



Title	Exploring the full catalytic cycle of rhodium(I)BINAP-catalysed isomerisation of allylic amines : a graph theory approach for path optimisation
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Exploring the Full Catalytic Cycle of Rhodium(I)-BINAP-Catalysed Isomerisation of Allylic Amines: A Graph Theory Approach for Path Optimisation

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1 Absolute energies of TSs and LMs

Table S1: The electronic and Gibbs free energies (60 °C) of simple molecules^a

Name	E	G
allylic amine	-330.647486	-330.471406
(<i>E</i>)-enamine	-330.653916	-330.476816
(<i>Z</i>)-enamine	-330.647281	-330.469767
TMA	-174.552133	-174.455988
BINAP-Rh(I)	-2489.986682	-2489.438835

^aThe energies are calculated at the B3LYP+D3(PCM)/BS3//B3LYP+D3/BS2 level. The energies are given in a.u.

Table S2: The electronic and Gibbs free energies of LMs and TSs in the dissociative mechanism

No.	E_{ONIOM}^a	G_{ONIOM}^a	E^b	G^b
1	-1125.730772	-1124.913096	-2820.684453	-2819.931331
4	-1125.740405	-1124.919239	-2820.691181	-2819.936397
5	-1125.720529	-1124.909197	-2820.674481	-2819.928267
8	-1125.720719	-1124.908826	-2820.677211	-2819.930078
22	-1125.723900	-1124.909316	-	-
33	-1125.721588	-1124.902540	-2820.679019	-2819.927520
36	-1125.721164	-1124.911588	-2820.663364	-2819.921637
45	-1125.712512	-1124.900701	-2820.669576	-2819.923703
46	-1125.720351	-1124.908783	-2820.672001	-2819.924606
47	-1125.730769	-1124.917743	-2820.660056	-2819.914195
53	-1125.715590	-1124.905836	-2820.660548	-2819.916040
54	-1125.731889	-1124.919010	-2820.681749	-2819.933746
95	-1125.727547	-1124.915314	-2820.659911	-2819.914335
96	-1125.737528	-1124.925292	-2820.684304	-2819.937191
102	-1125.720668	-1124.908160	-2820.658028	-2819.914839
107	-1125.712478	-1124.898816	-2820.664969	-2819.916859
113	-1125.703807	-1124.890748	-2820.661987	-2819.914623
114	-1125.712653	-1124.898140	-2820.662071	-2819.914568
116	-1125.707573	-1124.894602	-	-
123	-1125.700956	-1124.887932	-	-
TS ₁₋₄	-1125.724434	-1124.908375	-2820.676824	-2819.927279
TS ₁₋₃₃	-1125.708539	-1124.887994	-2820.668845	-2819.917529
TS ₄₋₅	-1125.716807	-1124.903738	-	-
TS ₄₋₄₅	-1125.707529	-1124.893881	-2820.667743	-2819.920404
TS ₅₋₃₆	-1125.705762	-1124.897195	-	-
TS ₈₋₂₂	-1125.707998	-1124.898483	-	-
TS ₂₃₋₄₉	-1125.694792	-1124.882959	-	-
TS ₃₃₋₁₁₄	-1125.697630	-1124.880858	-2820.661644	-2819.912385
TS ₃₆₋₉₃	-1125.694127	-1124.881821	-	-
TS ₄₅₋₄₆	-1125.712512	-1124.900721	-2820.664784	-2819.916537
TS ₄₆₋₄₇	-1125.719707	-1124.909562	-2820.660513	-2819.914719
TS ₄₇₋₄₈	-1125.713859	-1124.902802	-2820.659168	-2819.912130
TS ₄₈₋₅₃	-1125.715378	-1124.902716	-2820.660078	-2819.913601
TS ₅₃₋₅₄	-1125.715545	-1124.905765	-2820.660374	-2819.915930
TS ₉₅₋₉₆	-1125.723451	-1124.913136	-2820.659426	-2819.912741
TS ₉₇₋₁₀₁	-1125.720543	-1124.905600	-2820.665494	-2819.919089
TS ₉₇₋₁₁₅	-1125.694400	-1124.885121	-	-
TS ₁₀₂₋₁₀₇	-1125.711682	-1124.900373	-2820.655958	-2819.912780
TS ₁₀₇₋₁₁₃	-1125.702519	-1124.888569	-2820.657531	-2819.908350
TS ₁₁₃₋₁₁₄	-1125.703635	-1124.888731	-2820.661372	-2819.912018
TS ₁₁₆₋₁₂₃	-1125.698679	-1124.886908	-	-
TS ₁₂₄₋₁₂₇	-1125.694309	-1124.881770	-	-

^aThe energies are calculated at the ONIOM(B3LYP/BS1) (25 °C) level. ^bThe energies are calculated at the B3LYP+D3(PCM)/BS3//B3LYP+D3/BS2 (60 °C) level. The energies are given in a.u.

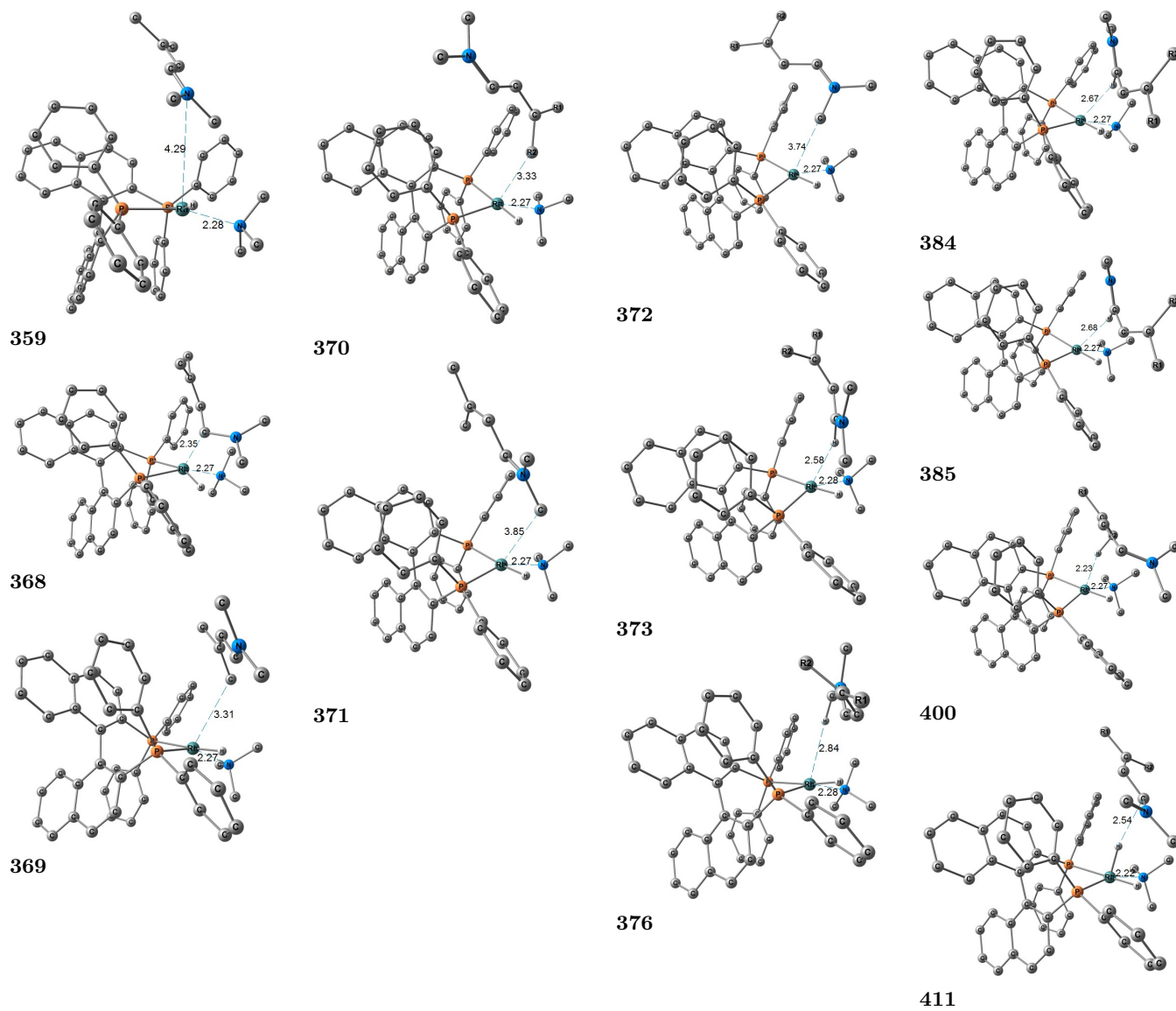
Table S3: The electronic and Gibbs free energies of LMs and TSs in the associative mechanism

No.	E_{ONIOM}^a	G_{ONIOM}^a	E^b	G^b
291	-1300.155345	-1299.226716	-2995.241576	-2994.379772
359	-1300.154670	-1299.227120	-2995.212374	-2994.354363
368	-1300.140555	-1299.205971	-2995.209142	-2994.343077
369	-1300.157997	-1299.230089	-	-
370	-1300.154705	-1299.227178	-	-
371	-1300.151196	-1299.227567	-	-
372	-1300.150897	-1299.222780	-	-
373	-1300.144374	-1299.216164	-	-
376	-1300.144018	-1299.215448	-	-
384	-1300.143256	-1299.214948	-	-
385	-1300.144023	-1299.216400	-	-
400	-1300.138067	-1299.209300	-	-
411	-1300.109017	-1299.184911	-	-
TS ₂₉₁₋₃₅₉	-1300.135983	-1299.209685	-2995.215337	-2994.355446

^aThe energies are calculated at the ONIOM(B3LYP/BS1) (25 °C) level. ^bThe energies are calculated at the B3LYP+D3(PCM)/BS3//B3LYP+D3/BS2 (60 °C) level. The energies are given in a.u.

