.726186
 N -2.024661 -0.469056 0.012742
 H -0.879658 -2.250257 -2.596414
 H 0.918034 0.451652 -3.257846
 C 2.332797 -0.324623 -1.835005
 H 3.167688 -0.197755 -2.530749
 H 2.251026 0.579662 -1.225051
 O -0.402373 -0.455567 2.946610
 C 0.618731 -0.235606 2.387682
 O 1.819810 -0.066435 2.407857
 H 0.355376 -0.233381 0.803361
 H 2.643047 -0.541482 0.910935
 C 3.396539 -2.394930 1.247759
 H 3.795713 -2.078488 2.210969

H 2.410181 -2.834726 1.395382
 H 4.065399 -3.112251 0.769650
 C 4.579130 -0.516337 0.163903
 H 4.998639 -0.272116 1.140291
 H 5.244737 -1.195937 -0.371628
 H 4.436994 0.397332 -0.410688
 N 3.257853 -1.188824 0.366816
 C 2.553332 -1.536969 -0.923488
 H 3.145043 -2.318872 -1.408435
 H 1.594127 -1.959059 -0.617416

D-TS5

1 1

C 0.628111 3.003846 -0.384165
 C -0.485654 2.722177 -1.214895
 H -0.504253 2.772090 -2.294634
 C -1.603257 2.393970 -0.357830
 H -2.611268 2.177643 -0.682525
 C 0.232639 2.849757 0.986336
 H 0.847401 3.039130 1.855081
 C -1.154784 2.484596 0.987514
 H -1.760015 2.308073 1.867321
 H 1.617117 3.279773 -0.726382
 Ru 0.002940 0.849878 -0.048684
 C 0.832526 -1.504767 1.449671
 C -1.344967 -0.894852 2.200559
 C 1.989752 -1.244065 0.621702
 H -1.200832 -1.792901 2.815764
 C 3.142166 -2.036205 0.616918
 C 2.894080 0.194620 -0.968504
 C 4.203907 -1.678260 -0.206921
 H 3.193554 -2.912061 1.255441
 C 4.074605 -0.541657 -1.010476
 H 2.749546 1.071448 -1.588091
 H 5.112675 -2.270200 -0.226071
 H 4.876630 -0.224539 -1.667655
 N -0.167104 -0.685322 1.352560
 N 1.865847 -0.135287 -0.165781
 H 0.822601 -2.350983 2.136864
 H -1.415050 -0.036566 2.876712
 C -2.648531 -1.017666 1.398361
 H -3.446084 -1.228027 2.118323
 H -2.885746 -0.053787 0.939661
 H -0.355206 -0.125674 -1.383969

H -1.079192 -0.598011 -0.941589
 C -1.595758 -2.722762 -1.815793
 H -1.245202 -2.306461 -2.764110
 H -0.739107 -3.151500 -1.289177
 H -2.322814 -3.517959 -2.026717
 C -3.255747 -0.951857 -1.727726
 H -2.844062 -0.495565 -2.631896
 H -4.061466 -1.642711 -2.009192
 H -3.673199 -0.159044 -1.104320
 N -2.179160 -1.644945 -1.001021
 C -2.623583 -2.125255 0.331444
 H -3.616112 -2.586547 0.232471
 H -1.939360 -2.921102 0.643311

D-TS6

1 1

C 3.914581 -1.396086 -0.989923
 C 3.075641 -1.147396 -2.125662
 H 2.669320 -1.887015 -2.800857
 C 2.947444 0.271960 -2.252298
 H 2.371085 0.785385 -3.010077
 C 4.296687 -0.141287 -0.429124
 H 4.938358 -0.001212 0.430784
 C 3.688729 0.899068 -1.208873
 H 3.816740 1.963511 -1.068874
 H 4.217849 -2.368975 -0.625638
 Ru 2.024690 -0.357482 -0.280531
 C 0.616270 -0.185491 2.243094
 C 1.859606 1.835677 1.898583
 C 0.264336 -1.495089 1.783674
 H 1.671645 1.985854 2.970915
 C -0.601976 -2.376543 2.453976
 C 0.640658 -3.076689 0.101672
 C -0.826368 -3.638147 1.931237
 H -1.076477 -2.054667 3.375466
 C -0.187750 -3.992530 0.729285
 H 1.141530 -3.307232 -0.831165
 H -1.482411 -4.339067 2.436155
 H -0.332554 -4.971280 0.285636
 N 1.450190 0.491298 1.482485
 N 0.882956 -1.842276 0.605056
 H 0.250955 0.201362 3.193109
 H 2.935712 1.919309 1.733787
 C 1.139166 2.911179 1.063878

H 1.677105 3.859062 1.161248
 H 1.190244 2.595192 0.016047
 H 0.661787 0.152369 -1.016692
 C -0.321664 3.075978 1.497250
 H -0.421077 3.766090 2.342038
 H -0.735098 2.110411 1.799659
 N -1.210062 3.565884 0.388393
 C -0.789683 4.886923 -0.159538
 C -2.644272 3.575280 0.801264
 H -1.142031 2.807826 -0.407312
 H -1.463264 5.160368 -0.972636
 H -0.833024 5.642882 0.628687
 H 0.225133 4.812514 -0.548371
 H -2.931311 2.568041 1.106871
 H -2.790131 4.275361 1.627035
 H -3.254427 3.873431 -0.052126
 O -1.211554 1.698177 -1.377626
 C -1.100504 0.539656 -0.914511
 C -1.609389 -0.653291 -1.688104
 H -1.005460 0.378982 0.172159
 C -3.045509 -0.848467 -1.226971
 H -1.008189 -1.535782 -1.464164
 H -1.548797 -0.432417 -2.756833
 C -4.047687 0.037387 -1.648524
 C -3.369027 -1.863042 -0.317537
 C -5.356135 -0.106361 -1.188048
 H -3.793519 0.835652 -2.340779
 C -4.678885 -2.005756 0.144940
 H -2.596004 -2.548339 0.017445
 C -5.674792 -1.129255 -0.289739
 H -6.129130 0.573946 -1.533515
 H -4.922372 -2.804212 0.839826
 H -6.694576 -1.243938 0.064995

