

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.

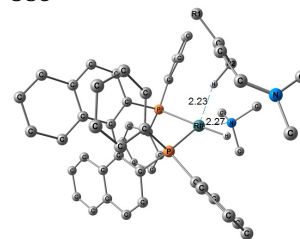
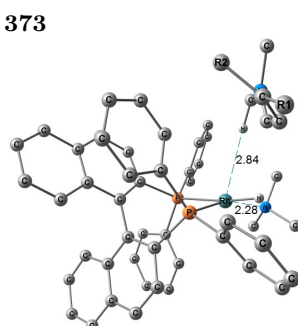
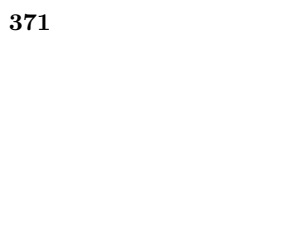
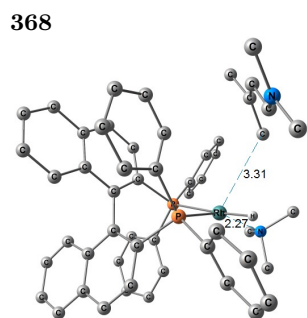
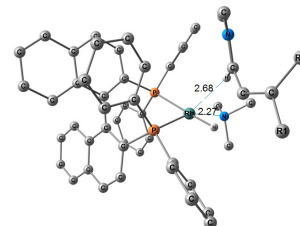
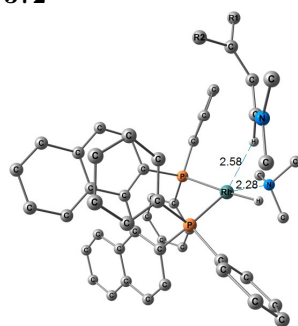
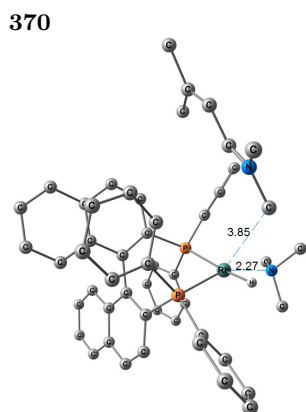
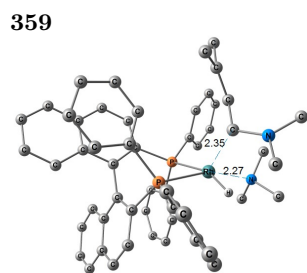
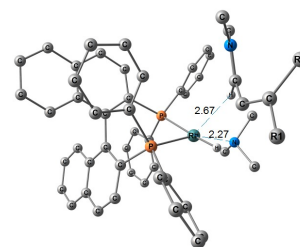
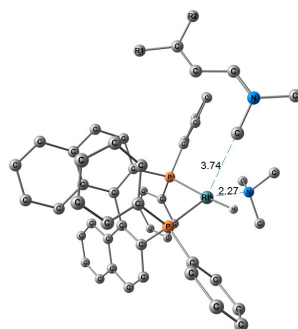
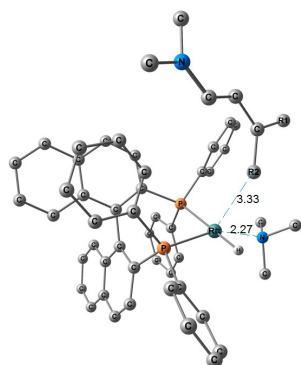
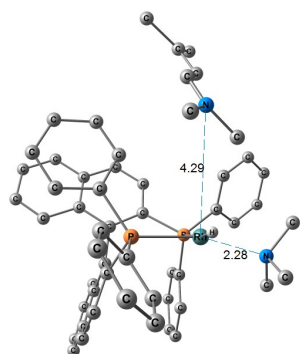
Table S3: The electronic and Gibbs free energies of LMs and TSs in the associative mechanism

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	C -2.291338 0.305728 2.578126
P 0.494486	-1.814103	0.491525	C -1.629483 0.428349 1.324665
P 0.317517	1.609213	-0.369799	H 0.110938 3.281680 2.044758
C 1.097704	-3.419748	-0.096172	H -1.005447 3.070348 4.132684
C 0.297682	-1.872559	2.329038	H -2.512640 1.857192 5.625236
C 1.238496	3.165421	-0.262384	H -4.049299 0.033126 6.013940
C -0.851799	1.673289	-1.799087	H -4.504077 -1.631013 4.248715
C -1.206244	-1.598527	-0.175986	H -3.424860 -1.493810 2.111418
C -0.709742	1.493709	1.145676	4
N 3.955237	-1.079972	-0.078643	Rh 2.004639 0.289252 -0.042967
C 4.660411	-0.009559	-0.889065	P 0.497158 -1.580335 -0.656250
C 3.713245	0.401633	-1.993150	P 0.180923 1.708698 0.672144
C 3.551712	1.665409	-2.483802	C 1.326183 -2.476824 -1.995982
C 2.663747	1.915273	-3.681528	C 0.027148 -2.766930 0.682825
C 4.350280	2.860265	-0.022171	C 0.876994 2.943625 1.804632
H 5.617734	-0.398519	-1.266607	C -0.822334 2.551460 -0.635300
H 4.881412	0.827040	-0.223289	C -1.099442 -0.966058 -1.320414
H 3.258754	-0.416982	-2.552279	C -1.015559 0.705069 1.641165
H 3.751180	3.775123	-2.006650	N 3.936096 -0.857725 0.102339
H 4.745013	2.758139	-1.009560	C 4.782020 0.399968 0.110707
H 5.202285	3.010125	-2.698318	C 3.836486 1.582038 0.123784
H 1.899300	2.667305	-3.445207	C 3.281299 2.105114 -1.046344
H 3.254132	2.327293	-4.509628	C 2.778134 3.535273 -1.049538
H 2.168320	1.005316	-4.025573	C 3.575307 1.578345 -2.438449
C 4.305123	-2.427922	-0.621410	H 5.438893 0.400219 0.985971
H 5.389673	-2.588261	-0.571537	H 5.417415 0.396952 -0.78796
H 3.816828	-3.201623	-0.028358	H 8.369947 2.211358 1.009774
H 3.976966	-2.509678	-1.657927	H 4.415568 2.143261 -2.869555