2 Molecular structures

2.1 Hydride complexes in the associative mechanism (ONIOM(B3LYP/BS1:UFF) level)



3 Cartesian coordinates

3.1 Dissociative mechanism (ONIOM(B3LYP/BS1:UFF) level)

```
1
Rh 1.969972 -0.127877 -0.369654
P 0.494486 -1.814103 0.491525
P 0.317517 1.609213 -0.369799
C 1.097704 -3.419748 -0.096172
C 0.297682 -1.872559 2.329038
C 1.238496 3.165421 -0.262384
C -0.851799 1.673289 -1.799087
C -1.206244 -1.598527 -0.175986
C -0.709742 1.493709 1.145676
N 3.955237 -1.079972 -0.078643
C 4.660411 -0.009559 -0.889065
C 3.713245 0.401633 -1.993150
C 3.551712 1.665409 -2.483802
C 2.663747 1.915273 -3.681528
C 4.350280 2.860265 -2.022171
H 5.617734 -0.398519 -1.266607
H 4.881412 0.827040 -0.223289
H 3.258754 -0.416982 -2.552279
H 3.751180 3.775123 -2.063655
H 4.745013 2.758139 -1.009600
H 5.202285 3.010125 -2.698318
H 1.899300 2.667305 -3.445207
H 3.254132 2.327293 -4.509628
H 2.168320 1.005316 -4.025573
C 4.305123 -2.427922 -0.621410
H 5.389673 -2.588261 -0.571537
H 3.816828 -3.201623 -0.028358
H 3.976966 -2.509678 -1.657927
C 4.321186 -1.008888 3.170990
H 4.043335 -0.029372 1.761789
H 3.768166 -1.780906 1.909093
H 5.397731 -1.175282 1.510063
C 3.161640 -3.571819 -1.459272
C 1.849123 -2.4786367 -1.957072
C 2.092889 -5.844678 -1.076605
C 1.860162 -5.689239 0.293662
C 3.169093 -4.471195 0.781235
H 1.185911 -2.740400 -2.125214
H 2.046484 -4.906577 -3.018439
H 2.475615 -6.785859 -1.455584
H 2.070515 -6.508097 0.975986
H 1.228334 -4.343489 1.839532
C 0.999427 -0.964194 3.134582
C 0.814664 -0.955677 4.251063
C -0.075121 -1.849415 5.117757
C -0.783519 -2.751391 4.323547
C -0.609252 -2.757278 2.935889
H 1.672059 -0.249302 2.679863
H 1.357489 -0.245568 5.129754
H -0.221841 -1.837565 6.193129
H -1.485428 -3.437054 4.778529
H -1.183870 -3.443294 2.326735
C 2.286594 3.247436 0.655996
C 3.003631 4.440690 0.808483
C 2.679168 5.546815 0.016684
C 1.652166 5.459552 -0.929101
C 0.937860 4.262616 -1.107315
H 2.525598 2.386343 1.261457
H 3.810579 4.509363 1.523341
H 3.239313 6.472031 0.127136
H 1.155869 6.316248 -1.554119
H 0.163509 4.192827 -1.812381
C -0.715970 0.752334 -2.847785
H 1.628133 0.745165 -3.980608
C 2.688370 1.651797 -3.930058
C -2.836188 2.565933 -2.886664
C -1.931103 2.571827 -1.820396
H 0.090905 0.030936 -2.829531
H -1.513781 0.027200 -4.708648
H -3.398966 1.641013 -4.750460
H 3.665000 3.260835 -2.890024
H -2.072016 3.266360 -1.002138
C -1.719900 -2.534666 -1.098141
C -2.908638 -2.366975 -1.703252
C 3.697266 -1.249382 -1.418046
C -4.931965 -1.068833 -2.062671
C -5.702224 -0.009578 -1.763555
C -5.290068 0.925979 -0.804760
C -4.114190 0.787126 -0.167072
C 3.263659 -0.306696 -0.452488
C -2.010006 -0.487533 0.196498
H 1.167270 -3.423062 -1.338159
H 3.257523 -3.108407 -2.415821
H -5.273460 -1.784346 -2.801363
H -6.656113 0.123009 -2.263461
H -5.929155 1.772239 -0.577162
H -3.829879 1.538283 0.567168
C -0.540104 2.437456 2.179839
H -1.173595 2.325559 3.360570
C -2.043937 1.257874 3.599119
C 2.693517 1.134629 4.838214
C -3.548981 0.121647 5.055181
C -3.808590 -0.822334 4.052060
C -3.205205 -0.737935 2.853126
C -2.291338 0.305728 2.578126
C -1.629483 0.428349 1.324665
H 0.110938 3.281680 2.044758
H -1.005447 3.070348 4.132684
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4
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P 0.497158 -1.580335 -0.656250
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C 0.027148 -2.766930 0.682825
C 0.876994 2.943625 1.804632
C -0.822334 2.551460 -0.635300
C -1.099442 -0.966058 -1.320414
C -1.015559 0.705069 1.641165
N 3.936096 -0.857725 0.102339
C 4.782020 0.399968 0.110707
C 3.836486 1.582038 0.123784
C 3.281299 2.105114 -1.046344
C 2.778134 3.535273 -1.049538
C 3.575307 1.578345 -2.438449
H 5.438893 0.400219 0.985971
H 5.417415 0.396952 -0.77796
H 8.36947 2.211358 1.00974
H 4.155568 2.143261 -2.869555
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C 1.170181 5.228222 2.566516
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H 2.035717 1.462851 2.829187
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C -4.255773 -2.863521 2.102931
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C -1.399007 -2.684774 -2.795923
C -2.440422 -0.687555 -0.826773
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H -1.903765 -6.943906 0.516503
H 0.541798 -9.020448 -2.133881
H -0.578099 -8.155560 -3.179961
H 0.666061 -7.262110 -2.298354
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H -1.392042 -10.082636 -0.784896
H -2.651617 -9.030565 -0.105416
C 1.874410 -5.571665 0.967273
H 2.325403 -5.210282 0.043567
H 2.343981 -5.068663 1.815548
H 2.025459 -6.654187 1.059831
C -0.226473 -5.691066 2.239610
H -1.247047 -5.309965 2.290021
H -0.228324 -6.783684 2.312159
H 0.344925 -5.282282 3.074594
C -0.356135 -2.722819 3.865882
C -0.444020 -3.270302 5.151661
C 0.724469 -3.504858 5.882876
C 1.973674 -3.202832 5.331030
C 2.050104 -2.651403 4.045549
H -1.248879 -2.555512 3.282415
H -1.410999 -3.522264 5.577641
H 0.663131 -3.934286 6.876761
H 2.879564 -3.405766 5.895435
H 3.013540 -2.453772 3.609411
C 3.249605 -2.044428 0.049152
C 4.556775 -1.757871 -0.357724
C 5.322860 -0.824841 0.341917
C 4.777649 -0.176207 1.450346
C 3.467834 -0.452427 1.855495
H 2.656138 -2.752640 -0.514092
H 4.970490 -2.256194 -1.223803
H 6.335354 -0.599893 0.021841
H 5.362630 0.556160 1.990174
H 3.046264 0.074210 2.702113
C -0.483294 -3.645974 -3.227324
C -0.785966 -4.476985 -4.312673
C -2.020318 -4.347999 -4.956796
C -2.950717 -3.401700 -4.514481
C -2.639106 -2.577698 -3.425090
H 0.464828 -3.738390 -2.720161
H -0.071775 -5.221827 -4.652471
H -2.261892 -4.990558 -5.796335
H -3.915368 -3.317633 -5.007355
H -3.370424 -1.876259 -3.063639
C -3.054166 -0.903270 0.415772
C -4.111183 -0.088556 0.835018
C -4.565383 0.949508 0.020772
C -3.960021 1.171443 -1.216352
C -2.898680 0.363860 -1.637473
H -2.697563 -1.694557 1.062684
H -4.571687 -0.261260 1.798177
H -5.381692 1.584569 0.350164
H -4.299119 1.982492 -1.846562
H -2.419738 0.560765 -2.588076
C -0.478978 0.392258 2.812170
H -1.181309 1.537948 2.843576
C -1.323761 2.313149 1.689201
C -2.074946 3.499426 1.719901
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53

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H 3.504067 -3.180189 -5.766921
C -0.166797 -5.789554 -1.470279
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H -1.220865 -5.517427 -1.397728
H -0.086050 -6.884135 -1.444573
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C 4.066023 -2.243679 -2.433836
C 5.415989 -2.577970 -2.594481
C 6.175456 -1.930409 -3.573462
C 5.588188 -0.962660 -4.394667
C 4.235816 -0.637709 -4.227308
H 3.465646 -2.749466 -1.693048
H 5.871588 -3.341619 -1.970674
H 7.220509 -2.187980 -3.705111
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C -0.271014 0.686010 -6.280259
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C 1.113670 2.438759 -5.369820
C 1.592495 1.557871 -4.394755
H -0.158726 -1.218443 -5.285210
H -0.999832 0.346222 -7.003384
H -0.198652 2.694721 -7.060348
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H 2.299276 1.910392 -3.654495
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C -4.721407 -4.971166 -3.686514
C -4.587686 -4.839090 -2.300629
C -3.579939 -4.020365 -1.774921
H -2.146224 -2.977111 -4.661284
H -3.945143 -4.416303 -5.621293
H -5.499819 -5.605767 -4.995570
H -5.258744 -5.377419 -1.637117
H -3.458354 -3.948518 -0.708807
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C -0.274738 -2.611864 1.969820
C -1.393503 -2.146591 2.661529
C -2.522731 -1.737421 1.951694
C -2.533549 -1.787362 0.554010
H 0.599293 -3.007261 0.045066
H 0.609135 -2.915956 2.513739
H -1.382070 -2.094176 3.745632

H -3.387838 -1.362184 2.481526
H -3.404623 -1.441214 0.012499
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C 2.338262 0.439589 0.741921
C 1.071685 0.844865 1.176159
C 0.882270 1.293861 2.493299
C -0.329988 1.708211 2.898453
C -1.419382 1.703359 2.016186
C -1.277197 1.280595 0.747461
C -0.024302 0.826591 0.276101
C 0.166253 0.368893 -1.056596
H 3.508171 -0.307092 -0.803747
H 3.183336 0.480195 1.422687
H 1.712389 1.313497 3.189578
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H -2.388397 2.044059 2.364308
H -2.145074 1.282727 0.101869
C -2.884543 -0.285075 -3.289081
C -3.165797 0.947057 -3.746455
C -2.346248 2.029267 -3.415940
C -2.631836 3.312093 -3.911309
C -1.855212 4.355208 -3.574730
C -0.754154 4.181824 -2.725150
C -0.449211 2.969023 -2.230494
C -1.233245 1.837725 -2.558848
C -0.939723 0.535973 -2.062611
H -3.560413 -1.076315 -3.555225
H -4.037643 1.099944 -4.375421
H -3.481473 3.469574 -4.565192
H -2.082370 5.344071 -3.959340
H -0.141628 5.038580 -2.465670
H 0.416061 2.879404 -1.588104

TS₁₋₃₃
Rh 0.539278 -0.075014 2.533176
P 2.380482 1.535475 2.928246
P 0.863968 -1.057060 4.666147
C 3.143766 1.838316 1.311873
C 1.860467 3.161849 3.637226
C -0.346915 -2.312961 5.279005
C 2.474659 -1.972535 4.759877
C 3.732650 0.929253 4.033117
C 0.993573 0.403753 5.794520
N -0.878112 -1.448781 1.645840
C -1.000371 -0.661953 3.583660
C -0.884175 0.803798 0.706482
C -0.181930 1.735389 -0.002825
C -0.321337 3.205661 0.320939
C 0.616087 1.433192 -1.249247
H -1.954570 -0.902665 -0.134359
H -0.193557 -0.978749 -0.304277
H -1.574748 1.167034 1.465823
H 1.465793 2.117158 -1.340341
H 0.999172 0.411125 -1.286087
H -0.010607 1.591190 -2.136733
H 0.654795 3.654635 0.544219
H -0.709419 3.741968 -0.554472
H -0.995489 3.385254 1.160191
C -2.218174 -1.582692 2.299455
H -2.940976 -2.019966 1.598941
H -2.132420 -2.245644 3.158851
H -2.570438 -0.608336 2.635574
C -0.284377 -2.800435 1.040829
H 0.706933 -2.682009 0.962817
H -0.191529 -3.321884 2.354512
H -0.923507 -3.390746 0.731371
C 3.451398 0.737258 0.511750
C 0.088248 0.913128 -0.723847
C 4.398645 2.203908 -1.161897
C 4.073804 3.312961 -0.374032
C 3.444638 3.125472 0.863467
H 3.205249 -0.252453 0.860251
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H 4.308656 4.314484 -0.723666
H 3.189553 3.981384 1.461992
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C 0.088243 4.664099 4.354741
C 1.034582 5.584656 4.805673
C 2.393247 5.295094 4.679297
C 2.807112 4.089125 4.104896
H -0.244526 2.738248 3.456005
H -0.966643 4.878131 4.458222
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H 3.131906 5.998087 5.039981
H 3.864030 3.868806 4.027811
C -0.006309 -3.672477 5.182261
C -0.875184 -4.675079 5.626870
C -2.117064 -4.328124 6.154309
C -2.499619 -2.989192 6.213339
C -1.624104 -1.991647 5.673961
H 0.924398 -3.969416 4.732070
H -0.590938 -5.720886 5.551759
H -2.795284 -5.101592 6.497199
H -3.483774 -2.726468 5.591528
H -1.995382 -0.999754 6.759149
C 3.211021 -2.218559 3.925252
C 4.398391 -2.956280 3.643796
C 4.853991 -3.472084 4.857515
C 4.113862 -3.256193 6.019874
C 2.929325 -2.513467 5.974888
H 2.856238 -1.838462 2.645581
H 4.962559 -3.128415 2.737492
H 5.777030 -4.041717 4.897068

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H 2.361572 -2.353207 6.882438
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C 6.029855 0.215685 4.227056
C 5.844755 -0.085326 5.579288
C 6.901358 -0.611739 6.340365
C 6.723083 -0.891725 7.642348
C 4.450601 -0.160289 7.564542
C 4.588356 0.151263 6.191558
C 3.517276 0.685470 5.421001
H 5.215533 0.920168 2.457378
H 6.997717 0.050758 3.763467
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H 7.543970 -1.296962 8.225026
H 5.363716 -0.898575 9.312117
H 3.508476 -0.010647 8.075035
C -0.198819 1.074587 6.121192
C -0.235118 2.152457 6.920552
C 0.949747 2.733935 7.368492
C 0.909875 3.879221 8.180564
C 2.046824 4.507709 8.518560
C 2.383344 4.043910 8.052504
C 3.360999 2.951409 7.272055
C 2.194877 2.228987 6.916232
C 2.226130 1.064231 6.088235
H -1.107478 0.794620 5.641424
H -1.188168 2.615847 7.156261
H -0.038618 4.270140 8.529418
H 2.009613 5.392668 9.145317
H 4.187852 4.578983 8.321283
H 4.336925 2.651702 6.921663

TS₄₋₅
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C 0.412516 2.582051 0.951204
C -0.635667 -2.874336 1.568237
C 0.871109 -2.586269 -0.994505
C 1.275748 1.163511 -1.496749
C 1.477347 -0.833855 1.265628
N -3.363205 -1.456832 -0.440969
C -4.223633 -0.241965 -0.766084
C -4.509636 0.616668 0.434117
C -5.703095 1.104070 0.828061
C -5.797234 2.007225 2.038433
C -7.021935 0.836990 1.038726
H -5.134620 -0.576196 -1.276014
H -3.643444 0.322657 -1.526567
H -3.623834 0.894016 1.014380
H -7.752169 0.445086 0.857227
H -7.439420 1.772551 -0.255397
H -6.952830 0.130415 -0.691634
H -6.206779 2.986915 1.760560
H -6.475939 1.582266 2.788536
H -4.821522 2.166241 2.507023
C -3.936754 -2.243953 0.693075
H -4.965740 -2.548754 0.466673
H -3.333219 -3.141368 0.839386
H -3.927565 -1.645376 1.601578
C -3.231926 -2.333214 -1.650030
H -4.200320 -2.780175 -1.909994
H -2.864076 -1.740813 -2.488412
H -2.518626 -3.129158 -1.429031
C -1.832716 2.322594 -2.686026
C -2.632323 3.153399 -3.480433
C -2.764759 4.505549 -3.149417
C -2.109600 5.023907 -2.027600
C -1.311566 4.184162 -1.239901
H -1.724801 1.276590 -2.929402
H -3.151392 2.753861 -4.347073
H -3.385380 5.153212 -3.758846
H -2.229631 6.071258 -1.764733
H -0.834621 4.577736 -0.359630
C -0.024568 2.175969 2.220477
C 0.477353 2.790092 3.372735
C 1.420630 3.813225 3.270827
C 1.861104 4.228552 2.012072
C 1.366937 3.608078 0.857122
H -0.743234 1.371410 2.310948
H 0.137075 2.463340 4.345860
H 1.813779 4.284509 4.166075
H 2.601429 5.006804 1.926858
H 1.737709 3.916861 -0.113407
C -1.307059 -2.387822 2.691619
C -1.909244 -3.270789 3.596179
C -1.853566 -4.647325 3.357436
C -1.209262 -5.139396 2.217724
C -0.607797 -4.247585 1.320268
H -1.359948 -1.321693 2.853013
H -2.426102 -2.892121 4.473321
H -2.323016 -5.335615 4.051542
H -1.186799 -6.208587 2.026298
H -0.146948 -4.626728 0.425512
C 0.452657 -2.330876 -2.308361
C 1.079971 -2.961296 -3.387892
C 2.133705 -3.849123 -3.168659
C 2.561930 -4.103414 -1.865466
C 1.944261 -3.467921 -0.783472
H -0.345623 -1.624146 -2.491512
H 0.751962 -2.750411 -4.396596
H 2.623123 -4.333293 -4.007835

H 3.386776 -4.780697 -1.689790
H 2.301714 -3.652603 0.221493
C 1.395952 1.506166 -2.857136
C 3.265014 0.994161 -3.636630
C 3.300655 0.098374 -3.107464
C 4.301807 -0.449118 -3.926161
C 5.215152 -1.287553 -3.408200