B-LAPS

0 1

C -0.658926 2.675063 -1.877545
 C -1.460239 2.856832 -0.706180
 H -2.525261 2.689184 -0.619518
 C -0.592486 3.368211 0.318013
 H -0.884127 3.595420 1.334670
 C 0.677847 3.047191 -1.583622
 H 1.517235 2.991693 -2.263074
 C 0.727154 3.483468 -0.208988

H	1.608626	3.785337	0.337499
H	-1.002047	2.270392	-2.821791
Ru	0.168452	1.351181	-0.166422
C	1.601605	-1.962989	-0.299616
C	2.321205	-2.231741	1.857015
C	2.876276	-2.232224	-0.812452
C	0.442241	-1.729936	-1.208940
C	3.634082	-2.469611	1.450443
H	2.059450	-2.235030	2.913066
C	3.911213	-2.482320	0.082067
H	3.049841	-2.199559	-1.882816
C	0.107102	-2.753391	-2.105964
H	4.412292	-2.646630	2.185677
H	4.918132	-2.670931	-0.278477
C	-1.477054	-0.578424	-1.788143
C	-1.058152	-2.675608	-2.858922
H	0.755741	-3.620593	-2.166903
C	-1.885222	-1.570424	-2.669175
H	-2.098766	0.288591	-1.609521
H	-1.329525	-3.470155	-3.547183
H	-2.832448	-1.469011	-3.187407
N	1.316067	-1.995692	1.007337
N	-0.315799	-0.610888	-1.096861
C	-3.283865	-2.428892	1.227998
C	-4.506888	-1.753598	1.194809
C	-4.534056	-0.362193	1.332103
C	-3.348027	0.350135	1.493871
C	-2.113479	-0.324973	1.529725
C	-2.091771	-1.726695	1.395991
H	-3.257636	-3.510025	1.121756
H	-5.433028	-2.305982	1.063800
H	-5.482061	0.168267	1.311623
H	-3.362497	1.431319	1.592455
H	-1.129910	-2.228840	1.409085
C	-0.877663	0.396510	1.647563
C	0.223506	0.869809	1.976508
H	1.080929	1.133547	2.563774
C	3.077536	1.108749	0.592237
O	2.999116	1.979392	1.458521
O	2.150673	0.639474	-0.179881
H	4.051348	0.608496	0.390597

H2-sol

0 1

H	0.000000	0.000000	0.372243
H	0.000000	0.000000	-0.372243

H2O-sol

0 1

O	0.000000	0.000000	0.118096
H	0.000000	0.762169	-0.472384
H	0.000000	-0.762169	-0.472384

HCOO--sol

-1 1

C	0.000005	0.332546	0.000146
O	-1.130332	-0.215542	-0.000028
H	-0.000003	1.453414	-0.000019
O	1.130329	-0.215544	-0.000079

HCOOH-sol

0 1

C	-0.125778	0.369301	-0.000006
O	-1.172812	-0.221800	0.000003
H	-0.038919	1.466072	0.000004
O	1.048802	-0.281741	-0.000002
H	1.785668	0.346448	0.000027

PhCCH-sol

0 1

C	-1.510402	1.208018	0.000050
C	-0.118690	1.212837	0.000002
C	0.592941	-0.000002	-0.000019
C	-0.118694	-1.212839	0.000009
C	-1.510406	-1.208015	0.000057
C	-2.209947	0.000002	0.000078
H	-2.049441	2.148372	0.000065
H	0.424865	2.150030	-0.000020
H	0.424858	-2.150034	-0.000007
H	-2.049448	-2.148368	0.000079
H	-3.293804	0.000004	0.000114
C	2.022003	-0.000003	-0.000071
C	3.228252	0.000001	-0.000117
H	4.292628	0.000003	-0.000166

PhCH2CH2OH-sol

0 1

C	0.790090	-1.202981	0.217367
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C 0.088725 -0.003135 0.389489
 C 0.775264 1.203275 0.204244
 C 2.126943 1.212343 -0.140539
 C 2.815094 0.009960 -0.307987
 C 2.141820 -1.198977 -0.127071
 H 0.273765 -2.147281 0.358775
 H 0.247527 2.142696 0.335772
 H 2.642499 2.156893 -0.275315
 H 3.866235 0.014971 -0.573635
 H 2.669193 -2.138463 -0.251073
 C -1.387634 -0.011461 0.710838
 H -1.644802 -0.890928 1.307997
 H -1.648462 0.873760 1.300405
 C -2.239958 -0.023529 -0.566226
 O -3.644095 -0.074728 -0.288449
 H -1.999562 0.850921 -1.183526
 H -2.019430 -0.917842 -1.153184
 H -3.896268 0.740130 0.160692

PhCH2CHO-sol

0 1

C 0.748768 -1.245303 0.135204
 C -0.047031 -0.133015 0.431394
 C 0.511014 1.146203 0.322476
 C 1.840708 1.309782 -0.064051
 C 2.627881 0.194827 -0.355207
 C 2.077928 -1.083380 -0.255957
 H 0.329529 -2.242552 0.218283
 H -0.096882 2.016405 0.546951
 H 2.261405 2.306419 -0.136631
 H 3.662006 0.321241 -0.654832
 H 2.683677 -1.954908 -0.477403
 C -1.504720 -0.296330 0.815553
 H -1.655084 -1.264308 1.307740
 H -1.838539 0.492451 1.491919
 C -2.378749 -0.286629 -0.419641
 O -3.312763 0.464406 -0.594900
 H -2.098807 -1.026920 -1.195457