C 4.321186	-1.008888	1.370990	H 2.716501 1.728748 -3.098117
H 4.043345	-0.029372	1.761789	H 3.832335 0.519431 -2.458431
H 3.768166	-1.780906	1.909093	H 1.845524 3.667262 -1.600585
H 5.397731	-1.175282	1.510063	H 3.527905 4.160100 -1.553532
C 1.361640	-3.571819	-1.459272	H 2.663421 3.934126 -0.038961
C 1.849123	-4.786367	-1.957072	C 4.453482 -1.858649 -0.876465
C 2.092889	-5.844678	-1.076605	H 4.390582 -1.460479 -1.889224
C 1.860162	-5.689239	0.293662	H 8.354751 -2.768342 -0.817017
C 1.369093	-4.471195	0.781235	H 5.496728 -2.115545 -0.653223
H 1.185911	-2.740400	-2.125214	C 3.893225 -1.476037 1.467439
H 2.046484	-4.906577	-3.018439	H 3.474357 -0.760244 2.176209
H 4.245615	-6.785859	-1.455584	H 4.903638 -1.763691 1.787556
H 2.070515	-6.508097	0.975986	H 3.268557 -2.369080 1.432706
H 1.228334	-4.343489	1.839532	C 1.809454 -1.741381 -3.079612
C 0.999427	-0.964194	3.134582	C 2.488449 -2.378496 -4.129441
C 0.814664	-0.955677	4.521063	C 2.698501 -3.759611 -4.070091
C -0.075121	-1.849415	5.117757	C 2.240691 -4.499035 -2.974762
C -0.783519	-2.751391	4.323547	C 1.560439 -3.851872 -1.934994
C -0.609252	-2.757278	2.935819	H 1.646376 -0.675197 -3.104702
H 1.672059	-0.249302	2.678589	H 2.856348 -1.806050 -4.971651
H 1.357489	-0.245568	5.129754	H 3.227968 -4.258241 -4.874442
H -0.221841	-1.837565	6.193129	H 2.424788 -5.568701 -2.927222
H -1.485428	-3.437054	4.778529	H 1.251755 -4.416442 -1.073976
H -1.183870	-3.443294	3.326735	C 0.455924 -2.542483 1.999196
C 2.286594	3.247436	0.655996	C 0.057625 -3.397629 3.031925
C 3.003631	4.440690	0.808483	-0.782485 -4.478844 2.765370
C 2.679168	5.546815	0.106684	C -1.231241 -4.698784 1.463015
C 1.652166	5.459552	-0.929101	C -0.843033 -3.840638 0.429052
C 0.937860	4.262616	-1.070315	H 1.072086 -1.683322 2.225888
C 2.525598	2.386343	1.261457	H 0.391692 -3.208551 4.042875
H 3.810579	4.509363	1.523341	H -1.096161 -5.137433 3.569054
H 3.239313	6.472031	0.127136	H -1.897720 -5.524307 1.252960
H 1.415869	6.316248	-1.554119	H -1.221609 -4.003882 -0.571861
H 0.163509	4.192827	-1.812381	C 1.791997 2.512843 2.767073
C -0.715970	1.752334	-2.847785	C 2.385060 3.428248 3.644608
C 1.628133	0.745165	-3.908068	C 2.067520 4.785804 3.543382
C 2.688370	1.651797	-3.930058	C 1.170181 5.228222 2.566516
C -2.836188	2.565933	-2.886664	C 0.581480 4.303758 1.694155