C 5.186698 -1.624638 -2.047757
C 4.243514 -1.120827 -1.232170
C 3.255332 -0.241851 -1.731058
C 2.239421 0.308617 -0.902521
H 0.699138 2.192874 -3.304650
H 2.416945 1.276459 -4.683914
H 4.347301 -0.195815 -4.978795
H 5.987422 -1.705571 -4.045586
H 5.935346 -2.301624 -1.650882
H 4.250428 -1.414235 -0.191067
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C 2.656448 -0.445556 3.332704
C 3.442273 0.535817 1.722673
C 4.404290 1.237794 3.467198
C 5.173911 2.165213 2.873774
C 5.032484 2.443800 1.507526
C 4.122930 1.792094 0.761501
C 3.284682 0.810271 1.340537
C 2.304988 0.103604 0.587390
H 1.158180 -1.863123 3.139638
H 2.800627 -0.679539 4.383216
H 4.534277 1.034172 4.523555
H 5.916457 2.702844 3.544295
H 5.665654 3.195722 1.049042
H 4.040214 2.047050 -0.286157

TS₄₋₄₅
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P 1.880261 -2.030527 -0.078311
P 1.629753 -2.300872 0.179884
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C 2.140059 -0.889921 -1.507240
C -3.042877 -3.085403 -0.630341
C -1.952377 -2.151294 1.988441
C 1.431471 -0.964177 1.347835
C -1.413298 -0.619264 -0.494043
N -0.361097 -6.192062 1.148918
C -0.141083 -6.273947 -0.310942
C 1.172719 -5.647643 -0.736411
C 1.388637 -5.065503 -1.990714
C 2.799994 -4.747821 -2.443013
C 0.389178 -5.120366 -3.133484
H -0.237944 -7.503627 -0.174777
H -0.986247 -5.721757 -0.780552
H 2.037078 -5.846980 -0.113042
C 0.431430 -4.208515 -3.735373
H 0.650291 -5.959101 -3.795244
H -0.643643 -5.271609 -2.811696
H 3.098447 -5.456190 -3.225841
H 2.880011 -3.745414 -2.875252
H 3.523550 -4.843292 -1.628106
C 0.566999 -7.016303 1.947450
H 1.601349 -6.725758 1.751549
H 0.368134 -6.846480 3.007594
H 4.058965 -8.095252 1.736392
C -1.771117 -6.430017 1.515682
H -2.415917 -5.736728 0.962435
H -2.106918 -7.458792 1.296717
H -1.902757 -6.242011 2.583146
C 3.962679 -3.892322 1.281052
C 4.558311 -4.603997 1.601348
C 5.765855 -4.296612 0.950261
C 5.793724 -3.289910 -0.020030
C 4.624694 -2.583918 -0.333219
H 2.461711 -4.124770 1.771024
H 4.532060 -5.393068 2.347571
H 6.659797 -8.464615 1.192052
H 7.623994 -3.066475 -0.534920
H 6.499350 -1.837388 -1.106187
C 1.406067 -1.074074 -2.687838
C 1.545043 -0.182518 -3.756380
C 2.412859 0.905375 -3.656379
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C 2.998317 0.217692 -1.408063
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H -4.275415 -3.202169 1.123954
C -1.162718 -2.870830 2.897411
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C -2.338383 -1.857603 4.784000
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C 2.166890 -1.072216 2.545846
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C -0.733468 1.928090 4.840098
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H 2.408570 -0.532745 4.565399
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C 1.018102 3.540431 -0.891517
C 0.827548 2.382122 -0.235629
C -0.168864 1.471792 -0.656061
C -0.398825 0.235580 0.007949
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H -1.331825 3.325262 -3.293307
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H 1.788923 4.226993 -0.558552
H 1.461661 2.158338 0.611979
TS₅₋₃₆
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C 0.141016 -2.405617 -1.362027
C -0.211354 3.220993 -1.420917
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C 0.946905 -1.337496 1.722263
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C -7.140240 -1.274293 -0.758263
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H -7.171087 -2.370720 -0.809653
H -8.106281 -0.951220 -0.350217
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H -4.884474 2.796203 -0.980987
C -3.237994 3.448614 -1.186109
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C -3.233885 2.702921 1.309259
H -4.209398 3.148218 1.537525
H -2.877112 2.129128 2.163651
H -2.517058 3.495038 1.082807
C -3.237881 -2.320495 2.135090
C -3.251279 -3.151467 2.780879
C -3.491529 -4.435049 2.281856
C -2.817821 -4.885018 1.141941
C -1.891227 -4.047821 0.506984
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H -4.210649 -5.080653 2.773950
H -3.021900 -5.876479 0.747053
H -1.400662 -4.385067 -0.388814
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C 0.395931 -2.356035 -3.779702
C 1.207077 -3.490168 -3.728921
C 1.487284 -4.083430 -2.497824
C 0.965997 -3.541679 -3.18534
H -0.748876 -0.924827 -2.652927
H 0.181270 -1.887211 -4.730389
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H 2.126160 -4.954985 -2.450601
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C -0.839767 2.940332 -2.635387
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C -1.116178 3.306366 -3.051421
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H 1.463622 6.115774 -3.683941
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H 0.354289 4.767072 -0.041483
C 0.084877 2.151089 2.423497
C 1.081623 2.584416 3.612046
C 2.247281 3.350469 3.575537
C 2.817284 3.681699 2.345889
C 2.229867 3.242715 1.154999
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C 3.942531 -0.339880 4.049497
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C 5.099107 0.892316 2.365729
C 4.170935 0.586254 1.441949
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C 2.047190 -0.552107 0.833531
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H 1.824180 -1.891023 4.498061
H 3.876811 -0.695518 5.071011
H 5.745698 0.686096 4.409715
H 5.948624 1.508244 2.091403
H 4.293354 0.974880 0.440059
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C 2.915076 0.605550 -3.238902
C 3.512053 -0.538968 -2.702665
C 4.440041 -1.275101 -3.456669
C 5.035331 -2.357018 -2.927624
C 4.744556 -2.764764 -1.618538
C 3.860836 -2.086335 -0.865284
C 3.201056 -0.945508 -1.379393
C 2.255233 -0.204253 -0.616887
H 1.603757 2.190698 -2.970568
H 3.178492 0.935784 -4.239247
H 4.685836 -0.972745 -4.467828
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H 3.658452 -2.441905 0.135831

TS₈₋₂₂
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P -4.437495 3.342737 -0.306001
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C -3.613162 4.751272 3.870903
C -3.471202 3.023438 -1.806135
C -6.219769 3.009780 -0.660866
C -6.216066 4.007898 2.757792
C -4.311366 5.120477 0.122156
N -2.266611 0.623449 2.519945
C -1.770323 0.701549 1.154717
C -0.532548 1.437171 0.860333
C 0.376055 1.102658 -0.089254
C 1.610376 1.953278 -0.282382
C 0.279805 -0.087470 -1.012478
H -1.847510 -0.264278 0.660430
H -3.030128 1.076696 0.260204
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H 1.700047 2.287090 -1.323238
H 1.607548 2.835551 0.363053
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H -0.561385 0.434695 3.764421
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C -4.178390 9.612638 2.364027
C -5.193839 8.984266 3.014636
C -5.498501 7.641849 2.644888
C -4.796342 7.009647 1.592712
C -5.087328 5.681290 1.173515
H -2.802575 5.532671 -1.366395
H -2.333973 7.757717 -0.664183
H -2.715929 9.631358 0.856860
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TS₂₃₋₄₉
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P 1.043606 -1.311369 -0.534211
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C -1.567187 1.796358 -1.627985
C 2.258545 -1.946712 -1.723163
C 0.951431 -2.468622 0.903669
C -1.335120 0.701254 1.159541
C -0.613190 -1.461381 -1.322731
N 4.356632 1.152142 -0.602887
C 3.760160 1.720720 0.492680
C 3.519068 1.020830 1.730393
C 2.949458 1.600520 2.844410
C 2.758307 0.788381 4.101303
C 2.594888 3.059184 2.976426
H 1.784832 2.741974 0.023448
H 3.805155 2.800593 0.505254
H 3.801126 -0.023400 1.793767
H 1.611123 3.170153 3.447045
H 3.315856 3.558807 3.637844
H 2.560553 3.591789 2.025646
H 3.252375 1.281681 4.948303
H 1.692612 0.726602 4.359096
H 3.157763 -0.224335 4.012352
C 4.797349 2.020420 -1.717015
H 5.875271 2.212672 -1.654603
H 4.577068 1.524783 -2.665034
H 4.251317 2.962812 -1.679762
C 4.962622 -0.193564 -0.581224
H 5.038963 -0.562272 -1.604999
H 5.966397 -0.159705 -0.141834
H 4.343682 -0.888961 -0.015995
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C -0.473625 5.938257 0.518130
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C -2.341433 5.122095 1.828802
C -2.067710 3.818509 1.396511
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C 2.492270 -1.215551 -2.888818
C 3.430855 -1.658213 -3.828858
C 4.152432 -2.830505 -3.583992
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C 0.718155 -4.173190 3.129852
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C -2.867036 -3.224320 3.891133
C -2.971755 -3.633715 2.554888
C -2.625045 -2.808541 1.551169
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TS₃₃₋₁₁₄
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C 0.144625 -2.380612 1.368970
C 0.982805 3.383286 -0.603543
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H 3.711116 -1.522383 0.893678
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H 5.089682 2.863793 2.033387
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C 1.257926 -5.209647 -3.255955
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C -0.861353 -3.798033 3.072205
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TS₃₆₋₉₃
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H -0.438503 -3.344684 3.138916
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C 3.487259 -1.889045 2.925894
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C 2.776567 -3.232773 4.796000
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H 0.837186 -2.780605 5.601306
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H 4.734313 3.608692 4.139132
H 6.235086 1.875081 4.991584
H 6.572413 -0.173044 6.229204
H 4.653752 -1.409672 7.169129
H 2.406906 -0.625460 6.863333

TS₄₅₋₄₆
Rh 1.778119 0.322566 -0.290212
P 0.383120 -1.575177 -0.772763
P 0.062397 1.664428 0.622877
C 1.259644 -2.492767 -2.060745
C 0.040982 -2.687448 0.657570
C 0.846055 2.801059 1.793394
C -0.932547 2.615695 -0.607778
C -1.223065 -1.008335 -1.430817
C -1.131453 0.631136 1.556153
N 4.677732 -1.019681 0.783718
C 4.178881 -0.246031 -0.342631
C 3.781853 1.162723 0.001643
C 3.328369 2.073878 -0.955664
C 3.113396 3.524597 -0.582859
C 3.420195 1.827888 -2.450652
H 4.817366 -0.292921 -1.248625
H 3.243866 -0.828564 -0.728899
H 3.948609 1.489033 1.023234
H 4.329617 2.310635 -2.837499
H 2.571902 2.275997 -2.974553
H 3.467265 0.769706 -2.716196
H 2.148481 3.901021 -0.938720
H 3.887934 4.140807 -1.055826
H 3.178966 3.686330 0.497017
C 4.645941 -2.472393 0.545652
H 3.623573 -2.778234 0.293362
H 4.939798 -2.992714 1.459642
H 5.315350 -2.795191 -0.271806
C 5.977682 -0.545836 1.301191
H 5.919362 0.515304 1.554277
H 6.800249 -0.687805 0.577613
H 6.215939 -1.098507 2.212156
C 1.756032 -1.782454 -3.154299
C 2.508544 -2.433222 -1.139415
C 2.778899 -3.799210 -4.010993
C 2.307266 -4.509851 -2.902363
C 1.554545 -3.848993 -1.923131
H 1.543969 -0.727617 -3.239265
H 2.885110 -1.883937 -4.997847
H 3.363589 -4.308418 -4.769337
H 2.534256 -5.567396 -2.798819
H 1.221182 -4.389881 -1.054677
C 0.644104 -2.432628 1.898076
C 0.348697 -3.232932 3.006414
C -0.550990 -4.293049 2.889388
C -1.154346 -4.553623 1.658465
C -0.866906 -3.753146 0.548399
H 1.333477 -1.604134 0.205565
H 0.816980 -3.022952 3.958443
H -0.783377 -4.909430 3.752065
H -1.860921 -5.367109 1.564311
H -1.357161 -3.950088 -0.396398
C 1.773448 2.279374 2.696425
C 2.440337 3.121272 3.594267
C 2.182179 4.495271 3.573377
C 1.269508 5.026984 2.656581
C 0.607619 4.175790 1.762228
H 1.970425 1.217327 2.697201
C 3.158163 2.713848 4.300726
H 2.698429 5.152747 4.264217
H 1.085672 6.097525 2.632914
H -0.064437 4.593163 1.034643
C -0.621368 2.527385 -1.972160
C -1.402213 3.192603 -2.922799
C -2.504729 3.948427 -2.523015
C -2.827113 4.035101 -1.168515
C -2.054718 3.363931 -0.215086
H 0.216578 1.924138 -2.294512
H -1.154360 3.111851 -3.972413
H -3.113432 4.459519 -3.262244

H -3.689459 4.607068 -0.853543
H -2.331085 3.414954 0.830319
C -1.512879 -1.180704 -2.797783
C -2.614139 -0.655762 -3.363493
C -3.523873 0.078739 -2.595156
C -4.667496 0.636420 -3.189655
C -5.553852 1.316775 -2.443485
C -5.354850 1.477145 -1.065170
C -4.271379 0.958923 -0.460040
C -3.305365 0.242275 -1.203046
C -2.144381 -0.317170 -0.601531
H -0.844218 -1.744299 -3.424425
H -2.795825 -0.804031 -4.423772
H -4.845346 0.517526 -4.251973
H -6.436863 1.742883 -2.908430
H -6.085129 2.027677 -0.482062
H -4.150465 1.114501 0.603509
C -1.160403 0.713422 2.963056
C -1.932897 -0.093069 3.711060
C -2.753720 -1.048873 3.105959
C -3.545096 -1.903009 3.891265
C -4.347128 -2.808700 3.307253
C -4.409043 -2.913929 1.911061
C -3.666341 -2.113835 1.125697
C -2.802604 -1.147013 1.692131
C -1.995437 -0.286090 0.896228
H -0.551813 1.435021 3.477156
H -1.914283 -0.001646 4.792942
H -3.516260 -1.835505 4.972418
H -4.957256 -3.464452 3.919755
H -5.064414 -3.651909 1.461226
H -3.736638 -2.237487 0.053703

TS₄₆₋₄₇
Rh 1.854531 0.280871 -0.288986
P 0.110255 1.732019 0.570882
P 0.422081 -1.614756 -0.715888
C 0.899337 2.905244 1.702671
C -0.906491 2.644254 -0.673138
C 1.274414 -2.579796 -1.985948
C 0.035421 -2.695970 0.728878
C -1.077432 0.732354 1.546822
C -1.178892 -1.036253 -1.383871
H 4.962981 -0.844050 0.736761
C 4.344530 -0.143413 -0.270796
C 3.833589 1.220309 -0.071622
C 3.278991 1.964051 -1.129579
C 2.993477 3.436992 -0.920602
C 3.404500 1.575274 -2.592133
H 4.760656 -0.359796 -1.253335
H 3.083678 -0.843904 -0.622190
H 3.986514 1.705449 0.884641
H 4.266186 2.099830 -3.030709
H 2.519661 1.887232 -3.153182
H 3.541511 0.504523 -2.751911
H 2.017469 3.725863 -1.321630
H 3.745782 4.033336 -1.451952
H 3.038938 3.720009 0.135207
C 4.614406 -0.588624 2.141658
H 3.556056 -0.818350 2.333975
H 4.799561 0.454636 2.405481
H 5.239679 1.214149 2.778299
C 5.429158 -2.201159 0.413706
H 4.600454 -2.927093 0.452929
H 6.201715 -2.504902 1.120886
H 5.854246 -2.215688 -0.592878
C 1.828202 2.409685 2.618847
C 2.507295 3.278331 3.481256
C 2.260346 4.652700 3.410906
C 1.347650 5.157966 2.479329
C 0.673941 4.280042 1.620385
H 2.017109 1.347569 2.656515
H 3.226591 2.891772 4.197865
H 2.786592 5.331078 4.073488
H 1.174415 6.228672 2.415410
H 0.006244 4.676721 0.877393
C -0.630630 2.498376 -2.040252
C -1.427587 3.134462 -2.997368
C -2.511932 3.917948 -2.601403
C -2.800585 4.060708 -1.244060