B-1-sol

0 1

C -2.553557 -1.743032 -0.322008
 C -3.097306 -0.483529 0.086529
 H -3.585863 -0.288330 1.029687

C -2.838458 0.490889 -0.915950
 H -3.151202 1.523563 -0.894606
 C -1.926599 -1.530497 -1.599617
 H -1.416253 -2.281228 -2.186240
 C -2.097483 -0.162526 -1.966810
 H -1.752532 0.295522 -2.882308
 H -2.633363 -2.679207 0.209204
 Ru -0.907463 -0.275909 -0.137072
 C 1.823810 0.912919 -0.275444
 C 0.207633 2.542308 -0.668769
 C 2.837913 1.870931 -0.356655
 C 2.061769 -0.519783 -0.044454
 C 1.167819 3.536848 -0.773093
 H -0.845740 2.762570 -0.771282
 C 2.509932 3.195339 -0.609782
 H 3.872193 1.585178 -0.225471
 C 3.328845 -1.087438 0.115358
 H 0.863245 4.556072 -0.972127
 H 3.286128 3.947366 -0.677920
 C 1.061442 -2.612061 0.165962
 C 3.446788 -2.458054 0.297933
 H 4.213364 -0.466220 0.096218
 C 2.289595 -3.236226 0.320260
 H 0.136858 -3.172723 0.188668
 H 4.422473 -2.911469 0.420631
 H 2.331476 -4.308669 0.459283
 N 0.518086 1.255260 -0.429977
 N 0.939866 -1.284641 -0.017103
 O -0.452758 0.069799 1.959074
 C -1.005723 0.960858 2.691263
 O -1.885479 1.775027 2.387003
 H -0.610699 0.962980 3.730029

B-2-sol

1 1

C 0.704658 -2.424329 1.747923
 C 0.497382 -3.141302 0.543214
 H -0.394214 -3.682049 0.266545
 C 1.697912 -3.021904 -0.239327
 H 1.861774 -3.451934 -1.215618
 C 2.019337 -1.849582 1.728204
 H 2.483063 -1.283139 2.521078
 C 2.630597 -2.241535 0.490451
 H 3.627425 -1.983156 0.165077

H -0.017158 -2.311343 2.543572
 Ru 0.845964 -0.961143 0.068593
 C 1.282541 1.985114 0.078707
 C 2.954313 0.898797 -1.128300
 C 1.886621 3.221157 -0.158751
 C 0.044150 1.804436 0.843726
 C 3.601568 2.095172 -1.394823
 H 3.333412 -0.041591 -1.502653
 C 3.059388 3.278776 -0.898284
 H 1.446439 4.127979 0.230979
 C -0.701741 2.849312 1.391770
 H 4.509743 2.090760 -1.982848
 H 3.539521 4.230611 -1.087238
 C -1.484468 0.244437 1.656168
 C -1.863550 2.565085 2.095740
 H -0.381280 3.873709 1.266203
 C -2.261428 1.237504 2.230686
 H -1.775334 -0.794043 1.712792
 H -2.451290 3.366562 2.525104
 H -3.163648 0.966615 2.762378
 N 1.826317 0.834685 -0.397376
 N -0.350657 0.512377 0.982812
 C -3.890349 1.161989 -1.292833
 C -4.776432 0.189401 -0.827860
 C -4.330346 -1.119039 -0.631662
 C -3.004612 -1.453955 -0.888807
 C -2.110366 -0.481602 -1.366495
 C -2.565527 0.832823 -1.563848
 H -4.229858 2.180719 -1.440705
 H -5.806678 0.449852 -0.614653
 H -5.013669 -1.877297 -0.266883
 H -2.649308 -2.462096 -0.712304
 H -1.873527 1.588705 -1.915004
 C -0.727220 -0.799252 -1.579676
 C 0.390242 -0.997060 -2.083480
 H 1.086534 -1.134637 -2.886629

B-3-sol

1 1

C 1.529832 -2.204674 2.047479
 C 0.170452 -2.549290 1.719520
 H -0.681810 -2.474153 2.377463
 C 0.179910 -3.138323 0.418296
 H -0.675893 -3.543350 -0.099560

C 2.344576 -2.525882 0.953375
 H 3.406267 -2.341687 0.878340
 C 1.514734 -3.077747 -0.085992
 H 1.856234 -3.470564 -1.031430
 H 1.854443 -1.729966 2.961835
 Ru 0.698745 -0.989132 0.180081
 C 2.030618 1.571139 -0.518837
 C 2.707281 -0.135350 -1.960980
 C 2.850813 2.483830 -1.182512
 C 1.181447 1.906221 0.631831
 C 3.542842 0.724921 -2.656841
 H 2.608242 -1.175504 -2.236669
 C 3.615936 2.057761 -2.259782
 H 2.892090 3.514998 -0.862432
 C 1.090607 3.178351 1.197877
 H 4.117243 0.349999 -3.493278
 H 4.256482 2.756663 -2.782604
 C -0.330623 1.066428 2.198572
 C 0.264583 3.381202 2.294982
 H 1.657478 4.001420 0.786936
 C -0.456214 2.305328 2.807323
 H -0.875087 0.204483 2.556314
 H 0.185200 4.363797 2.742516
 H -1.111331 2.415779 3.660972
 N 1.973325 0.272661 -0.911930
 N 0.468288 0.866869 1.136645
 C -5.426564 0.526611 -1.685544
 C -5.716961 0.589344 -0.322972
 C -4.716130 0.287586 0.605397
 C -3.442781 -0.069232 0.176946
 C -3.135849 -0.128353 -1.194668
 C -4.149642 0.171431 -2.118626
 H -6.194771 0.755127 -2.416055
 H -6.709426 0.866247 0.013457
 H -4.931205 0.328383 1.667579
 H -2.676677 -0.309257 0.904922
 H -3.933816 0.128184 -3.180914
 C -1.791511 -0.486973 -1.676399
 C -0.729704 -0.685333 -0.920377
 H -1.645666 -0.589447 -2.752372