C -2.012277 3.418427 -0.283792
H 0.192337 1.873177 -2.358681
H -1.206335 3.009715 -4.048629
H -3.133030 4.406678 -3.345449
C -3.649033 4.654316 -0.931375
H -2.263202 3.512841 0.764995
C 1.751064 -1.910051 -3.113596
C 2.485436 -2.596169 -4.088320
C 2.759922 -3.956210 -3.914919
C 2.311812 -4.625237 -2.771310
C 1.577290 -3.929063 -1.802670
H 1.535401 -0.859501 -3.234586
H 2.845023 -2.078594 -4.973382
H 3.331033 -4.492614 -4.664853
H 2.544604 -5.677417 -2.631945
H 1.268130 -4.436810 -0.905878
C 0.579437 -2.401465 1.987298
C 0.248450 -3.178097 3.102355
C -0.630134 -4.254414 2.974297
C -1.178970 -4.552437 1.726724
C -0.857230 -3.773968 0.610241
H 1.243285 -1.555293 2.101264
H 0.670109 -2.936208 4.068478
H -0.890456 -4.852785 3.841696

H -1.870291 -5.377912 1.623512
H -1.307097 -3.999391 -0.348204
C -1.109543 0.872249 2.949099
C -1.876242 0.090067 3.728241
C -2.688566 -0.896153 3.161412
C -3.477035 -1.721612 3.979598
C -4.273628 -2.654225 3.431623
C -4.332996 -2.816033 2.040739
C -3.592501 -2.045161 1.224655
C -2.733443 -1.052979 1.752680
C -1.929539 -0.220891 0.923474
H -0.510088 1.621404 3.434007
H 1.861974 0.226985 4.805448
H -3.451154 -1.609587 5.057136
H -4.881880 -3.287380 4.069265
H -4.984385 -3.574520 1.620230
H -3.660763 -2.212000 0.158366
C -1.486219 -1.257999 -2.740192
C -2.586794 -0.742114 -3.315007
C -3.481780 0.029413 -2.566576
C -4.626525 0.574100 -3.170926
C -5.501260 1.287347 -2.442193
C -5.289064 1.495236 -1.072314
C -4.203885 0.991123 -0.458409
C -3.248929 2.241687 -1.183530
C -2.086518 -0.304897 -0.572007
H -0.834833 -1.857147 -3.351264
H -2.781437 -0.929894 -4.366759
H -4.815003 0.418077 -4.226600
H -6.385329 1.703132 -2.914507
H -6.010316 2.071535 -0.503400
H -4.073166 1.183817 0.597818
TS₄₇₋₄₈
Rh 1.852031 0.276628 -0.447491
P 0.037701 1.885320 0.503460
P 0.399881 -1.666916 -0.615170
C 0.872512 3.037263 1.623574
C -0.930911 2.820763 -0.754740
C 1.163599 -2.923053 -1.689628
C 0.013949 -2.445926 1.014534
C -1.186294 0.938386 1.480582
C -1.206830 -1.131937 -1.323207
N 4.636007 -1.503420 0.204796
C 4.138496 -0.531916 -0.616272
C 3.964266 0.839790 -0.234883
C 3.533311 1.868923 -1.084330
C 3.475040 3.285036 -0.549231
C 3.602342 1.809588 -2.601263
H 4.160647 -0.793420 -1.665343
H 2.027375 -0.096194 -1.907057
H 4.170149 1.112682 0.800373
H 4.457793 2.410544 -2.940413
H 7.703898 2.244273 -3.049495
H 3.720776 0.800226 -2.998018
H 5.723858 3.802826 -0.884826
C 4.329852 3.861923 -0.924882
H 3.507443 3.320364 0.543800
C 4.824104 -1.298646 1.646668
H 3.51425 -0.361997 1.840621
H 3.433381 -2.114453 2.037783
H 5.865933 -1.290068 2.184210
C 4.689433 -2.892677 -0.268012
H 0.505262 -2.919680 -1.351440
H 3.895689 -3.496717 0.193094
H 5.655899 -3.341005 -0.025397
C 1.730324 2.508955 2.589669
C 2.435281 3.57681 3.451542
C 2.289821 4.742877 3.327116
C 1.452463 5.278261 2.342845
C 0.750098 4.420336 1.486661
H 1.844884 1.438100 2.664813
H 3.097938 2.947069 4.208182
H 8.37419 5.405386 3.988414
H 1.358816 6.355574 2.726727
H 0.137704 4.835140 0.706030
C -0.649881 2.651084 -2.117995
C -1.411172 3.313025 -3.086721
C -2.460785 4.149838 -2.705846
C -2.749751 4.321875 -1.351766
C -1.998070 3.653759 -0.379826
H 0.152275 1.992385 -2.424528
H -1.187802 3.170105 -4.135281
H -3.052744 4.660325 -3.459038
H -3.568255 4.961771 -1.050627
H -2.246325 3.775499 0.666818
C 1.564471 -2.579112 -2.985708
C 2.219168 -3.511148 -3.800318
C 2.490940 -4.789686 -3.307570
C 2.115333 -5.136232 -2.007440
C 1.459321 -4.198194 -1.200774
H 1.343509 -1.600541 -3.377120
H 2.517094 -3.246361 -4.811086
H 3.001951 -5.513535 -3.932954
H 2.346232 -6.125298 -1.621505
H 1.218168 -4.459626 -0.185947
C 0.619164 -1.956779 2.181159
C 0.306102 -2.509340 3.427324
C -0.611687 -3.556006 5.523207
C -1.216700 -4.050266 2.366469
C -0.912401 -3.496673 1.118657
H

H -1.937217 -4.854126 2.434639
H -1.401167 -3.875305 0.230115
C -1.299139 1.179666 2.864372
C -2.109360 0.452637 3.652195
C -2.892293 -0.570625 3.110487
C -3.736909 -1.329277 3.937275
C -4.513808 -2.290246 3.410643
C -4.497469 -2.547854 2.033182
C -3.700429 -1.844417 1.209476
C -2.855587 -0.828328 1.716018
C -1.991727 -0.066664 0.878063
H -0.731742 1.969089 3.325017
H -2.158177 0.667506 4.715507
H -3.772202 -1.140751 5.003825
H -5.166674 -2.870325 4.054677
H -5.136682 -3.325663 1.629435
H -3.713161 -2.084120 1.055069
C -1.539030 -1.514086 -2.637347
C -2.597543 -0.999500 -3.286540
C -3.430793 -0.069905 -2.658049
C -4.530806 0.472788 -3.342219
C -5.360886 1.325505 -2.718890
C -5.148505 1.679052 -1.379493
C -4.105471 1.180977 -0.692147
C -3.192338 0.294394 -1.308662
C -2.075942 -0.252420 -0.615260
H -0.945393 -2.243717 -3.154733
H -2.808139 -1.314216 -4.304534
H -4.722405 0.201395 -4.373755
H -6.210867 1.738908 -3.251892
H -5.835347 2.363696 -0.893925
H -3.974721 1.485472 0.337382

TS₄₈₋₅₃

Rh -1.089394 0.639227 -1.982600
P -0.561722 0.962081 -4.293469
P -3.487104 1.410855 -2.188557
C 1.243266 1.030472 -4.450128
C -1.205893 -0.332858 -5.444680
C -4.439785 0.454570 -0.990433
C -3.821034 3.213139 -1.961451
C -1.272381 2.556611 -4.867194
C -4.148968 0.977859 -3.841461
N -2.452717 0.793665 1.934438
C -1.608406 0.223650 1.066598
C -0.686684 0.898524 0.248028
C 0.408553 0.222861 -0.436753
C 1.709842 1.005892 -0.510301
C 0.643397 -1.269285 -0.179992
H -1.634714 -0.860351 1.051168
H -0.050728 -0.457353 -2.363064
H -0.594183 1.973250 0.366472
H 1.061923 -1.419403 0.824901
H 1.366541 -1.658946 -0.901454
H -0.266053 -1.868340 -0.278010
H 2.361971 0.603261 -1.291016
H 2.248301 0.912455 0.443744
H 1.541513 2.068298 -0.701697
C -3.266221 -0.022328 2.858465
H -3.239476 -1.066305 2.542895
H -4.302027 0.323072 2.844549
H -2.878176 0.056654 3.878459
C -2.533062 2.259314 2.080024
H -2.734911 2.718667 1.107484
H -1.599006 2.665978 2.749813
H -3.348670 2.502491 2.759413
C 1.951753 1.941010 -3.666618
C 3.350140 1.989924 -3.720334
C 4.040094 1.098164 -4.546251
C 3.330883 0.158883 -5.308379
C 1.939632 0.122127 -5.249465
H 1.409945 2.621104 -3.027567
H 3.899577 2.710127 -3.120153
H 5.123469 1.128385 -4.589278
H 3.880622 -0.543911 -5.935632
H 1.408187 -0.625610 -5.811819
C -1.913319 -1.433778 -4.938937
C -2.448073 -2.392021 -2.580996
C -2.284921 -2.262063 -7.185575
C -1.583364 -1.170428 -7.697398
C -1.052623 -0.205524 -6.835539
H -2.060552 -1.535973 -3.871639
H -2.998768 -3.231744 -5.404060
H -2.706839 -3.002762 -7.857654
H 1.464672 -1.057264 -8.766690
H -0.529011 0.648923 -7.244943
C -4.213345 -0.921116 -0.905428
C -4.965694 -1.716393 -0.032445
C -5.946185 -1.123904 0.769368
C -6.162371 0.256968 0.713602
C -5.398492 1.045603 -0.156608
H -3.462127 -1.366614 -1.537641
H -4.792508 -2.786869 0.044725
H -6.529581 -1.733936 1.449680
H -6.907968 0.716075 1.356212
H -5.542727 2.109556 -0.170871
C -2.768820 0.075637 -1.622251
C -2.991088 0.451064 -1.498461
C -4.264018 0.980234 -1.713641
C -5.315780 0.130193 -2.056605
C -5.096228 3.755408 -2.190926
H -1.774943 3.676648 -1.464579
H -2.170682 6.105442 -1.237128
H -4.434306 7.048025 -1.618983

H -6.302615 5.535490 -2.234467
H -5.913956 3.108633 -2.482138
C -0.417121 3.644390 -5.134928
C -0.886501 4.878623 -5.387726
C -2.262748 5.120693 -5.418502
C -2.750777 6.413113 -5.671550
C -4.073876 6.632584 -5.750171
C -4.984012 5.578825 -5.589819
C -4.554378 4.328125 -5.345418
C -3.172468 4.048893 -5.236463
C -2.678066 2.740071 -4.976949
H 0.647265 3.507736 -5.150628
H -0.189769 5.690742 -5.573798
H -2.064401 7.239910 -5.811756
H -4.444734 7.632965 -5.947991
H -6.047645 5.777815 -5.662974
H -5.290402 3.545628 -5.219755
C -5.166609 0.007455 -3.951093
C -5.628903 -0.412367 -5.141322
C -5.116750 0.119858 -6.327743
C -5.595617 -0.327045 -7.570091
C -5.119143 0.203003 -8.708787
C -4.142862 1.208031 -8.675869
C -3.658776 1.661037 -7.505085
C -4.123543 1.130896 -6.279031
C -3.632038 1.578185 -5.019878
H -5.606811 -0.421686 -3.068614
H -6.408568 -1.167344 -5.178020
H -6.355541 -1.098074 -7.618477
H -5.495818 -0.144381 -9.665315
H -3.774889 1.623629 -9.607780
H -2.898938 2.430216 -7.527808

TS₅₃₋₅₄

Rh 1.411235 1.254484 -0.141509
P -0.883214 1.846715 0.106677
P 1.001444 -1.197103 -0.362627
C -0.917628 3.485638 0.875545
C -1.901706 1.878119 -1.435140
C 2.295464 -1.810278 -1.471063
C 0.954097 -2.216113 1.177180
C -1.685822 0.648717 1.240975
C -0.598668 -1.485469 -1.206899
N 5.058675 -0.490353 0.609103
C 4.389349 0.495584 -0.004501
C 3.569543 1.448706 0.622414
C 3.108497 2.665014 -0.024749
C 3.005168 3.887625 0.877878
C 3.599565 3.007461 -1.433920
H 4.554417 0.560876 -1.074812
H 1.248932 2.710935 -0.702005
H 3.485088 1.419521 1.703199
H 4.649124 3.329815 -1.399427
H 3.011364 3.832530 -1.842787
H 3.511245 2.168715 -2.130925
H 2.286421 4.611969 0.482529
H 3.983346 4.384277 0.936698
H 2.700525 3.621083 1.892748
C 5.986731 -1.363134 -0.135722
H 5.894808 -1.163363 -1.204747
H 5.742731 -2.412643 0.048745
H 7.018555 -1.175778 0.175720
C 4.992407 -0.681250 2.070285
H 3.951863 -0.718578 2.400247
H 5.502576 0.134939 2.592568
H 5.475845 -1.623769 2.324723
C -0.142773 3.700513 2.015342
C -0.086488 4.968102 0.670502
C -0.793427 6.029131 2.034312
C -1.545531 5.828057 0.872680
H -1.596121 4.555105 0.289886
H 0.405881 2.875686 2.445054
H 0.506671 5.132148 3.503038
H -0.751142 7.014110 2.486530
H -2.079185 6.660125 0.421271
H -2.147904 4.413895 -0.622865
C -1.304089 1.611433 -2.675996
C -2.075666 1.578098 -3.842009
C -3.450647 1.807751 -3.782888
C -4.053584 2.072315 -2.553101
C -3.288108 2.099644 -1.383106
H -0.241141 1.414972 -2.731201
H -1.604321 1.363705 -4.791637
H -4.049362 1.774443 -4.687746
H -5.121250 2.237899 -2.498998
H -3.770256 2.282597 -0.431304
C 2.576962 -1.071554 -2.622033
C 3.553542 -1.510350 -3.524448
C 4.251284 -2.693926 -3.264263
C 3.985754 -3.428173 -2.104212
C 3.012852 -2.976015 -1.203315
H 2.025175 -0.165254 -2.814816
H 3.770595 -0.938980 -4.422662
H 5.010486 -3.037743 -3.958217
H 4.546727 -4.334480 -1.894495
H 2.842325 -3.518138 -0.291223
C 1.177935 -1.605357 2.419058
C 1.087804 -2.347512 3.601275
C 0.769785 -3.705257 3.556853
C 0.536541 -4.319510 3.268053
C 0.616414 -3.579006 1.142118
H 1.407177 -0.548401 2.465413
H 1.262065 -1.863688 4.525241
H 0.698156 -4.279247 4.475246

H 0.278168 -5.368929 2.285782
H 0.407096 -4.059514 0.194990
C -2.018987 1.047774 2.550703
C -2.457334 0.174262 3.474106
C -2.615703 -1.177158 3.152443
C -3.060279 -2.090436 4.122373
C -3.248252 -3.381022 3.799741
C -3.010980 -3.833600 2.494551
C -2.584185 -2.989056 1.538957
C -2.358892 -1.624238 1.831651
C -1.904717 -0.700024 0.850154
H -1.929971 2.077459 2.843557
H -2.690084 0.523189 4.475893
H -3.259520 -1.760007 5.135012
H -3.593337 -4.081465 4.553196
C -3.172535 -4.879106 2.255653
H -2.403594 -3.381369 0.547348
C -0.611738 -2.034506 -2.505690
C -1.749660 -2.189043 -3.204432
C -2.977683 -1.817220 -2.649658
C -4.164000 -1.971687 -3.385343
C -5.345438 -1.634948 -2.841704
C -5.413616 -1.128781 -1.536482
C -4.299471 -0.965251 -0.801245
C -3.030740 -1.299515 -1.330388
H -1.827679 -1.134928 -0.587828
H 0.304612 -2.351659 -2.971253
H -1.712063 -2.609784 -4.204816
H -4.135038 -2.367670 -4.393638
H -6.258684 -1.759862 -3.414306
H -6.377808 -0.866224 -1.116923
H -4.397388 -0.562110 0.197463

TS₉₅₋₉₆

Rh 1.454144 1.207406 -0.224898
P -0.795199 1.807844 0.338294
P 0.984454 -1.157353 -0.699815
C -0.679902 3.316528 1.329750
C -1.974851 2.067314 -1.059190
C 2.174725 -1.653581 -1.971450
C 1.056088 -2.340842 0.716482
C -1.493016 0.477458 1.385236
C -0.693842 -1.330165 -1.412733
N 4.501418 -0.369693 1.443653
C 3.899863 0.753460 1.032768
C 3.677776 1.201295 -0.292553
C 3.223054 2.560045 -0.550480
C 3.280293 3.013439 -2.004293
C 3.559077 3.685247 0.433674
H 1.525739 2.799312 -0.178743
H 3.587382 1.406511 1.838711
H 4.035422 0.620173 -1.135780
H 2.967249 4.575848 0.203514
H 4.620711 3.945696 0.339398
H 3.354554 3.424082 1.474288
H 4.285470 3.394352 -2.231160
H 2.567019 3.821387 -2.186869
H 3.057372 2.194157 -2.691865
C 4.645663 -0.671661 2.881652
H 5.705065 -0.672281 3.157660
H 4.226063 -1.658130 3.099753
H 4.120772 0.079066 3.473229
C 5.079433 -1.376542 0.540834
H 4.978649 -1.069387 -0.499014
H 4.571677 -2.336641 0.679090
H 6.141936 -1.507464 0.765438
C 0.299009 3.375944 2.323467
C 0.481397 4.546465 3.069568
C -0.309825 5.667108 2.799326
C -1.270688 5.623101 1.783921
C -1.444535 4.447109 1.042647
H 0.909291 2.506730 2.519739
H 1.234086 4.589711 3.852111
H -0.171992 6.577350 3.372853
H -1.870607 6.502671 1.566373
H -2.159911 4.428776 0.239649
C -1.519394 1.978864 -2.382998
C -2.412922 2.112841 -3.450654
C -3.769347 2.333806 -3.209587
C -4.231398 2.420835 -1.896212
C -3.343601 2.279597 -0.824917
H -0.471830 1.790773 -2.580982
H -2.050420 2.035934 -4.466773
H -4.462706 2.430979 -4.039110
H -5.284035 2.578011 -1.702804
H -3.717406 2.322737 0.190105
C 2.352255 -0.810506 -3.069546
C 3.297624 -1.119232 -4.055061
C 4.075942 -2.273782 -3.926801
C 3.915228 -3.112539 -2.819251
C 2.965268 -2.795193 -1.840160
H 1.746562 0.078116 -3.154375
H 3.432267 -0.466975 -4.913218
H 4.813765 -2.515627 -4.683859
H 4.535264 -3.998498 -2.714451
H 2.871876 -3.420181 -0.970351
C 1.389226 -1.874012 1.995879
C 1.387403 -2.744425 3.091002
C 1.055194 -4.088578 2.920908
C 0.717838 -4.560803 1.652137
C 0.706292 -3.691544 0.556407
H 1.629678 -0.829255 2.142384
H 1.642638 -2.369473 0.072497
H 1.053016 -4.761953 3.772082

H 0.448097 -5.599200 1.515782
H 0.417900 -4.062607 -0.418711
C -1.648877 0.697092 2.767865
C -2.009412 -0.286895 3.610139
C -2.254315 -1.577153 3.129342
C -2.617415 -2.606554 4.013059
C -2.880417 -3.838056 3.544864
C -2.801588 -4.113354 2.172778
C -2.456349 -3.154049 1.295790
C -2.160413 -1.844574 1.739633
C -1.787606 -0.803515 0.844625
H -1.474499 1.673145 3.184179
H -2.107243 -0.076642 4.671062
H -2.691980 -2.413910 5.076824
H -3.161893 -4.628680 4.232650
H -3.019998 -5.114327 1.816968
H -2.396735 -3.411835 0.247129
C -0.838709 -1.712243 -2.761555
C -2.039515 -1.765401 -3.363453
C -3.202602 -1.453284 -2.653129
C -4.454984 -1.502111 -3.286870
C -5.573692 -1.227002 -2.595801
C -5.101118 -0.891297 -1.536870
C -4.329452 -0.832498 -0.595236
C -3.122454 -1.106637 -1.280129
C -1.852911 -1.048950 -0.639622
H 0.024436 -1.978288 -3.345542
H -2.104042 -2.057483 -4.407351
H -4.527923 -1.766824 -4.335154
H -6.538468 -1.269764 -3.090629
H -6.426602 -0.676226 -0.697670
H -4.325726 -0.559646 0.451246

TS₉₇₋₁₀₁

Rh 2.027263 0.156237 -0.816994
P 0.226352 -1.804759 -0.298399
P 0.289788 1.836952 -0.767104
C 0.610385 -3.237548 -1.344805
C 0.113823 -2.373051 1.455728
C 0.863097 3.556002 -0.777845
C -1.043734 1.793597 -2.043520
C -1.501098 -1.290917 -0.683156
C -0.414777 1.500591 0.885777
N 4.233319 0.744344 0.284096
C 4.51076 0.517759 0.768131
C 3.863488 -0.711620 0.101124
C 4.012929 -0.883766 -1.304559
C 3.888293 -2.284166 -1.863177
C 4.853036 0.018926 -2.193082
H 4.420856 1.369067 0.159194
H 2.859505 1.374125 -1.276658
H 6.264474 -1.592454 0.686155
H 4.37665 0.130325 -3.172222
H 5.014244 1.019333 -1.789470
H 3.835013 -0.447594 -2.357525
H 5.363462 -2.277079 -2.824773
H 4.836600 -2.709470 -2.048430
H 3.357930 -2.957794 -1.184771
C 4.107546 -0.277567 3.135927
H 4.998257 -0.240862 3.706883
C 3.229828 -0.070760 3.755495
H 4.031060 -1.273931 2.705583
C 4.426123 2.119015 2.586497
H 3.545448 2.433089 3.517139
C 4.505388 2.162106 3.234991
H 5.362578 2.803933 1.748173
C 0.669949 -3.059824 -2.728086
C 0.996861 -4.131001 -3.568572
C 1.286675 -5.380608 -3.012786
C 2.166607 -5.558327 -1.626071
C 0.926737 -4.481101 -0.794583
H 4.586625 -2.088553 -3.143602
H 1.034096 -3.994579 -4.645569
H 5.465099 -6.212484 -3.658142
H 1.505588 -6.525820 -1.197764
H 0.947700 -4.610806 0.273467
C 0.924411 -1.782255 2.432001
C 0.821101 -2.171673 3.771819
C -0.101861 -3.146178 4.151825
C -0.927584 -3.726988 3.188778
C -0.830398 -3.336522 1.849368
H 1.609891 -0.998340 2.147445
H 1.449030 -1.703357 4.516643
H -0.185014 -3.442389 5.192650
H -1.654339 -4.473798 3.478632
H -1.487682 -3.781052 1.113110
C 1.838997 3.940019 -1.697187
C 2.76177 5.269610 -1.752983
H 1.706970 6.221166 -0.901260
C 0.688413 5.854178 -0.016640
C 0.257389 4.522539 0.029601
H 2.26164 3.219794 -2.398194
H 3.038411 5.568690 -2.467138
H 2.037900 7.253000 -4.945886
H 0.225318 6.604242 0.618526
H -0

H -3.976704 3.310979 -2.891250
H -2.213787 3.383379 -1.166597
C -2.251715 -2.027482 -1.622617
C -3.505606 -1.683274 -1.965082
C -4.123763 -0.576689 -1.375022
C -5.430652 -0.214887 -1.740593
C -6.030552 0.835005 -1.154799
C -5.366475 1.581173 -0.171197
C -4.114598 1.265597 0.205509
C -3.438447 0.173284 -0.385998
C -2.112122 -0.187227 -0.021540
H -1.834894 -2.905970 -2.081040
H -4.042733 -2.275579 -2.699649
H -5.964780 -0.781706 -2.494027
H -7.041410 1.107666 -1.440089
H -5.871684 2.422815 0.290419
H -3.634867 1.871817 0.962058
C 0.289784 2.021647 1.987686
C -0.051472 1.738297 3.255825
C -1.103430 0.856688 3.522837
C -1.454053 0.553584 4.848475
C -2.437724 -0.324903 5.103434
C -3.122623 -0.955323 4.055724
C -2.814857 -0.692413 2.773246
C -1.795106 0.233358 2.451327
C -1.431496 0.533482 1.107566
H 1.149653 2.652578 1.813778
H 0.513846 2.174195 4.073883
H -0.931282 1.022388 5.673767
H -2.703628 -0.555226 6.129830
H -3.907063 -1.668211 4.285294
H -3.359924 -1.212981 1.998341
TS₉₇₋₁₁₅
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P 0.169943 -1.659022 0.082432
P 0.069017 1.946496 -0.511223
C 0.784049 -3.141432 -0.767594
C -0.034832 -2.071006 1.870058
C 0.560169 3.685818 -0.538713
C -1.048193 1.733200 -1.966323
C -1.543594 -1.316267 -0.929609
C -0.869047 1.664804 1.033761
N 5.651437 -0.782750 1.414017
C 4.382128 -0.546934 1.189096
C 3.668549 -0.793201 -0.071041
C 3.779161 0.086859 -1.227189
C 3.576041 -0.513461 -0.610196
C 4.767118 1.250771 -1.246608
H 2.628465 1.654570 0.157631
H 3.841292 -0.130184 2.037163
H 3.475380 -1.852824 -2.061214
H 4.426507 0.202201 -1.942354
H 4.888797 1.724067 -0.268921
H 5.751644 0.910026 -1.604399
H 3.097307 0.210383 -3.726492
H 4.543026 -0.785424 -3.060510
H 2.959755 -1.414095 -2.579701
C 6.562342 -1.361480 0.397426
H 7.355774 -0.642974 0.178024
H 7.004371 -2.276182 0.800079
H 6.002208 -1.584471 -0.507772
C 6.281233 -0.486897 2.725951
H 5.540324 -0.059354 3.401185
H 6.680607 -1.410993 3.150740
H 7.097494 0.224606 2.578795
C 0.928710 -3.110770 -2.155026
C 1.444841 -4.216986 -2.840825
C 1.834760 -5.352363 -2.124407
H 1.718014 -5.380200 -0.731226
C 1.198653 -4.268412 -0.055801
H 0.630728 -2.226810 -2.695961
H 1.549052 -4.195199 -3.921866
H 2.240196 -6.210408 -2.649146
H 2.041844 -6.256538 -0.176599
H 1.148689 -4.277585 1.019556
C 0.693205 -1.364357 2.837860
C 0.511309 -1.633780 4.198224
C -0.398051 -2.609996 4.606733
C -1.127568 -3.317295 3.650470
C -0.954716 -3.046496 2.289292
H 1.388544 -0.593965 2.532266
H 1.075947 -1.078712 4.934821
H -0.539946 -2.815602 5.662986
H -1.838579 -4.070847 3.961168
H -1.537659 -3.589568 1.556520
C 1.775777 4.036945 -1.120121
C 2.173764 5.378962 -1.170522
C 1.335383 6.368750 -0.646820
C 0.099730 6.023435 -0.089408
C -0.288705 4.678505 -0.046053
H 2.390295 3.273721 -1.565512
H 3.120259 5.655631 -1.626830
H 1.637179 7.409652 -0.688313
H -0.555712 6.797960 0.299220
H -1.246910 4.407802 0.368308
C -0.740753 0.774794 -2.943018
C -1.580563 0.589259 -4.045989
C -2.729862 1.366221 -4.192877
C -3.034087 2.334828 -3.236444
C -2.198267 2.522822 -2.130673
H 0.149241 0.168902 -2.838702
H -1.336760 -0.160503 -4.786133
H -3.383552 1.218857 -5.046764

H -3.926663 2.936850 -3.341438
H -2.458373 3.265322 -1.389781
C -2.135048 -2.165555 -1.448829
C -3.353942 -1.924748 -1.962545
C -4.094270 -0.815985 -1.541361
C -5.362198 -0.559830 -2.088263
C -6.083189 0.490451 -1.661319
C -5.586193 1.341548 -0.664447
C -4.376591 1.128863 -0.116435
C -3.576049 0.041688 -0.537957
C -2.288031 -0.211069 0.009834
H -1.617993 -3.047303 -1.781743
H -3.766113 -2.600982 -2.705375
H -5.768970 -1.209388 -2.854378
H -7.063331 0.681086 -2.086289
H -6.187870 2.180857 -0.332405
H -4.027253 1.813875 0.644232
C -0.426134 2.353407 2.179036
C -0.928027 2.108443 3.041089
C -1.893369 1.113176 3.581941
C -2.408598 0.850707 4.861785
C -3.320568 -0.119731 5.037457
C -3.768418 -0.884825 3.952122
C -3.297393 -0.664809 2.711878
C -2.339514 0.348370 2.472921
C -1.809415 0.608095 1.176907
H 0.360448 3.087335 2.085725
H -0.562684 2.671397 4.254865
H -2.073647 1.427448 5.718781
H -3.715212 -0.317257 6.028735
H -4.501429 -1.666774 4.118358
H -3.661916 -1.288277 1.907261

TS₁₀₂₋₁₀₇
Rh 1.948273 0.018678 -0.553871
P 0.242330 -1.792126 -0.312328
P 0.292721 1.767409 -0.464949
C 0.652636 -3.160889 -1.428416
C 0.126834 -2.440629 1.414015
C 0.952002 3.451442 -0.380499
C -0.972399 1.853686 -1.807048
C -1.480045 -1.270858 -0.708887
C -0.520511 1.390261 1.126334
N 4.520881 1.538235 1.228189
C 4.278248 0.812458 0.092311
C 3.956005 -0.616649 1.450161
C 3.842895 -1.408518 -1.007001
C 3.867176 -2.912525 -0.820991
C 4.200593 -0.945358 -2.405504
H 4.857195 1.149057 -0.765424
H 3.019145 1.295819 -0.548026
H 3.943983 -1.106097 1.110687
H 3.512593 -1.390388 -3.132139
H 4.163163 0.137372 -2.563209
H 5.210375 -1.295712 -2.665229
H 3.419879 -3.435921 -1.670341
H 4.910604 -3.249702 -0.763694
H 3.362357 -2.230800 0.095598
C 3.935240 1.125953 2.512261
H 4.143863 1.892949 3.257459
H 2.846537 1.003994 2.416266
H 4.367380 0.184418 2.859268
C 4.862856 2.961430 1.084346
H 3.956784 3.588170 1.080497
H 5.504985 3.274807 1.908843
H 5.397137 3.121157 0.145621
C 0.869298 -2.872449 -3.767728
C 1.197259 -3.893065 -3.677420
C 1.320751 -5.207103 -3.216059
C 1.125027 -5.500030 -1.862644
C 0.795452 -4.471932 -0.970199
H 0.777301 -1.855076 -3.119240
H 1.360091 -3.669247 -4.727906
H 1.578793 -6.001227 -3.908100
H 1.239152 -6.520074 -1.506239
H 0.680173 -4.697140 0.074875
C 0.986916 -1.945008 2.404144
C 0.873899 -2.382607 3.727464
C -0.102316 -3.315138 4.078974
C -0.699516 -3.807162 3.103091
C -0.866209 -3.365225 1.780121
H 1.731784 -1.205793 2.147797
H 1.541638 -1.988098 4.481357
H -0.191859 -3.650066 5.107545
H -1.736463 -4.521027 3.371721
H -1.560007 -3.736054 1.036641
C 2.032738 3.796270 -1.109990
C 2.539203 5.101990 -1.791488
C 1.934040 6.070799 -0.372712
C 0.812979 5.745656 0.397339
C 0.313744 4.437304 0.376125
H 2.456567 3.061411 -1.855182
H 3.386312 5.368835 -1.804752
H 2.319361 7.084461 -0.364800
H 0.325483 6.510434 0.995508
H -0.576148 4.195142 0.934445
C -0.835705 1.059133 -2.953863
C -1.790115 1.115186 -3.975003
C -2.884180 1.974331 -3.868277
C -3.016991 2.784620 -2.746019
C -2.065107 2.731665 -1.771725
H 0.012029 0.395552 -3.047932
H -1.677583 0.489410 -4.849693
H -3.626667 2.014347 -4.658981

H -3.864133 3.451094 -2.650027
H -2.187540 3.356618 -0.842990
C -2.169369 -1.916070 -1.756902
C -3.414651 -1.562842 -2.119672
C -4.082666 -0.532886 -1.451552
C -5.376296 -0.153813 -1.845626
C -6.019975 0.830268 -1.195886
C -5.414712 1.490668 -0.117787
C -4.177735 1.155232 0.289630
C -3.458118 0.126974 -0.363026
C -2.144374 -0.250998 0.031098
H -1.707242 -2.724104 -2.294809
H -3.902299 -2.082338 -2.938991
H -5.863979 -0.652754 -2.674783
H -7.019920 1.117331 -1.504602
H -5.953670 2.281878 0.392371
H -3.744555 1.696701 1.119606
C 0.083264 1.895413 2.293136
C -0.324238 1.537731 3.522706
C -1.350490 0.600939 3.681769
C -1.770134 0.220718 4.966847
C -2.740594 -0.695887 5.117426
C -3.344366 -1.288260 3.999849
C -2.967638 -0.952622 2.753217
C -1.955104 0.011511 2.541102
C -1.521702 0.389984 1.239229
H 0.921701 2.570502 2.205844
H 0.165572 1.960384 4.394841
H -1.314112 0.662899 5.844815
H -3.061323 -0.984367 6.113067
H -4.122241 -2.029911 4.145479
H -3.451126 -1.444669 1.920686

TS₁₀₇₋₁₁₃
Rh 1.856669 -0.012090 -0.614132
P 0.215172 -1.753969 -0.350910
P 0.231138 1.761986 -0.561966
C 0.634345 -3.139178 -1.440879
C 0.133805 -2.350026 1.395947
C 0.962209 3.413868 -0.519602
C -1.056319 1.857181 -1.880053
C -1.522309 -1.256401 -0.725585
C -0.553131 1.433617 1.050056
N 4.078029 1.323610 1.625873
C 4.039889 0.789149 0.296556
C 3.818942 -0.682073 0.136918
C 3.835309 -1.312903 -1.111950
C 3.916887 -2.823924 -1.149429
C 4.226353 -0.929999 -2.407883
H 4.864743 1.150135 -0.346356
H 3.131249 1.324862 -0.262688
H 3.798375 -1.302473 1.022512
H 3.598527 -0.993833 -3.228039
H 4.142302 0.458920 -2.375168
H 5.266164 -0.883813 -2.660498
H 3.448905 -3.238980 -2.046872
H 4.972557 -3.124106 -1.180278
H 3.464240 -3.289572 -0.269196
C 4.595322 0.507395 2.734349
H 5.656908 0.235072 2.614089
H 4.493451 1.085594 3.654645
H 4.010683 -0.405741 2.861605
C 4.393595 2.755881 1.679722
H 3.714896 3.307120 1.017352
H 4.237966 3.126706 2.694116
H 5.428778 2.984680 1.375057
C 0.793102 -2.884737 -2.804204
C 1.121339 -3.921505 -3.686336
C 1.310345 -5.215158 -3.190630
C 1.179081 -5.471494 -1.822016
C 0.845068 -4.428277 -0.948770
H 0.653614 -1.881818 -3.173005
H 1.235738 -3.725195 -4.748646
H 1.570088 -6.021228 -3.868035
H 1.344949 -6.474851 -1.439601
H 0.778320 -4.623216 1.066568
C 0.958095 -1.766625 2.369347
C 0.869484 -2.165162 3.706741
C -0.051045 -3.140551 4.090508
C -0.888745 -3.713414 3.133042
C -0.808579 -3.312847 1.795435
H 1.646474 -0.981167 2.091443
H 1.507026 -1.701064 4.446945
H -0.123863 -3.443006 5.130359
H -1.615639 -4.458491 3.427070
H -1.480805 -3.746079 1.065892
C 2.087287 3.671331 -1.300285
C 2.656727 4.950826 -1.319532
C 2.074227 5.977729 -0.569381
C 0.917007 5.735294 0.178242
C 0.354520 4.452680 0.187657
H 2.499294 2.884740 -1.911911
H 3.536359 5.152398 -1.924336
H 2.508461 6.971318 -0.585264
H 0.452496 6.543152 0.736731
H -0.555608 4.267598 0.735663
C -0.954529 1.049819 -3.021526
C -1.930864 1.107344 -4.021710
C -3.012619 1.979808 -3.898778
C -3.111273 2.801772 -2.776156
C -2.137317 2.747459 -1.773653
H -0.117500 0.374401 -3.127317
H -1.845099 4.471864 -4.892379
H -3.772232 2.020754 -4.672967

H -3.949025 3.478099 -2.672615
H -2.234404 3.380141 -0.901904
C -2.221425 -1.928006 -1.749696
C -3.474603 -1.591821 -2.101273
C -4.141306 -0.554060 -1.443822
C -5.442330 -0.191015 -1.828596
C -6.084628 0.800758 -1.189281
C -5.470590 1.485160 -0.131320
C -4.226491 1.165428 0.266903
C -3.508062 0.129750 -0.375194
C -2.187102 -0.232179 0.009590
H -1.759974 -2.743510 -2.276641
H -3.969565 -2.131017 -2.903243
H -5.936714 -0.708412 -2.642304
H -7.090155 1.075541 -1.490868
H -6.008384 2.282407 0.370551
H -3.786654 1.725406 1.080932
C 0.032683 1.958212 2.195808
C -0.321381 1.632098 3.438461
C -1.349877 0.703676 3.631910
C -1.752269 0.351768 4.930502
C -2.716898 -0.565071 5.114164
C -3.330867 -1.186717 4.018110
C -2.971666 -0.877886 2.759436
C -1.968218 0.087236 2.512802
C -1.553110 0.437387 1.197571
H 0.923155 2.615643 2.082179
H 0.185736 2.067659 4.294011
H -1.286125 -0.814874 5.792160
H -3.023754 -0.832083 6.120077
H -4.102436 -1.929203 4.150460
H -3.461830 -1.391887 1.944229
TS₁₁₃₋₁₁₄
Rh 1.822666 0.022184 -0.706399
P 0.233470 -1.720118 -0.343778
P 0.170690 1.787449 -0.610973
C 0.668542 -3.137579 -1.386442
C 0.195224 -2.245129 1.428157
C 0.927176 3.427542 -0.571634
C -1.116687 1.864298 -1.931292
C -1.516392 -1.274799 -0.717066
C -0.616160 1.481451 1.005306
N 3.987642 0.902869 1.955498
C 4.050212 0.678091 0.515523
C 3.737728 -0.733969 0.090841
C 3.825311 -1.171308 -1.236387
C 3.942782 -2.650457 -1.522968
H 4.272038 -2.273352 -2.374420
H 4.994933 1.031742 0.049095
H 3.271476 1.369645 0.060348
H 3.646920 -1.480108 0.871765
H 3.773298 -0.561817 -3.304693
H 4.079632 0.789666 -2.196605
H 5.354384 -3.384059 -2.535987
H 3.484586 -2.926861 -2.476114
H 5.006715 -2.911413 -1.599215
H 3.512023 -3.265808 -0.728147
C 4.993593 0.152665 2.733480
H 6.028004 0.467351 2.504534
H 4.809207 0.319210 3.796852
H 4.908274 -0.919031 2.541499
C 3.967046 2.335114 2.299764
H 3.165402 2.834455 1.743579
H 3.765504 2.449806 3.366469
H 4.915693 2.850768 2.064285
H 0.767190 -2.941879 -2.765364
C 1.089279 -4.009556 -3.612392
C 1.337944 -5.272469 -3.066353
C 1.269111 -5.468287 -1.683259
C 0.936707 -4.395929 -0.845460
H 0.582223 -1.960918 -3.173179
H 1.154857 -3.860042 -4.686371
H 1.595075 -6.101516 -3.716439
H 1.480417 -6.447582 -1.262793
H 0.916328 -4.543091 0.219675
C 1.001439 -1.588673 2.370816
C 0.939337 -1.936689 3.723548
C 0.063131 -2.932730 4.154473
C -0.757666 -3.577246 3.228474
C -0.740467 -3.228042 1.875185
H 1.653351 -0.785419 2.058513
H 1.564206 -1.417139 4.437401
H 0.011125 -3.195824 5.206163
H -1.451212 -4.338636 3.558816
H -1.363879 -3.717103 1.170015
C 2.165370 3.616541 -1.180182
C 2.774377 4.877725 -1.166105
C 2.123624 5.952620 -0.551151
C 0.865451 5.773856 0.033805
C 0.265671 4.508430 0.012717
H 2.633672 2.793727 -1.693381