B-6-sol

0 1

C 2.719678 -1.149226 0.676015

C 3.092600 -0.721755 -0.629925
 H 3.377227 -1.362900 -1.450293
 C 3.092539 0.721959 -0.629762
 H 3.377138 1.363318 -1.449972
 C 2.524965 -0.000172 1.503639
 H 2.270647 -0.000307 2.553006
 C 2.719582 1.149086 0.676287
 H 2.632591 2.177388 0.998346
 H 2.632779 -2.177611 0.997831
 Ru 1.009070 -0.000021 -0.262529
 C -1.850076 0.728544 0.008826
 C -0.509929 2.639036 -0.040991
 C -3.001664 1.522227 0.085726
 C -1.850101 -0.728499 0.008825
 C -1.610646 3.468900 0.050374
 H 0.492403 3.038899 -0.108256
 C -2.889283 2.901782 0.108515
 H -3.977231 1.057558 0.129504
 C -3.001718 -1.522141 0.085704
 H -1.468462 4.541919 0.067702
 H -3.772263 3.525478 0.169584
 C -0.510019 -2.639038 -0.040969
 C -2.889385 -2.901700 0.108495
 H -3.977269 -1.057440 0.129459
 C -1.610765 -3.468862 0.050381
 H 0.492299 -3.038937 -0.108215
 H -3.772388 -3.525366 0.169545
 H -1.468620 -4.541886 0.067715
 N -0.604024 1.287988 -0.063643
 N -0.604066 -1.287986 -0.063629
 H 0.664035 -0.000032 -1.850620

B-TS2-sol

0 1

C -0.364241 -2.715731 -0.942524
 C -0.933421 -1.722355 -1.788128
 H -1.920991 -1.299971 -1.681586
 C 0.030908 -1.358890 -2.779913
 H -0.116704 -0.661836 -3.590627
 C 0.954651 -3.006029 -1.444592
 H 1.653010 -3.711747 -1.018871
 C 1.192370 -2.176961 -2.560322
 H 2.107370 -2.137190 -3.133883
 H -0.862379 -3.210895 -0.123223

Ru 0.811377 -0.799611 -0.748060
 C 3.204791 0.728884 0.130567
 C 2.651891 1.248427 -2.073839
 C 4.261330 1.642071 0.100914
 C 2.858105 -0.098545 1.292835
 C 3.691203 2.161008 -2.167280
 H 1.982136 1.067402 -2.903171
 C 4.510542 2.364185 -1.057867
 H 4.882520 1.787672 0.973522
 C 3.551688 -0.078391 2.503929
 H 3.845547 2.702104 -3.091609
 H 5.327383 3.074052 -1.094249
 C 1.407991 -1.728814 2.109687
 C 3.153133 -0.918826 3.534480
 H 4.394197 0.584731 2.640743
 C 2.064786 -1.764370 3.330138
 H 0.536998 -2.338055 1.922319
 H 3.682611 -0.913817 4.479082
 H 1.716571 -2.436218 4.103655
 N 2.411888 0.538574 -0.956499
 N 1.789297 -0.917072 1.108294
 C -0.274163 0.744001 -0.261776
 C -0.997087 1.731453 -0.790527
 C -1.874389 2.763940 -0.207163
 H -0.886566 1.761421 -1.874975
 C -2.835765 2.470617 0.775578
 C -1.787854 4.086331 -0.674909
 C -3.652043 3.472620 1.299421
 H -2.965771 1.448935 1.111202
 C -2.607797 5.084827 -0.155554
 H -1.064033 4.328587 -1.445707
 C -3.539564 4.784602 0.840341
 H -4.386750 3.221797 2.056430
 H -2.518545 6.099614 -0.527316
 H -4.176731 5.562347 1.245331
 O -0.312668 1.018997 1.604275
 H -0.808207 1.818007 1.835271
 H -0.830009 0.219059 1.992112
 O -4.266494 -1.195217 -1.160743
 O -1.601985 -0.994401 2.472780
 C -4.692262 -2.335992 -1.177862
 C -2.369280 -1.463706 1.591768
 O -4.434298 -3.271324 -0.291353
 H -5.357087 -2.706892 -1.971928

O -2.961754 -2.573239 1.653506
H -2.537420 -0.860206 0.681998
H -3.821591 -2.931180 0.475419

B-TS5-sol

O 1

C -1.408925 -2.832848 0.069786
C -2.378187 -1.808900 -0.243089
H -3.218975 -1.504303 0.359967
C -2.014346 -1.230802 -1.486777
H -2.543732 -0.430448 -1.982345
C -0.462180 -2.859919 -0.989868
H 0.400165 -3.509340 -1.043911
C -0.827289 -1.881640 -1.968723
H -0.327236 -1.696595 -2.907125
H -1.415639 -3.480241 0.933339
Ru -0.398059 -0.842334 -0.017909
C 2.226138 0.576304 0.100922
C 3.595214 0.795198 0.276125
C 2.477218 -1.664182 0.687404
C 4.414397 -0.256633 0.659820
H 4.015527 1.777672 0.113232
C 3.842441 -1.511408 0.868972
H 1.990455 -2.615742 0.850976
H 5.477237 -0.101165 0.796205
H 4.439193 -2.361741 1.172262
N 1.676065 -0.651020 0.304985
H -0.519483 -0.536670 1.639703
C -3.197022 1.359833 1.810822
O -3.726964 1.004516 0.753852
H -3.758077 2.030985 2.496207
O -2.030300 1.053714 2.250207
H -1.245594 0.135825 1.584434
C 1.269719 1.612942 -0.304782
C 1.610625 2.943567 -0.557546
C -0.973273 2.065206 -0.758432
C 0.623057 3.844315 -0.931969
H 2.635665 3.273290 -0.461249
C -0.693103 3.395382 -1.031040
H -1.982857 1.679016 -0.781472
H 0.874478 4.877799 -1.135250
H -1.498543 4.063375 -1.307636
N -0.015603 1.181970 -0.416634