H 3.738985 5.028376 -1.642605
H 2.588762 6.932241 -0.542417
H 0.356899 6.615497 0.495744
H -0.705593 4.363428 0.457768
C -1.009338 1.037558 -3.058865
C -1.988996 1.065816 -4.056963
C -3.081939 1.925430 -3.945009
C -3.190050 2.761863 -2.834161
C -2.213266 2.736574 -1.8

H -4.038927 3.425170 -2.737205
H -2.324829 3.374068 -0.967908
C -2.210728 -1.991013 -1.714713
C -3.469595 -1.684844 -2.073176
C -4.150021 -0.637278 -1.446989
C -5.457156 -0.305598 -1.839337
C -6.114412 0.692744 -1.226033
C -5.510256 1.414694 -0.187572
C -4.260708 1.125590 0.216968
C -3.526054 0.085226 -0.399040
C -2.198800 -0.245478 -0.007051
H -1.743480 -2.819590 -2.213896
H -3.959172 -2.257693 -2.854913
H -5.944462 -0.853121 -2.637450
H -7.124640 0.943090 -1.533101
H -6.060251 2.216125 0.293966
H -3.829170 1.714145 1.015090
C -0.053134 2.090242 2.142507
C -0.455581 1.786590 3.388623
C -1.434506 0.809219 3.596725
C -1.842960 0.480312 4.899464
C -2.767909 -0.473794 5.097252
C -3.335233 -1.155968 4.012053
C -2.968740 -0.870481 2.749972
C -2.003452 0.129059 2.488849
C -1.582445 0.456512 1.169891
H 0.749606 2.799234 2.024429
H 0.005468 2.282647 4.237261
H -1.414113 0.992009 5.752947
H -3.079646 -0.722865 6.106251
H -4.076156 -1.926378 4.195823
H -3.421568 -1.430548 1.943424
TS₁₁₆₋₁₂₃
Rh -2.652511 -2.666394 1.495124
P 1.687211 -0.850337 2.739279
P -1.584346 -1.922213 -0.654003
P -3.122205 -0.632824 0.426190
C 0.148564 -0.806691 2.937740
C -1.027779 -3.390307 -1.559701
C -2.702070 -0.931921 -1.742857
C -2.235987 0.585543 1.750857
C -0.109942 -0.842205 -0.420332
N -5.322454 -4.236818 3.529436
C -4.844552 -3.381398 2.577339
C -4.588109 -3.709395 1.160559
C -3.694378 -4.666840 0.655002
C -3.819876 -5.011097 -0.818590
C -2.912817 -5.685768 1.462600
H -3.353191 -3.104122 2.933793
H -5.179662 -2.359400 2.738809
H -5.208055 -3.173059 0.449194
H -3.386672 -6.675944 1.393509
H -2.806492 -5.417901 2.513493
H -1.907321 -5.790179 1.041189
H -4.591742 -5.780940 0.904619
H -2.891912 -5.433266 -1.214565
H -4.102406 -4.148431 -1.428802
C -5.451197 -5.689593 3.363761
H -6.363663 -6.011132 3.873111
H -4.603081 -6.233662 3.795835
H -5.535271 -5.935051 2.305785
C -5.525695 -3.724390 4.892664
H -4.679923 -3.990147 5.540551
H -6.440645 -4.145493 5.315392
H -5.612276 -2.634877 4.869091
C -2.489615 -1.754592 5.234399
C -2.928193 -1.613377 6.557098
C -3.159328 -0.336146 7.076494
C -2.927856 0.795950 6.289393
C -2.486606 0.643129 4.969056
H -2.249291 -2.732345 4.851275
H -3.070456 -2.488153 7.185393
H -3.492948 -0.222342 8.102080
H -3.074646 1.787360 6.708874
H -2.262212 1.515894 4.377434
C 0.924491 -1.902559 2.533083
C 2.315682 -1.879558 2.677152
C 2.946179 -0.768606 3.238124
C 2.180622 0.317496 3.662266
C 0.789324 0.299437 3.519320
H 0.444582 -2.769459 2.100621
H 2.902941 -2.727164 2.351463
H 4.026058 -0.749743 3.345853
H 2.663215 1.183388 4.095122
H 0.209686 1.154022 3.841014
C -0.239707 -4.322927 -0.883923
C 0.199838 -5.483497 -1.532145
C -0.166176 -5.711731 -2.862082
C -0.972074 -4.790846 -3.539095
C -1.406047 -3.632485 -2.881636
H 0.031247 -4.138331 0.143010
H 0.817783 -6.206817 -1.007615
H 0.167805 -6.610890 -3.368163
H -1.268284 -4.981680 -4.566902
H -2.055935 -2.946775 -3.394649
C -4.026581 -0.689935 -1.351051
C -4.866834 0.103040 -2.139147
C -4.392624 0.671342 -3.321593
C -3.072263 0.448571 -3.712798
C -2.226155 -0.337480 -2.924175
H -4.396323 -1.099058 -4.021620
H -5.884973 0.284478 -1.822499
H -5.044437 1.291436 -3.928867
H -2.694472 0.897900 -4.621302
H -1.197039 -0.484060 -3.226211
C -3.532794 1.074944 1.996799
C -4.091407 2.034330 1.239460
C -3.408336 2.546435 0.131572
C -3.996794 3.541506 -0.665747
C -3.353676 4.007842 -1.748996
C -2.093440 3.507116 -2.103063
C -1.498334 2.552529 -1.365999
H -2.128977 2.035775 -2.016354
H -1.537471 1.020972 0.594176
H -4.112166 0.654399 2.805561
H -5.088886 2.392681 1.475583
H -4.973647 3.937693 -0.414621
H -3.813412 4.777273 -2.360569
H -1.595996 3.893378 -2.986106
H -0.532455 2.186182 -1.684719
C 1.147481 -1.280865 -0.884817
C 2.267063 -0.556852 -0.711689
C 2.218394 0.680644 -0.063216
C 3.392468 1.426270 0.131730
C 3.341090 2.620321 0.745482
C 2.120314 3.140202 1.197648
C 0.974761 2.456261 1.028533
C 0.976974 1.194078 0.390273
C -0.211282 0.435947 0.199344
H 1.238471 -2.218902 -1.402265
H 3.214966 -0.938969 -1.078372
H 4.346492 1.044668 -0.212509
H 4.251812 3.192002 0.891632
H 2.102834 4.106693 1.689892
H 0.056152 2.889141 1.400765
TS₁₂₄₋₁₂₇
Rh 1.710280 0.100773 -0.581483
P 0.171021 -1.684476 -0.229505
P -0.002710 1.842587 -0.467482
C 0.710159 -3.087972 -1.241578
C 0.030012 -2.224310 1.533734
C 0.717406 3.492735 -0.307502
C -1.218616 1.924660 -1.855810
C -1.564829 -1.289722 -0.713011
C -0.864226 1.469887 1.095527
N 5.346982 0.791808 1.252470
C 3.926576 0.475575 1.237399
C 3.523335 -0.738429 0.379153
C 3.749558 -0.889977 -1.001555
C 3.947367 -2.260679 -1.607135
C 4.275949 0.237845 -1.866017
H 3.388602 1.381360 0.905607
H 3.568648 0.282981 2.258554
H 3.352660 -1.661183 0.930889
H 3.853732 0.183465 -2.874993
H 4.091530 1.231922 -1.450294
H 5.368184 0.156469 -1.963700
H 5.543068 -2.325213 -2.621327
H 5.024069 -2.462627 -1.681436
H 3.512195 -3.056502 -0.996579
C 6.298161 -0.271158 1.553761
H 6.620425 -0.848540 0.669021
H 7.194812 0.160991 2.011105
H 5.860355 -0.971954 2.273672
C 5.864395 2.019938 0.663246
H 5.081169 2.786002 0.654313
H 6.629422 2.402996 1.271682
H 6.241224 1.902382 -0.368217
C 0.860105 -2.898482 -2.616640
C 1.275033 -3.954643 -3.437323
C 1.565432 -5.198004 -2.867761
C 1.447353 -5.385473 -1.486934
C 1.023939 -4.324865 -0.675660
H 0.644851 -1.930585 -3.042333
H 1.381193 -3.810492 -4.508799
H 1.894457 -6.017428 -3.497345
H 1.692558 -6.348370 -1.047337
H 0.969075 -4.463269 3.895989
C 0.739970 -1.548926 2.536713
C 0.595836 -1.913924 3.878989
C -0.268364 -2.948389 4.237734
C -0.994676 -3.613751 3.249981
C -0.858848 -3.247066 1.907255
H 1.378287 -0.718243 2.276642
H 1.145816 -1.379747 4.641826
H -0.384677 -3.225529 5.280722
H -1.678798 -4.405857 3.523116
H -1.446111 -3.754358 1.152521
C 2.052023 3.684883 -0.647871
C 2.642176 4.948300 -0.517490
C 1.879909 6.020429 -0.041815
C 0.535833 5.833258 0.298214
C -0.042713 4.564841 0.161916
H 2.615616 2.860476 -1.039286
H 3.682118 5.101095 -0.792244
H 2.330737 7.001674 0.058100
H -0.052426 6.669035 0.666684
H -1.070589 4.409073 0.442782
C -1.017065 1.134121 -2.997090
C -1.938875 1.154334 -0.4048910
C 3.069551 1.967740 -3.976987
C 3.275600 2.763010 -2.850142
C -2.357511 2.744962 -1.794836
H -0.146603 0.494604 -3.060962
H -1.773369 0.534555 -4.919445
H -3.786982 1.979427 -4.791398
H -4.157143 3.386125 -2.782304
H -2.554270 3.340893 -0.916609
C -2.175748 -2.019706 -1.754558
C -3.418112 -1.747264 -2.189562
C -4.167688 -0.726238 -1.600000
C -5.458264 -0.431919 -2.069418
C -6.184618 0.537081 -1.487855
C -5.670016 1.264783 -0.406113
C -4.438847 1.011244 0.071967
C -3.633120 0.003625 -0.508862
C -2.322268 -0.289328 -0.387079
H -1.658069 -2.834139 -2.225344
H -3.841531 -2.329114 -3.002753
H -5.877400 -0.985407 -2.901434
H -7.181705 0.758462 -1.854407
H -6.274948 2.041756 0.048910
H -4.077116 1.603568 0.901353
C -0.403283 2.088906 2.273255
C -0.879923 1.758645 3.486223
C -1.836651 0.746437 3.618570
C -2.323356 0.391857 4.887254
C -3.226948 -0.594363 5.013210
C -3.694031 -1.284770 3.886261
C -3.250829 -0.975140 2.654867
C -2.304246 0.058458 2.468815
C -1.805560 0.413609 1.184504
H 0.377354 2.831321 2.216714
H -0.500544 2.265475 4.368465
H -1.973300 0.909986 5.772286
H -3.599924 -0.862879 5.996157
H -4.419660 -2.080951 4.012397
H -3.627619 -1.542108 1.814685

3.2 Associative mechanism (ONIOM(B3LYP/BS1:UFF) level)

291
Rh -0.738339 0.677285 0.484699
P 0.050475 -1.452071 0.829321
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H 5.259045 4.239946 1.597585
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H 3.518587 2.495055 -1.920658
C 1.674798 -0.646851 3.064821
C 2.924767 -0.360647 3.468574
C 3.934178 -0.118232 2.532131
C 5.236922 0.189702 2.957097
C 6.213757 0.384411 2.055576
C 5.951232 0.278390 0.682897
C 4.716297 -0.013580 0.237689
C 3.651484 -0.215517 1.145965
C 2.306966 -0.522530 1.746848
H 0.941254 -0.846930 3.823841
H 3.150783 -0.323384 4.530209
H 5.464534 0.265871 4.013854
H 7.218864 0.619239 3.390293
H 6.755869 0.435848 -0.027061
H 5.551190 -0.076259 -0.829937
H 1.488928 -0.137587 -3.012090
C 1.918324 -1.306521 -3.517843
C 2.423985 -2.296591 -2.675800
C 2.868996 -3.521757 -3.206201
C 3.382604 -4.463878 -2.397986
C 3.494108 -4.239555 -1.019031
C 3.087129 -3.079465 -0.47397

H 3.718933 -5.407821 -2.814217
H 3.912394 -5.014304 -0.385643
H 3.180532 -2.953805 0.596011
N -2.103532 3.282365 0.647243
C -1.985618 3.526253 1.125019
H -0.936100 3.482473 2.414639
H -2.527786 2.744203 2.654824
H -2.397216 4.514018 2.382419
C -1.399966 4.382352 -0.079210
H -1.562419 4.265247 -1.152558
H -0.331613 4.335447 0.130451
H -1.785554 5.365146 0.226414
C -3.547797 3.312650 0.260221
H -4.072905 2.531487 0.808347
H -3.631349 3.123564 -0.811219
H -3.991870 4.293057 0.489726
411
Rh -1.280696 1.106889 0.918191
P -0.445415 -1.039077 1.555528
P 0.605380 1.531301 -0.822664
C -1.283316 -1.416640 3.147891
C -0.602642 -2.479329 0.432232
C -0.932224 2.427435 -2.235894
C 2.083939 2.444446 -0.194147
C 1.348290 -0.842729 1.913379
C 1.281668 -0.052381 -1.448637
N -4.469754 -1.764405 0.287835
C -4.449421 -0.823871 -0.713414
C -4.245307 -1.152366 -0.299863
C -4.464282 -0.313999 -3.144026
C -4.179603 -0.752389 -4.559201
C -5.000967 1.087321 -2.950369
H -2.397749 0.783861 1.958136

H -4.827875 0.143994 -0.420477
H -3.884310 -2.150920 -2.321805
H -4.279926 1.731167 -2.417849
H -5.924028 1.090668 -2.355369
H -5.223974 1.569839 -3.905739
H -3.399041 -0.133638 -5.026310
H -5.071909 -0.655068 -5.193151
H -3.846775 -1.794019 -4.602110
C -4.214053 -3.080753 0.195571
H -4.275939 -3.683625 1.085943
H -2.389127 0.445145 0.050618
H -4.020908 -3.533043 -0.761668
C -4.817169 -1.240273 1.641133
H -4.034646 -0.550516 1.967972
H -4.896959 -2.066541 2.344687
H -5.772463 -0.716608 1.586946
C -1.335872 -0.427129 4.133847
C -2.040889 -0.647071 5.323602
C -2.721510 -1.853889 5.509374
C -2.708281 -2.830654 4.509277
C -1.996558 -2.602099 3.325207
H -0.817607 0.506806 3.977385
H -2.066921 0.114004 6.098534
H -3.274538 -2.028348 6.425890
H -3.264047 -3.754622 4.644151
H -2.040802 -3.330786 2.534717
C -1.154005 -2.312747 -0.847264
C -1.194576 -3.381663 -1.749344
C -0.699979 -4.632186 -1.381656
C -0.145867 -4.808342 -0.114367
C -0.084973 -3.737849 0.783330
H -1.515658 -1.344221 -1.157593
H -1.611292 -3.233296 -2.735498

H -0.735804 -5.460679 -2.081616
H 0.254805 -5.771285 0.171221
H 0.375614 -3.879863 1.752519
C -1.232596 1.911644 -2.856680
C -1.819062 2.588319 -3.933837
C -1.276085 3.800915 -4.367471
C -0.156438 4.339876 -3.727462
C 0.428481 3.652471 -2.656868
H -1.648493 0.978049 -2.507753
H -2.692798 2.181118 -4.432096
H -1.730251 4.330407 -5.197869
H 0.250420 5.292255 -4.056093
H 1.265644 4.090486 -2.143434
C 2.127476 2.864867 1.142685
C 3.261360 3.509887 1.647193
C 4.364722 3.739290 0.824562
C 4.333659 3.317685 -0.505047
C 3.206504 2.662117 -1.010759
H 1.286392 2.671887 1.794574
H 3.284823 3.823409 2.682002
H 5.245601 4.236149 1.218849
H 5.190378 3.482307 -1.144646
H 3.202872 2.317520 -2.036969
C 1.810933 -0.793474 3.243120
C 3.081720 -0.475756 3.545831
C 4.004009 -0.199714 2.531912
C 5.328696 0.140669 2.851123
C 6.224001 0.361603 1.874101
C 5.854133 0.249628 0.526834
C 4.594972 -0.073173 0.182162
C 3.612143 -0.300335 1.172811
C 2.269274 -0.640718 0.848526
H 1.146688 -1.018406 4.057005

H 3.393100 -0.439399 4.585706
H 5.639561 0.219766 3.886251
H 7.246804 0.621009 2.127112
H 6.594638 0.426951 -0.245462
H 4.349602 -0.141496 -0.869010
C 1.158008 -0.365197 -2.817879
C 1.571523 -1.539729 -3.323209
C 2.160691 -2.498993 -2.495022
C 2.580143 -3.730420 -3.024284
C 3.166065 -4.642742 -2.231341
C 3.370470 -4.380682 -0.869847
C 2.982466 -3.213337 -0.326413
C 2.355431 -2.222035 -1.117733
C 1.925420 -0.975728 -0.579316
H 0.730585 0.345808 -3.501476
H 1.447432 -1.741632 -4.382888
H 2.436370 -3.951903 -4.075212
H 3.848657 -5.591851 -2.646686
H 3.846123 -5.131893 -0.248660
H 3.149105 -3.058945 0.730770
N -2.231216 3.112525 1.026314
C -1.920864 3.563841 2.429156
H -0.838977 3.634909 2.557399
H -2.321693 2.837653 3.136016
H -2.366395 4.549518 2.617500
H -2.326258 4.144607 0.066519
C -1.030071 3.870786 -0.944602
H -0.638150 4.198640 0.119414
H -2.146977 5.129636 0.303591
C -3.719793 2.998766 0.853596
H -4.112563 2.301196 1.591680
H -3.927140 2.616641 -0.146501
H 4.192180 3.981673 0.979757

3.3 Simple molecules (B3LYP+D3/BS2 level)

N,N,N-3-trimethylbut-2-en-1-amine (Reactant)

N -1.784101 -0.372984 0.116110
C -0.688743 -0.085139 -0.818263
C 0.611315 -0.681709 -0.350531
C 1.776705 -0.062004 -0.110648
C 2.988354 -0.842688 0.342669
C 2.019621 1.420634 -0.260522
H -0.597287 1.000972 -1.010685
H -0.957600 -0.546037 -1.779678
H 0.557611 -1.758459 -0.187117
C 2.153318 1.838637 0.676359
H 2.781254 1.611756 -1.029509
H 1.122966 1.983305 -0.529312
H 3.819856 -0.725023 -0.366785
H 3.529213 -0.473080 1.311597
H 2.776383 -1.911898 0.443271
C -3.077514 -0.052848 -0.469499
H -3.221273 -0.624741 -1.393117
H -3.877047 -0.327527 0.227710
H -3.193839 1.023962 -0.711615
C -1.601478 0.312181 1.389305
H -0.633631 0.040757 1.820337
H -1.635293 1.471218 1.292779
H -2.389174 0.008686 2.087929

BiNAP-Rh(I)

Rh -0.000031 -2.460104 -0.000022
P -1.546401 -0.952108 -0.440608
P 1.546374 -0.952154 0.440593
C -2.760540 -1.852166 -1.478764
C -2.466758 -0.262137 0.978209
C 2.760486 -1.852254 1.478748
C 2.466758 -0.262185 -0.978028
C -0.912245 0.496969 -1.380088
C 0.912255 0.496929 1.380091
C -2.276307 -2.630612 -2.550935
C -3.154636 -3.385269 -3.327354
C -4.521401 -3.383361 -3.035850
C -5.006469 -2.625900 -1.967279
C -4.134194 -1.865692 -1.187059
H -1.212970 -2.635404 -2.780205
H -2.772133 -3.976561 -4.154070
H -5.205511 -3.974805 -3.637179
H -6.067784 -2.626942 -1.736971
H -4.523364 -1.287858 -0.356073
C -2.273941 -0.781825 2.265604

C -2.956892 -0.231040 3.349733
C -3.839810 0.833127 3.153341
C -4.044054 1.346559 1.870000
C -3.356693 0.806666 0.844462
H -1.571574 -1.597340 2.413956