B-TS6- α -sol

O 1

C -2.020668 0.769147 1.668016
C -1.618209 -0.542430 2.084920
H -2.143980 -1.459816 1.877038
C -0.435073 -0.418011 2.872657
H 0.095365 -1.232514 3.343165
C -1.066168 1.681177 2.180823
H -1.073939 2.749558 2.019104
C -0.085239 0.964098 2.938453
H 0.747637 1.391076 3.475700
H -2.893568 1.015884 1.086963
Ru 0.021077 0.236460 0.774518
C 2.884449 0.139703 0.002028
C 2.208455 -1.857675 0.994281
C 4.185003 -0.346604 -0.139777
C 2.452715 1.472464 -0.426855
C 3.483304 -2.390806 0.888743
H 1.385435 -2.434027 1.387527
C 4.491429 -1.622652 0.311667
H 4.949611 0.265745 -0.596317
C 3.282264 2.407767 -1.049104
H 3.669388 -3.396446 1.242133
H 5.496730 -2.011668 0.209070
C 0.649704 2.944328 -0.550006
C 2.765782 3.641161 -1.419203
H 4.318650 2.173452 -1.246598
C 1.422826 3.915345 -1.166029
H -0.401210 3.104601 -0.352552
H 3.398746 4.374880 -1.902424
H 0.974330 4.860138 -1.443071
N 1.910960 -0.615440 0.574146
N 1.149943 1.753438 -0.175495
C -3.794881 -1.288939 -0.408851
C -3.061491 -0.461847 -1.265269
C -3.580853 0.803892 -1.570589
C -4.781106 1.240919 -1.013319
C -5.492879 0.411818 -0.142984
C -4.998470 -0.858579 0.151432
H -3.411902 -2.275328 -0.169061
H -3.035404 1.456517 -2.244740
H -5.161959 2.226860 -1.256474
H -6.424582 0.751293 0.295350
H -5.545595 -1.512826 0.821436

C -1.739669 -0.906565 -1.835408
H -1.545856 -1.950438 -1.583678
H -1.780314 -0.836475 -2.931089
C -0.535764 -0.041058 -1.413585
H -0.339335 -1.119987 0.059057
H -0.773441 1.004276 -1.614038
O 0.599611 -0.356847 -2.165761
H 0.804172 -1.326232 -2.064901
O 1.223549 -2.952320 -2.055380
C 0.683803 -3.770901 -1.256931
O -0.127989 -3.524004 -0.340524
H 0.980361 -4.837890 -1.398249

A-X

1 1
C -2.730736 -1.859543 0.666274
C -2.523554 -2.399284 -0.622907
H -3.229898 -2.386965 -1.442327
C -1.192832 -2.976953 -0.662730
H -0.745308 -3.469882 -1.515569
C -1.516804 -2.048808 1.430671
H -1.368144 -1.774136 2.466438
C -0.593805 -2.794980 0.604929
H 0.393826 -3.125261 0.896542
H -3.625106 -1.360614 1.015615
Ru -1.017199 -0.803427 -0.232575
C 0.810381 1.467189 0.030665
C 2.136371 -0.548439 -0.061108
C -0.502996 2.113962 0.033890
H 2.119878 -1.178500 -0.958490
C -0.669703 3.493953 0.106545
C -2.800197 1.770676 -0.077716
C -1.964929 4.019731 0.088732
H 0.198298 4.141502 0.172671
C -3.043939 3.144987 -0.008573
H -3.610854 1.055195 -0.152449
H -2.123409 5.091363 0.147611
H -4.065100 3.508702 -0.027319
N 0.859242 0.182588 -0.055865
N -1.561112 1.259144 -0.049489
H 1.700252 2.089580 0.103971
H 2.088438 -1.236654 0.791203
C 3.421012 0.275517 -0.008605
H 3.452756 0.882753 0.903389

H 3.473597 0.960571 -0.862718
C 4.661161 -0.645448 -0.032820
H 4.617803 -1.342892 0.814615
H 4.643621 -1.261916 -0.941645
C 5.907337 0.114091 0.021088
C 6.923024 0.763882 0.067075
H 7.830437 1.322617 0.106791

D-X

1 1
C -1.331673 -3.043612 -0.216555
C -0.117701 -2.869499 -0.987221
H 0.016773 -3.164452 -2.020086
C 0.857934 -2.249038 -0.171050
H 1.870340 -2.004599 -0.460992
C -1.101851 -2.500790 1.071061
H -1.810559 -2.464779 1.888180
C 0.240694 -1.962371 1.101844
H 0.720057 -1.509080 1.959161
H -2.240964 -3.513810 -0.565117
Ru -0.864393 -0.872440 -0.372970
C -0.753672 2.042789 -0.590726
C 1.403479 1.222011 -1.197778
C -2.109322 1.818393 -0.087036
H 1.614956 0.458969 -1.952942
C -3.028383 2.843602 0.116570
C -3.634475 0.212427 0.622361
C -4.300883 2.523079 0.598874
H -2.752084 3.869969 -0.100890
C -4.607459 1.188833 0.853164
H -3.831273 -0.837407 0.807268
H -5.035467 3.302890 0.770021
H -5.581448 0.895517 1.228263
N 0.016672 1.024172 -0.760777
N -2.409347 0.513426 0.169070
H -0.420884 3.061338 -0.800004
H 1.517863 2.207044 -1.668092
C 2.364210 1.076317 -0.010757
H 2.237438 1.920199 0.676052
H 2.097567 0.172569 0.543148
C 3.824980 1.016236 -0.476704
H 4.041628 1.914994 -1.066361
H 3.954439 0.153193 -1.165398
N 4.759692 0.974334 0.638206

C	6.115018	1.323672	0.215712
H	6.540703	0.609920	-0.513949
H	6.118751	2.319671	-0.237345
H	6.774792	1.349265	1.087538
C	4.745548	-0.307295	1.335983
H	5.453621	-0.278545	2.168439
H	3.757417	-0.509901	1.760072
H	5.021865	-1.157638	0.681769

B-3'

O 1

C	0.102586	-2.374086	1.205978
C	-0.176086	-2.721215	-0.146551
H	-1.144243	-2.588179	-0.606923
C	1.022617	-3.255225	-0.725900
H	1.136516	-3.633452	-1.732317
C	1.465620	-2.729347	1.489489
H	1.972365	-2.619246	2.438381
C	2.023121	-3.261438	0.295481
H	3.046078	-3.595364	0.168962
H	-0.622135	-1.915056	1.871195
Ru	1.383196	-1.055513	-0.147593
C	3.532655	0.964400	0.157916
C	4.267189	-0.828025	-1.152952
C	4.783556	1.582174	0.034359
C	2.399174	1.524710	0.902540
C	5.526507	-0.265642	-1.306031
H	4.002776	-1.771762	-1.614154
C	5.789199	0.964552	-0.697917
H	4.965134	2.537722	0.510809
C	2.405918	2.775446	1.524236
H	6.277980	-0.780748	-1.893580
H	6.761683	1.435640	-0.797097
C	0.182518	1.162925	1.564551
C	1.257845	3.220515	2.175253
H	3.290932	3.399659	1.486975
C	0.127988	2.406220	2.194045
H	-0.679167	0.499355	1.567804
H	1.246256	4.195783	2.651730
H	-0.820437	2.687135	2.648134
N	3.293841	-0.238778	-0.431867
N	1.293383	0.731683	0.940062
C	0.601159	-0.128040	-1.547857
C	-0.032569	0.655533	-2.395926

C	-1.295290	1.356543	-2.059476
H	0.422813	0.833975	-3.371826
C	-2.235713	0.782438	-1.188932
C	-1.549543	2.627865	-2.599684
C	-3.402104	1.471984	-0.855003
H	-2.076636	-0.213859	-0.790781
C	-2.711082	3.319236	-2.256224
H	-0.831091	3.075684	-3.282052
C	-3.638321	2.745973	-1.381519
H	-4.148428	0.989213	-0.230030
H	-2.895809	4.302896	-2.679537
H	-4.552245	3.276027	-1.129561
O	-2.866653	2.116812	2.644672
H	-3.101894	2.226677	1.713642
H	-2.727058	1.146804	2.719289
O	-5.982592	-0.372570	0.034317
O	-2.282337	-0.553324	2.278614
C	-6.038822	-1.383469	-0.648678
C	-3.198355	-1.036321	1.561450
O	-5.123554	-2.317952	-0.766248
H	-6.924281	-1.620851	-1.267996
O	-3.032780	-1.810386	0.570988
H	-4.242152	-0.745887	1.793862
H	-4.283409	-2.096808	-0.192847

B-4'

O 1

C	0.184986	-2.780166	-1.472625
C	-0.351326	-1.673233	-2.186031
H	-1.361435	-1.296913	-2.099533
C	0.677608	-1.106889	-3.003388
H	0.563929	-0.281731	-3.692499
C	1.556077	-2.937571	-1.882683
H	2.241730	-3.695924	-1.528595
C	1.855412	-1.908331	-2.809297
H	2.814472	-1.745903	-3.285234
H	-0.363424	-3.410272	-0.787267
Ru	1.277895	-0.872838	-0.824046
C	3.186296	0.781357	0.691541
C	3.141352	1.409276	-1.559071
C	4.078392	1.823436	0.978095
C	2.683036	-0.177220	1.672441
C	4.029884	2.448531	-1.335612
H	2.725887	1.212924	-2.540162

C 4.508250 2.665321 -0.037506
 H 4.426710 1.973205 1.993357
 C 3.034849 -0.186847 3.028967
 H 4.333277 3.081197 -2.162630
 H 5.196624 3.476873 0.173934
 C 1.324943 -2.053310 1.985906
 C 2.519711 -1.162860 3.869490
 H 3.706779 0.568692 3.419268
 C 1.649869 -2.118940 3.330733
 H 0.632303 -2.752890 1.535405
 H 2.783934 -1.179802 4.921695
 H 1.216863 -2.900110 3.945900
 N 2.721827 0.579421 -0.578366
 N 1.825526 -1.109044 1.156811
 C -0.068800 0.527402 -0.178316
 C -0.309387 1.748308 -0.710511
 C -1.379068 2.682637 -0.305437
 H 0.375263 2.092120 -1.481374
 C -2.702488 2.245033 -0.088236
 C -1.111523 4.055250 -0.137262
 C -3.703905 3.128354 0.318069
 H -2.974699 1.214616 -0.292795
 C -2.113251 4.941173 0.254463
 H -0.101120 4.418377 -0.309722
 C -3.412638 4.481415 0.496420
 H -4.706340 2.739646 0.469414
 H -1.879940 5.995781 0.378117
 H -4.189086 5.175012 0.806619
 O -0.843120 0.111463 0.928043
 H -1.444662 0.828313 1.201211
 H -1.332611 -1.423685 0.995225
 O -5.216018 0.149517 0.183391
 O -1.820742 -2.300307 0.990277
 C -6.204834 -0.519799 -0.063305
 C -3.078931 -2.040644 0.690266
 O -6.289039 -1.837176 -0.063486
 H -7.177519 -0.071194 -0.323398
 O -3.928580 -2.911642 0.568261
 H -3.326187 -0.976500 0.558811
 H -5.406701 -2.254528 0.178602