H -2.793416 -0.627206 4.347640
H -4.365077 1.266258 3.999354
H -4.721546 2.180923 1.717334
C -3.493720 1.230397 -0.206632
C 2.276232 -2.630690 2.550911
C 3.154541 -3.385376 3.327325
C 4.5421305 -3.383504 3.035819
C 5.006395 -2.626050 1.967253
C 4.134140 -1.865814 1.187038
H 1.212896 -2.635453 2.780182
H 2.772022 -3.976661 4.154038
H 5.205400 -3.974971 3.637144
H 6.067710 -2.627120 1.736944
H 4.523325 -1.287983 0.356057
C 2.273929 -0.781839 -2.265155
C 2.956894 -0.231046 -3.349731
C 3.839842 0.833092 -3.153314
C 4.044101 1.346486 -1.869961
C 3.356726 0.806586 -0.784435
H 1.571541 -1.597333 -2.413987
H 2.793406 -0.627184 -4.347647
H 4.365120 1.266229 -3.999317
H 4.721619 2.180826 -1.717274
H 3.493766 1.230290 0.206669
C -1.098200 0.540590 -2.788131
C -0.470770 1.496195 -3.549020
C 0.372479 2.465329 -2.950995
C 1.044525 3.443964 -3.705573
C 1.851436 4.386226 -3.135190
C 2.019143 4.386335 -1.729462
C 1.386322 3.446992 -0.947118
C 0.544901 2.456178 -1.527914
C -0.104747 1.444946 -0.744562
H -1.743956 -0.184920 -3.269056
H -0.619932 1.519335 -4.625409
H 0.905599 3.436562 -4.808480
H 2.358280 5.132805 -3.739462
H 2.655637 5.133830 -1.264786
H 1.532027 3.456510 1.026551
C 1.098208 0.540526 2.788134
C 0.470801 1.496137 3.549034

C -0.372419 2.465302 2.951019
C -1.044442 3.443943 3.730610
C -1.851327 4.386235 3.135237
C -2.019027 4.386370 1.729509
C -1.386228 3.447021 0.947153
C -0.544835 2.456177 1.527937
C 0.104785 1.444934 0.744574
H 1.743943 -0.185009 3.269051
C 0.619960 1.519259 4.625424
H -0.905521 3.436521 4.808517
H -2.358155 5.132817 3.739518
H -2.655499 5.133889 1.264841
H -1.531927 3.456562 -0.126517
(E)-N,N,N-3-trimethylbut-1-en-1-amine (Product)
N -1.944311 0.134999 -0.265488
C -0.628603 -0.292086 -0.450723
C 0.485484 0.177647 0.136357
C 1.876969 -0.282307 -0.223997
C 2.699972 0.866970 -0.837951
C 2.599147 -0.864965 1.005500
H 1.794753 -1.078526 -0.978859
H -0.542283 -1.078497 -1.200978
H 4.627680 0.946378 0.905692
H 3.610088 -1.206288 0.748997
H 2.693939 -0.106090 1.793479
H 2.043583 -1.711851 1.423199
H 2.798649 1.695338 -0.124014
H 3.711423 0.534753 -1.104907
H 2.215047 1.258829 -1.738715
C -2.968186 -0.896770 -0.348741
H -3.019456 -1.529243 0.555417
H -3.949395 -0.432651 -0.498371
H -2.766503 -1.547381 -1.206223
C -2.177814 1.137215 0.756440
H -1.948197 0.772858 1.774092
H -1.553966 2.015684 0.560999
H -3.226925 1.447472 0.727301
(Z)-N,N,N-3-trimethylbut-1-en-1-amine (Product)
N -1.765644 0.115569 -0.200753
C -0.792370 -0.783951 -0.635326
C 0.551315 -0.803458 -0.528787
C 1.535157 0.083872 0.201525
C 2.556461 -0.785664 0.959353
C 2.260047 1.031751 -0.775036

H 1.018192 0.694934 0.946928
H -1.244859 -1.592889 -1.209283
H 1.029368 -1.603135 -1.096096
H 0.091002 1.651614 -0.253551
H 2.786050 0.458046 -1.548868
H 1.550724 1.695119 -1.282953
H 3.117963 -1.422266 0.262841
H 3.280674 -0.163676 1.499958
H 2.057044 -1.440769 1.681804
C -3.043011 -0.456008 1.195245
H -0.306047 -0.853743 1.225548
H -3.827328 0.307457 0.130946
H -3.309606 -1.275363 -0.480439
C -1.413187 1.334011 0.499711
H -1.126566 1.170031 1.552920
H -0.587616 1.831853 -0.014500
H -2.275955 2.010491 0.489924
tetrahydrofuran (THF)
O -0.000001 1.251576 -0.000003
C -1.164210 0.429942 -0.133350
C -0.732301 -0.996037 0.243788
C 0.732304 -0.996034 -0.231790
C 1.164208 0.429945 0.134354
H -1.528401 0.475643 -1.172940
H -1.951928 0.824119 0.518757
H -1.345724 -1.764120 -0.249425
H -0.786488 -1.145404 1.317062
H 1.345730 -1.764117 0.249421
H 0.786492 -1.145396 -1.317064
H 1.528390 0.475645 1.172947
H 1.951930 0.824125 -0.518746
trimethylamine (TMA)
N -0.000005 0.000000 -0.375237
C -1.384366 0.106386 0.061403
H -1.966731 -0.738630 -0.329195
H -1.826696 1.029865 -0.329158
H -1.494662 0.114850 1.165477
C 0.600049 -1.252081 0.061408
H 1.620952 -1.330400 -0.329279
H 0.021433 -2.096099 -0.329082
H 0.647950 -1.351764 1.165480
C 0.784315 1.145692 0.061406
H 0.341629 2.069014 -0.329132
H 1.805214 1.067061 -0.329233
H 0.846857 1.236923 1.165480

3.4 Dissociative mechanism (B3LYP+D3/BS2 level)

1
Rh -1.894600 0.329882 -0.015482
P -0.556215 -1.456880 0.332145
P -0.115965 1.658326 -0.360307
C -1.472170 -2.646138 1.405328
C 0.056224 -2.430215 -1.093925
C -0.651718 3.037950 -1.411162
C 0.724374 2.413122 1.083589
C 0.970812 -1.067475 1.324852

C 1.254844 0.855702 -1.331231
N -3.544830 1.877133 0.328525
C -4.613402 0.828824 0.307387
C -4.167161 -0.218132 -0.684775
C -4.202643 -1.567189 -0.515442
C -3.794469 -2.492719 -1.631033
C -4.790812 -2.257477 0.684066
H -4.704807 0.407029 1.310268
H -5.587544 1.273749 0.051112

H -3.929889 0.157806 -1.681188
H -5.813969 -2.571487 0.433212
H -4.231246 -3.161308 0.934791
H -4.844350 -1.629817 1.574933
H -2.997772 -3.167155 -1.296752
H -4.643092 -3.124956 -1.922079
H -3.440796 -1.954059 -2.513577
C -3.400314 2.487763 1.667171
H -3.181330 1.710919 2.403354

H -2.565976 3.192495 1.648540
H -4.317235 0.3019548 1.963743
C -3.870349 2.934165 -0.652732
H -3.947509 2.505213 -1.652148
H -4.826852 3.411733 -0.391760
H -3.084972 3.687975 -0.660510
C -2.112337 -2.135303 2.550598
C -2.793887 -2.980832 3.424025
C -2.872651 -4.349855 3.151999

C -2.268675 -4.862329 2.002780
C -1.568092 -4.018515 1.135027
H -2.065750 -1.068276 2.756778
H -3.270413 -2.572100 4.310707
H -3.407270 -5.010361 3.828326
H -2.334541 -5.923417 1.779749
H -1.097036 -4.436427 0.252235
C -0.362130 -2.075049 -2.383897
C -0.127309 -2.760158 -3.495561
C -1.035822 -3.807298 -3.326690
C -1.455830 -4.168260 -2.043872
C -0.974649 -3.479348 -0.931671
H -1.047335 -1.241184 -2.506334
H -0.89193 -2.468341 -4.492938
H -1.425373 -4.334444 -4.192586
H -2.176594 -4.969414 -1.911686
H -1.332906 -3.738860 0.060843
C -1.340452 2.790448 -2.605985
C -1.822660 3.819175 -3.411978
C -1.652878 5.151006 -3.021564
C -0.990767 5.443042 -1.828308
C -0.486504 4.412940 -1.028534
H -1.514380 1.755820 -2.891168
H -2.343743 3.583079 -4.335596
H -2.038251 5.954449 -3.642465
H -0.859768 6.475323 -1.516502
H -0.027225 4.659453 -0.106022
C -0.220602 2.183293 2.371086
C -0.872587 2.171115 3.485724
C -2.029358 3.475651 3.321676
C -2.534574 3.712588 2.040469
C -1.889814 3.179842 0.925613
H -0.660406 1.560201 2.914335
H -0.486677 2.512669 4.481581
H -2.543480 3.877714 4.189632
H -3.443111 4.292916 1.911655
H -2.303562 3.340558 -0.066224
C -1.003912 -1.337850 2.709777
C -2.035979 -0.889653 3.508970
C -3.108781 -0.149185 2.956345
C -4.170911 0.340184 3.762265
C -5.121705 1.043220 3.202196
C -5.231413 1.285733 1.807628
C -4.212933 0.828866 1.001876
C -3.118695 0.098565 1.546378
C -2.027961 -0.370653 0.739402
H -0.211756 -1.914073 3.180314
H -2.039654 -1.108554 4.573917
H -4.146511 0.144554 4.831266
H -6.022950 1.410509 3.825334
H -6.056458 1.840611 1.370091
H -4.238874 1.031536 -0.062222
C -1.385673 1.109911 -2.725004
C -2.264264 0.394040 -3.500908
C -3.080068 -0.616710 -2.937684
C -3.975542 -1.381638 -3.731359
C -4.774999 -2.344652 -3.159702
C -4.708498 -2.580728 -1.765482
C -3.845869 -1.859029 -0.971670
C -3.002452 -0.856058 -1.528480
C -2.072741 -0.104471 -0.733605
H -0.798574 1.889191 -3.191663
H -2.346175 0.606922 -4.563897
H -4.020017 -1.188064 -4.800067
H -5.459824 -2.922603 -3.773441
H -5.342491 -3.341338 -1.318799
H -3.800917 -2.059369 0.092172

4
Rh 1.984026 0.126728 0.171132
P -0.469915 -1.548995 -0.345134
P -0.286665 1.615822 0.417188
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C -0.719232 -3.470044 -2.682178
C -0.265710 -4.454288 -2.570517
C -1.062525 -4.522648 -1.424475
C -0.882813 -3.601123 -0.394282
H -1.670989 -1.776316 -1.735113
H -1.337640 -3.416727 -3.573825
H -0.415644 -5.166702 -3.376591
H -1.836159 -5.279685 -1.341555
H -1.521729 -3.638765 0.483474
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C -2.440830 3.061245 -3.616812
C -2.096926 4.416364 -3.654428
C -0.125033 4.909228 -2.782991
C -0.492314 4.056638 -1.874415
H -2.107526 1.162545 -2.659602
H -3.197453 2.670545 -4.291491
H -2.587745 5.083331 -4.357131
H -0.858006 5.961838 -2.803779
H -0.247940 4.461262 -1.193668
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C -1.364540 3.325012 2.782987
C -2.507486 3.978622 2.317281
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H -1.102409 3.368233 3.836237
H -1.315648 4.534231 3.007170
H -3.748230 4.399934 0.603624
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C -4.771791 0.948115 3.060940
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H -6.259789 1.918914 0.166279
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C -3.330164 -2.330925 -3.815371
C -4.234592 -3.160628 -3.193697
C -4.439936 -3.059304 -1.796612
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C -2.008416 -0.333906 -0.897295
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H -1.530716 -0.561568 -4.772899
H -3.166055 -2.395725 -4.887866
H -4.794605 -3.890748 -3.770635
H -5.157628 -3.713949 -1.310473
H -3.905100 -2.083237 0.020642

TS3-114
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P -0.254689 -1.597595 -0.537484
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C -0.005581 -2.464176 1.057058
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C -0.896322 2.102770 -1.616312
C -1.477977 -1.080389 -0.976440
C -0.622734 1.196448 1.219956
N -3.401838 1.065553 2.054733
C -2.84066 0.464022 1.044325
C -3.742820 -0.828282 0.454623
C -3.902321 -1.234738 -0.859927
C -3.859655 -2.709926 -1.186696
C -4.515212 -0.383315 -1.952893
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H -5.572352 -0.656360 -2.087752
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C -1.464849 -4.684452 -3.786077

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C -1.589887 5.379251 0.878089
C -0.843121 4.202282 0.806648
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H -3.960555 4.677809 1.463100
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H -1.285210 6.167345 1.560654
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C -2.643493 2.917715 -3.639681
C -2.767447 3.451242 -2.353514
C -1.894260 3.050849 -1.345135
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H -1.542203 1.572079 4.916411
H -3.328713 3.228087 -4.423029
H -3.551125 4.169798 -2.133906
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C -3.311312 -1.216444 4.797743
C -3.835202 -1.644218 3.554658
C -3.310608 -1.72571 2.372187
C -2.236629 -0.239134 2.369489
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H -3.737323 -1.595268 5.722207
H -4.657326 -2.353754 5.354012
H -3.718267 -1.513248 1.427724

TS45-46
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P -0.430095 -1.468792 -0.603992
C -0.724835 2.780267 1.793023
C -0.805226 2.501123 -0.709614
C -1.385997 -2.518454 -1.777889
C -0.095869 -2.579047 0.748651
C -1.212700 0.607416 1.462935
C -1.125558 -0.953102 -1.455109
N -4.927575 -0.846349 0.945709
C -3.00162 -0.174352 -0.186992
C -3.786206 1.212367 0.138173
C -3.319282 2.098294 -0.816764
C -3.017719 3.531856 -0.452242
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C -4.702811 -2.816299 1.601511
C -3.874752 -1.996627 0.868375
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C -5.353297 1.493323 -1.412195
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C -2.127581 -0.311302 -0.724875
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H -2.341163 -0.554333 -4.623018
H -4.430064 0.746323 -4.607851
H -6.236870 1.886271 -3.355869
H -6.150103 1.990989 -0.866863
H -4.275716 0.989668 0.358268

TS₄₆₋₄₇
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C 0.225394 -3.021020 -1.861623
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C -0.610909 1.100634 1.445537
C -1.617802 -0.894675 -1.075214
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C 4.159519 -0.686932 0.032994
C 3.891352 0.483318 -0.455634
C 3.297334 0.522057 -1.763334
C 3.041725 1.901771 -2.335309
C 3.625472 -0.487091 -2.848947
H 4.657513 -1.519505 -0.644315
H 2.496125 -1.840275 -0.437619
H 3.966635 1.408949 0.104835
H 4.588240 -0.223069 -3.313005
H 2.869139 -0.440833 -3.637698
H 3.627178 -1.520519 -2.503104
H 2.219644 1.896368 -3.054415
H 3.941578 2.230399 -2.876370
H 2.827700 2.647022 -1.566837
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H 4.980610 1.120488 1.922893
H 5.801710 -0.026940 2.994608
H 4.024321 -0.050290 2.869903
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H 5.584908 -2.856748 0.761005
H 4.821405 -2.642301 2.353200
H 6.512503 -2.134599 2.097608
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C 3.374485 3.659529 2.318270
C 3.335397 4.961728 1.806076

C 2.429587 5.276700 0.793536
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C -2.114668 3.512032 -3.160611
C -2.157163 4.009603 -1.856125
C -1.349575 3.448845 -0.867846
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H -2.754951 3.940910 -3.925681
H -2.836511 4.817633 -1.602629
H -1.410611 3.819565 0.151623
C 0.742219 -2.628402 -3.107685
C 0.973024 -3.568228 -4.109733
C 0.706796 -4.920381 -3.872805
C 0.204668 -5.320085 -2.634240
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H 0.893472 -5.656599 -4.649274
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C -1.027365 -3.807775 3.418496
C -1.917413 -3.905376 2.346675
C -1.619717 -3.290412 1.131481
H 1.404086 -1.944669 1.932743
H 0.860368 -3.021277 4.103410
H -1.270926 -4.271696 4.369758
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C -1.008991 0.828107 3.837702
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C -3.253226 -0.445776 -2.822756
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C -5.082334 2.484620 -0.391834
C -3.999831 1.781933 0.087131
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C -2.210483 0.060127 -0.246599
H -1.719514 -1.902517 -2.998458
H -3.655643 -0.652430 -3.811317
H -5.359021 1.095262 -3.492315
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H -5.557842 3.234107 0.234433
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TS₄₇₋₄₈
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C 0.023395 -2.218442 -1.636883
C 0.358243 3.456705 -1.057685
C 1.024690 2.246301 1.520727
C 0.424294 -1.450200 1.147846
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C -3.813532 0.414277 -0.760385
C -3.055388 1.293182 -1.640431
C -2.693586 0.670731 -2.976702
C -3.432235 2.760921 -1.799609
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H -3.957251 -0.612647 -1.081417
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H -2.577051 3.341075 -2.143613
H -3.777369 3.220553 -0.863280
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H -3.540774 0.773037 -3.671824
H -2.457791 -0.392615 -0.891372
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H -5.285726 -1.666630 0.083634
H -6.895141 -0.892603 0.018622
H -6.302828 -1.647361 1.520322
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H -5.659627 1.810987 2.405745
H -5.960393 0.204014 3.105545
H -7.165867 0.939650 2.021891
C -2.905466 -2.340971 1.431603
C -3.868045 -3.231342 1.904746
C -4.126647 -4.417920 1.212837

C -3.413659 -4.702734 0.048025
C -2.415645 -3.833173 -0.402562
H -2.747420 -1.399680 1.952551
H -4.426990 -2.991211 2.805385
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H -3.619254 -5.613148 -0.507754
H -1.858703 -4.086299 -1.297580
C 0.161133 -1.512247 -2.839237
C 0.868171 -2.066763 -3.905866
C 1.443349 -3.332307 -3.780755
C 1.317245 -4.040311 -2.582725
C 0.618339 -3.484758 -1.512676
H -0.242345 -0.510755 -2.921272
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H 1.782883 -5.015300 -2.474482
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H 0.760715 6.813657 -0.635352
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C 2.331657 2.726127 1.695799
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H 2.409578 2.902417 5.091590
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H 2.969577 2.891638 0.831863
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C 0.940458 -1.837700 3.501371
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C 3.870547 -0.130095 1.935088
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H 0.659891 -2.245917 4.469826
H 2.785245 -1.454238 5.427255
H 5.018303 -0.423600 5.126371
H 5.704509 0.414421 2.880499
H 4.182535 0.250123 0.970061
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C 3.673669 -0.720626 -2.296783
C 4.631277 -1.525650 -2.969383
C 5.047553 -2.721286 -2.431158
C 4.515157 -3.161449 -1.195714
C 3.578812 -2.407081 -0.525848
C 3.125855 -1.162659 -1.049818
C 2.149974 -0.352173 -0.374060
H 2.056108 2.255521 -2.575820
H 3.688364 0.880651 -3.751601
H 5.033991 -1.174169 -3.915924
H 5.785367 -3.327582 -2.948637
H 4.845982 -4.106534 -0.774565
H 3.174917 -2.765442 0.413347

TS₉₅₋₉₆
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P 1.080980 -1.011281 -0.593222
C -0.880682 3.236961 1.457877
C -1.853185 2.015813 -1.022079
C 2.258596 -1.830760 -1.762210
C 1.090319 2.066500 0.907274
C -1.400408 0.370226 1.391921
C -0.584511 -1.275072 -1.376370
N 4.500200 -0.042272 1.252670
C 3.964582 1.043000 0.693612
C 3.669166 1.268247 -0.673376
C 3.158476 2.544140 -1.095743
C 2.926891 2.753664 -2.578602
C 3.581037 3.836679 -0.406931
H 1.410963 2.894411 0.049680
H 3.811517 1.858589 1.390627
H 3.907472 0.514376 -1.414660
H 2.879969 4.641700 -0.644393
H 4.572960 4.130076 -0.779913
H 3.636880 3.761146 0.680963
H 3.823903 3.196398 -3.037160
H 2.101236 3.455261 -2.736738
H 2.699855 1.826679 -3.108329
C 4.680140 -0.128548 2.701158
H 5.734737 -0.310930 2.935396
H 4.080316 -0.953783 3.100494
H 4.365246 0.802819 3.175699
C 4.842000 -1.262741 0.527464
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C -4.096914 2.209307 -1.924643
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H -1.771698 2.580459 -4.383127
H -4.235054 2.566638 -4.045481
H -5.171765 2.177932 -1.776897
H -3.663879 1.797832 0.139558
C 2.615546 -1.121206 -2.923079
C 3.537125 -1.640915 -3.831758
C 4.131746 -2.881795 -3.588368
C 3.788233 -3.595845 -2.439412
C 2.857270 -3.078373 -1.534831
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H 1.088883 -4.169586 4.181434
H 0.360219 -5.197574 2.040954
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C -1.766292 -0.506560 3.636883
C -2.129002 -1.770547 3.111569
C -2.481782 -2.855184 3.957794
C -2.848153 -4.071628 3.428780
C -2.873551 -4.250533 2.025024
C -2.526923 -3.220251 1.179772
C -2.141905 -1.948097 1.690929
C -1.752001 -0.861651 0.835386
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H -1.773348 -0.360983 4.714286
H -2.463345 -2.702924 5.033991
H -3.126225 -4.893484 4.083736
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C -1.864079 -1.519366 -3.435443
C -3.079158 -1.339400 -2.731651
C -4.333497 -1.350348 -3.397879
C -5.506382 -1.202734 -2.698384
C -5.466359 -1.037776 -1.288440
C -2.468688 -1.010647 -0.616964
C -3.032562 -1.154109 -1.312981
C -1.761174 -1.094705 -0.646910
H 0.246510 -1.671370 -3.348388
H -1.895651 -1.685444 -4.509326
H -4.348762 -1.484862 -4.476401
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H -4.257524 -0.873010 0.457703

TS₉₇₋₁₀₁
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C 1.817735 -2.990600 -0.518270
C 0.157103 -2.127976 1.671811
C -0.023450 3.137043 1.497459
C -1.118627 3.88215 -1.126494
C -0.544081 -1.435273 -1.164681
C -1.646459 0.715767 1.143382
N 4.58647 -0.386469 -0.356629
C 4.538216 0.519687 0.019462
C 3.766948 1.314087 -0.834779
C 2.935125 2.428786 -0.399460
C 2.504668 3.378517 -1.509909
C 3.329165 3.193212 0.859333
H 4.469254 0.666408 1.092003
H 1.955607 0.726842 1.393218
H 3.865377 1.145943 -1.096634
H 4.225944 3.798466 0.658513
H 2.53895 3.876576 1.161581
H 3.545026 2.548689 1.716136
H 1.617485 3.947956 -1.215443
H 3.303210 4.104870 -1.725643
H 2.278027 2.856830 -2.444977
H 5.799212 -0.576097 -1.763526
H 0.631440 0.388289 -2.226798
H 6.680398 -1.216490 -1.831368
H 4.981690 -1.046802 -2.324851
C 6.031296 -1.318623 0.612723
H 7.118692 -1.360166 0.495180
H

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H 1.304986 -4.296353 -0.587876
H 3.521661 -1.751563 -0.876138
H 4.948321 -3.608256 -1.734232
H 4.025664 -5.915082 -1.843136
H 1.689938 -6.346021 -1.110351
H 0.288369 -4.505420 -0.275223
C 0.692444 -1.599043 2.855370
C 0.244861 -2.049425 4.098489
C -0.745896 -3.030203 4.171699
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C -0.834348 -3.116973 1.757610
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H -1.101023 -3.374451 5.138759
H -2.075291 -4.305823 3.045858
H 1.293010 -3.508578 0.856404
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C 0.847976 3.928181 3.626163
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C -0.202671 4.466891 1.093201
H 0.689582 1.855522 3.096321
H 1.257852 3.713239 4.608907
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H 0.007279 6.542720 1.618518
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C -1.271295 2.549606 -3.543007
C -2.458391 3.272696 -3.422537
C -2.982905 3.549211 -2.156773
C -2.324489 3.099674 -1.014029
H 0.306815 1.528958 -2.504603
H -0.872236 3.212997 -4.524751
H -2.982646 6.607917 -4.312488
H 3.914176 4.099848 -2.061070
H -2.750942 3.292294 -0.033365
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C -1.076364 -1.571773 -3.421573
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C -4.415574 -0.028520 -4.163017
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C -3.907360 0.141156 -1.796442
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H -1.754830 -0.786049 -0.907953
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H -5.700116 0.891795 -2.678113
H -4.181673 4.70012 -0.801442
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C -5.113255 -2.776221 2.464821
C -4.691614 -3.108243 1.155030
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C -2.179345 -0.390153 4.679666
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H -4.913816 -1.387910 4.089200
H -5.847099 -3.392262 3.971860
H -5.107140 -3.984132 0.664979
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TS₁₀₂₋₁₀₇
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P 0.135519 -1.708422 -0.370624
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C -0.237932 -2.432627 1.272486
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C -1.516976 -1.075592 -0.947618
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H 3.616413 -2.173645 -2.633273
H 4.379409 -0.646938 -2.174990
H 5.227741 -2.187783 -1.919711
H 2.965260 -3.871015 -0.943903
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H 2.771787 -3.418809 0.764619
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H 5.814697 2.425426 0.305759
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C 1.070150 -5.169873 -3.326296
C 0.544486 -5.480181 -2.071178
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C -3.712320 -0.857573 4.633166
C -4.217973 -1.216605 3.361726
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TS₁₀₇₋₁₁₃
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C 0.685744 -2.999456 -1.474955
C -0.028140 -2.327688 1.307286
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C 3.859422 -1.588378 -0.781123
C 3.802935 -3.086140 -0.602817
C 4.275049 -1.126185 -2.157281
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H 3.277507 1.307605 -0.042165
H 3.781964 -1.241069 1.321326
H 3.620201 -1.560367 -2.918626
H 4.270534 -0.040706 -2.281224
H 5.291574 -1.491395 -2.366979
H 3.324298 -3.584832 -1.447021
H 4.833712 -3.464026 -0.544890
H 3.284850 -3.373891 0.315898
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H 6.148121 2.466387 1.176650
H 6.156172 1.779969 2.821439
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H 3.872548 2.384730 3.263823
H 3.625577 3.137799 1.665660
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C 1.477832 -3.679436 -3.671847
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C 0.562510 -2.455003 3.656177
C -0.493743 -3.340378 3.876894
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C -1.094435 -3.212514 1.537610
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H -0.682108 -3.725215 4.874761
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C -1.821877 2.913440 -1.589985
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TS₁₁₃₋₁₁₄
Rh 1.801434 0.207740 -0.696725
P 0.445002 -1.554557 -0.472867
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C 0.957313 -2.901157 -1.609026
C 0.451377 -2.230450 1.232325
C 0.667547 3.379311 -0.229047
C -1.264197 1.880022 -1.680094
C -1.373812 -1.333528 -0.830244
C -0.723832 1.167174 1.179508
N 3.626259 1.257345 1.984775
C 3.957902 1.067504 0.578535
C 3.767383 -0.358867 0.104534
C 3.940965 -0.765446 -1.208308
C 4.136844 -2.229712 -1.515624
C 4.361600 0.169757 -2.322584
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H 3.299245 1.754943 -0.004184
H 3.715391 -1.125182 0.872441
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H 4.202393 1.230006 -2.101209
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H 5.617855 1.032349 2.755007
H 4.286526 0.575781 3.909211
H 4.646403 -0.459755 2.681336
C 3.503714 2.680430 2.302216
H 2.750036 3.144869 1.659753
H 1.85644 2.793526 3.343287
H 4.454208 3.231571 2.172576
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C 1.506114 -3.544640 -3.889946
C 1.803885 -4.840202 -3.454517
C 1.687637 -5.161052 -2.101727
C 1.261590 -4.199674 -1.180951
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H 1.603302 -3.284952 -4.940251
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C 1.160112 -2.104073 3.545459
C 0.351309 -3.196807 3.859240
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H 1.737457 -1.610930 4.322314
H 0.304856 -3.565855 4.879528
H -1.067521 -4.638619 3.106645
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C -2.910656 -1.367198 5.011122
C -3.442952 -1.914907 3.819878
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C -2.087327 -0.393115 2.484609
H -1.646713 0.123655 1.219829
H 0.611099 2.421465 3.547788
H -0.130745 1.565899 4.521799
H -1.557439 0.066806 5.854309
H -3.239017 -1.747217 5.974129
H -4.174656 -2.715640 3.876981
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3.5 Associative mechanism (B3LYP+D3/BS2 level)

291

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P 0.322059 -1.073981 -0.975492
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C 0.356570 -2.417866 0.268229
C 0.008000 2.776109 1.886711
C -1.942658 2.374912 -0.296577
C -1.449429 -0.946590 -1.500633
C -1.387003 0.229866 1.568715
N 5.179355 -0.696613 -0.813003
C 3.899484 -0.579792 -0.146232
C 3.970558 -0.188972 1.311551
C 4.328659 -1.012189 2.309271
C 4.305204 -0.550883 3.745033
C 4.746329 -2.445085 2.094127
H 3.228406 0.177906 -0.674732
H 3.377001 -1.533937 -0.264747
H 3.690289 0.832430 1.555521
H 4.940891 -2.671429 1.044217
H 3.973239 -3.130757 2.466795
H 5.662024 -2.662997 2.667880
H 5.301084 -0.628474 4.200494
H 3.639530 -1.187065 4.345219
H 3.964113 0.485779 3.842051
C 6.032405 0.477388 -0.709892
H 5.647727 1.341625 -1.287321
H 7.028421 0.238830 -1.096490
H 6.133338 0.773763 0.337506
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H 4.459853 -2.079346 -2.218965
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C 1.508640 -0.846804 -3.497758
C 2.225948 -1.271315 -4.615254
C 2.695294 -2.585649 -4.685300
C 2.443997 -3.467947 -3.632829
H 1.723945 -3.045880 -2.512460
H 1.144752 0.177213 -3.447684
H 2.420201 -0.577539 -5.428399
H 3.255429 -2.918717 -5.554140
H 2.810261 -4.489550 -3.679665
H 1.546134 -3.742574 -1.701009
C 1.045645 -2.218902 1.471547
C 1.049378 -3.215254 2.448707
C 0.372856 -4.416560 2.228839
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C -0.326545 -3.626070 0.503487
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H 1.568883 -3.044507 3.387384
H 0.368628 -5.187547 2.993728
H -0.853239 -5.548387 0.860599
H -0.891054 -3.776016 -0.862886
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C 1.656100 3.294537 3.602727
C 1.046846 4.534331 3.819776
C -0.074331 4.894800 3.071021
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C -6.386274 0.235517 -1.871382
C -6.091791 0.194185 -0.487389
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C -2.437240 -0.688973 -0.549182
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C -3.543080 -4.100255 3.164903
C -3.828499 -4.001044 1.718181
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C -2.641255 -1.874994 1.661725
C -2.139700 -0.752266 0.920197
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368
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