B-4''

0 1

C -2.311059 -2.324117 -1.791082

C -1.444736 -3.086736 -0.946416
 H -0.504861 -3.532089 -1.243503
 C -1.997824 -3.119806 0.364124
 H -1.583881 -3.647349 1.212631
 C -3.438948 -1.922255 -0.988467
 H -4.280091 -1.333928 -1.332402
 C -3.254292 -2.413216 0.324430
 H -3.927829 -2.267865 1.158745
 H -2.201520 -2.182860 -2.858153
 Ru -1.496222 -0.956265 -0.164325
 C -0.987893 1.399636 1.539300
 C -0.857694 -0.569498 2.787964
 C -0.615061 2.152435 2.659547
 C -1.282845 1.965904 0.223840
 C -0.506271 0.125449 3.934011
 H -0.942915 -1.649195 2.777831
 C -0.374287 1.517384 3.868852
 H -0.501045 3.225828 2.574328
 C -1.211046 3.328707 -0.087072
 H -0.325273 -0.417578 4.855198
 H -0.080080 2.090050 4.742047
 C -1.937061 1.478362 -1.963202
 C -1.514504 3.762652 -1.368491
 H -0.878088 4.037270 0.660119
 C -1.900598 2.815738 -2.322691
 H -2.217144 0.707009 -2.672029
 H -1.432155 4.812481 -1.625829
 H -2.149899 3.104939 -3.337695
 N -1.099158 0.041037 1.606382
 N -1.627284 1.042124 -0.720973
 C 0.511023 -0.843039 -0.610490
 C 1.568096 -1.010048 0.240750
 O 0.801088 -0.607626 -1.941136
 C 3.015471 -1.046557 -0.019297
 H 1.296693 -1.189944 1.277636
 H -0.050326 -0.514331 -2.386667
 C 3.612011 -0.968862 -1.297984
 C 3.882906 -1.142935 1.091773
 C 4.999086 -0.981818 -1.442636
 H 2.980687 -0.905992 -2.173855
 C 5.266126 -1.157000 0.942190
 H 3.452451 -1.201615 2.089268
 C 5.837832 -1.073419 -0.330232
 H 5.427828 -0.920163 -2.439835

H 5.901015 -1.230282 1.821580
H 6.917234 -1.079656 -0.451299
C 1.887399 2.432902 -0.963265
O 1.789331 3.595010 -1.278738
H 2.102081 1.615109 -1.673157
O 1.724995 2.015746 0.302311
H 1.717676 1.029478 0.325258

B-5'

O 1

C -2.946861 -2.300928 -1.148652
C -2.407430 -2.924334 0.020941
H -1.722042 -3.762418 0.038127
C -2.922986 -2.254355 1.169396
H -2.733379 -2.527031 2.198678
C -3.847414 -1.272171 -0.695951
H -4.405697 -0.602612 -1.338015
C -3.851377 -1.251541 0.711105
H -4.414217 -0.572908 1.337344
H -2.819678 -2.627940 -2.172411
Ru -1.627689 -0.792662 -0.007353
C -0.540872 1.796724 0.918162
C -0.921351 0.369542 2.728482
C 0.036261 2.756100 1.758204
C -0.704960 1.970983 -0.532777
C -0.403953 1.296397 3.621552
H -1.279816 -0.600289 3.051186
C 0.100020 2.500465 3.122329
H 0.518155 3.631899 1.323019
C -0.324720 3.123692 -1.231078
H -0.372935 1.060910 4.679958
H 0.558318 3.226362 3.786282
C -1.497157 0.985232 -2.498478
C -0.575397 3.193853 -2.594849
H 0.239727 3.900522 -0.718960
C -1.182205 2.112756 -3.240914
H -1.937011 0.103498 -2.949024
H -0.276858 4.074968 -3.153558
H -1.388998 2.128863 -4.305584
N -0.987777 0.607509 1.403366
N -1.268477 0.914918 -1.171576
C 0.240334 -1.325950 -0.255443
C 1.461945 -0.813293 0.460227
O 0.556273 -2.248062 -1.160735

C 2.790897 -1.464606 0.142134
H 1.242267 -0.870362 1.534479
H -0.258745 -2.491007 -1.628961
C 3.789711 -0.719263 -0.497063
C 3.049743 -2.794979 0.497597
C 5.024798 -1.307113 -0.782298
H 3.588956 0.323053 -0.737731
C 4.282392 -3.380061 0.210994
H 2.278807 -3.376078 0.999589
C 5.274297 -2.635560 -0.433708
H 5.796297 -0.720749 -1.274265
H 4.471066 -4.412896 0.491848
H 6.236766 -3.088502 -0.656085
C 2.704252 3.309729 -0.092947
O 2.044824 4.341155 0.207296
H 3.811587 3.450121 -0.198572
O 2.271780 2.141583 -0.296172
H 1.528706 0.267418 0.248767

B-6'

O 1

C -1.187828 -2.886787 0.215251
C -2.254281 -1.919038 0.172097
H -2.956831 -1.704967 0.964637
C -2.252510 -1.314195 -1.115837
H -2.942933 -0.545787 -1.432196
C -0.549091 -2.861566 -1.062637
H 0.301969 -3.466225 -1.351888
C -1.217456 -1.921398 -1.899091
H -0.969289 -1.688615 -2.925544
H -0.951615 -3.546688 1.037865
Ru -0.301734 -0.826077 -0.031148
C 1.311071 1.644868 -0.224508
C -0.927658 2.073002 -0.751843
C 1.626122 3.000035 -0.400114
C 2.277829 0.610176 0.117179
C -0.665512 3.417159 -0.953567
H -1.927616 1.668512 -0.842575
C 0.637385 3.899024 -0.768496
H 2.644229 3.341057 -0.251067
C 3.644354 0.833746 0.344486
H -1.476498 4.077542 -1.241381
H 0.870029 4.949627 -0.908100
C 2.573883 -1.681255 0.472750

C	4.482661	-0.232922	0.628081
H	4.041233	1.841182	0.297334
C	3.931642	-1.521108	0.685668
H	2.096525	-2.651830	0.532610
H	5.541085	-0.071501	0.804220
H	4.545623	-2.388480	0.902897
N	0.031013	1.183770	-0.390538
N	1.745669	-0.647918	0.191754
H	-0.312059	-0.513339	1.550871
C	-3.497590	1.303612	1.514689
O	-3.789840	1.068163	0.358863
H	-4.165526	1.847780	2.204522
O	-2.377476	0.975034	2.142489
H	-1.758394	0.442489	1.564358

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0 1

C	0.276354	-2.126059	2.184552
C	1.490223	-2.181774	1.414430
H	1.672719	-2.832532	0.570049
C	2.399065	-1.216818	1.927952
H	3.391835	-1.027333	1.544736
C	0.462450	-1.116422	3.183409
H	-0.269317	-0.823061	3.925972
C	1.768784	-0.567884	3.044030
H	2.203450	0.210393	3.656552
H	-0.587288	-2.766036	2.071689
Ru	0.543996	-0.163700	1.104058
C	0.275864	2.503409	-0.134990
C	2.471168	1.709883	-0.310266
C	0.625547	3.672888	-0.823941
C	-1.069917	2.180261	0.325131
C	2.870502	2.852600	-0.983827
H	3.147853	0.881678	-0.147897
C	1.934562	3.861160	-1.242484
H	-0.127869	4.424532	-1.030793
C	-2.200702	2.986480	0.129921
H	3.898574	2.936277	-1.318698
H	2.218649	4.763648	-1.774049
C	-2.379470	0.573976	1.411330
C	-3.437617	2.570715	0.598791
H	-2.104149	3.931999	-0.391399
C	-3.523698	1.334851	1.254520
H	-2.402845	-0.403207	1.876077

H	-4.318830	3.186691	0.452217
H	-4.470281	0.955484	1.622826
N	1.206148	1.536351	0.141417
N	-1.163688	0.974209	0.969668
C	-2.080728	-2.459122	-0.738258
C	-1.895836	-1.605878	-1.832566
C	-2.963300	-0.795521	-2.239455
C	-4.190583	-0.840730	-1.574951
C	-4.368131	-1.707134	-0.495281
C	-3.308384	-2.516484	-0.078198
H	-1.251793	-3.073250	-0.401239
H	-2.835350	-0.128764	-3.089378
H	-5.007224	-0.204796	-1.904633
H	-5.324918	-1.752135	0.017500
H	-3.437361	-3.192594	0.762768
C	-0.564934	-1.525462	-2.538732
H	0.096832	-2.356738	-2.282010
H	-0.714624	-1.567880	-3.628939
C	0.182158	-0.218829	-2.297498
H	0.164505	-0.716388	-0.353350
H	-0.444188	0.646684	-2.017055
O	1.358053	-0.048978	-2.615621
H	2.331334	-1.356218	-2.343794
O	2.765826	-2.237806	-2.136246
C	3.775839	-2.090055	-1.290045
O	4.177675	-1.051242	-0.806395
H	4.229499	-3.071652	-1.068639

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C	-0.494003	-1.590903	-2.296894
C	0.290524	-2.579664	-1.605085
H	1.295850	-2.886751	-1.857988
C	-0.495746	-3.076475	-0.524183
H	-0.190648	-3.828729	0.191450
C	-1.795073	-1.565887	-1.680713
H	-2.609095	-0.909934	-1.959701
C	-1.801853	-2.472104	-0.607754
H	-2.616095	-2.623727	0.087422
H	-0.203914	-1.055305	-3.190050
Ru	-0.028034	-0.890063	-0.218117
C	-2.812384	0.994910	0.279088
C	-4.996688	0.427329	-0.146759
C	-2.795220	0.245931	1.462765

C	-1.636175	1.810352	-0.145735	O	-0.066727	-0.841378	1.895217
C	-5.076499	-0.358483	1.003906	C	1.179799	-1.025643	1.543611
H	-5.853962	0.523798	-0.810440	H	1.577038	-2.050996	1.615395
C	-3.951664	-0.439969	1.825989	C	2.183733	0.068307	1.896437
H	-1.890202	0.187146	2.053864	H	1.648638	1.022356	1.884102
C	-1.863003	3.158245	-0.457687	H	2.482689	-0.099515	2.944300
H	-5.995833	-0.881652	1.247659	C	3.424555	0.152558	1.036551
H	-3.969371	-1.030970	2.737027	C	4.094294	-0.994531	0.584852
C	0.630629	2.079839	-0.546214	C	3.944808	1.403603	0.675971
C	-0.801438	3.983577	-0.802370	C	5.237036	-0.892067	-0.208419
H	-2.880678	3.527552	-0.417856	H	3.717037	-1.977481	0.849171
C	0.478043	3.429814	-0.829790	C	5.089492	1.511699	-0.116928
H	1.603956	1.611923	-0.593148	H	3.444623	2.304694	1.024123
H	-0.966031	5.030838	-1.036892	C	5.739456	0.361657	-0.565691
H	1.352242	4.020864	-1.081150	H	5.736719	-1.794623	-0.550008
N	-3.898075	1.102068	-0.507296	H	5.471297	2.493687	-0.383398
N	-0.396898	1.259777	-0.220151	H	6.628479	0.439761	-1.184946
H	1.413637	-0.454615	-0.691106				

1. D. G. Johnson, J. M. Lynam, J. M. Slattery and C. E. Welby, *Dalton Trans.*, 2010, **39**, 10432-10441.