C -1.931103	2.571827	-1.820396	H 2.035717 1.462851 2.829187
H 0.090905	0.030936	-2.829531	H 3.091407 3.090580 4.397765
H -1.513781	0.027200	-4.708648	H 2.526555 5.500286 4.217841
H -3.398966	1.641013	-4.750460	H 0.942037 6.286905 2.479091
H -3.665000	3.260835	-2.890024	H -0.071953 4.655935 0.917729
H -2.072016	3.266360	-1.002138	C -0.513456 2.351571 -1.988963
C -1.719900	-2.534666	-1.098141	C -1.296474 2.934193 -2.990660
C -2.908638	-2.366975	-1.703252	C -2.404997 3.711123 -2.653978
C -3.697266	-1.249382	-1.418046	C -2.732956 3.899166 -1.311388
C -4.931965	-1.068833	-2.062671	C -1.957100 3.312098 -0.306579
C -5.702224	-0.009578	-1.763555	H 0.326875 1.727417 -2.262214
C -5.290068	0.925979	-0.804760	H -1.046741 2.769715 -4.029872
C -4.114190	0.787126	-0.167072	H -3.016571 4.156330 -3.432338
C -3.263659	-0.306696	-0.452488	H -3.603573 4.482694 -1.044212
C -2.010066	-0.487533	0.196498	H -2.241359 3.437840 0.730317
H -1.167270	-3.423062	-1.338159	H -1.406384 -1.147555 -2.684933
C -3.257523	-3.108407	-2.415821	C -2.526433 -0.651333 -3.238480
H -5.273460	-1.784346	-2.801363	C -3.446695 0.057608 -2.461328
H -6.656113	0.123009	-2.263461	C -4.611515 0.582874 -3.044322
H -5.929155	1.772239	-0.577162	C -5.507268 1.241322 -2.290114
H -3.829879	1.538283	0.557168	C -5.296389 1.411768 -0.915010
C -0.540104	2.437456	2.179839	C -4.192723 0.924125 -0.321105
C -1.173595	3.235559	3.360570	C -3.216941 0.228198 -1.072592
C -2.043937	1.257874	3.599119	C -2.034499 -0.301011 -0.482591
C -2.693517	1.134629	4.838214	H -0.744349 -1.703867 -3.322290
C -3.548981	0.121647	5.055814	H -2.717456 -0.808189 -4.295827
C -3.808590	-0.822334	4.052060	H -4.797683 0.456776 -4.104345
C -3.205205	-0.737935	2.853126	H -6.406451 1.642485 -2.746119
			H -6.033717 1.945530 -0.325200
			H -4.063947 1.089180 0.739893
			C -1.054294 0.834578 3.045124
			C -1.821822 0.045495 3.816745
			C -2.627648 -0.940569 3.241407
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			C -4.203432 -2.709433 3.494959
			C -4.255773 -2.863521 2.102931
			C -3.516955 -2.082933 1.294646
			C -2.666991 -1.088133 1.831995
			C -1.867313 -0.243612 1.011132
			H -0.460624 1.580230 3.539620
			H -1.811957 0.175885 4.894785
			C 1.326183 -2.476824 -1.995982
			H -4.810012 -3.350428 4.126249
			H -4.899204 -3.624549 1.675024
			H -3.577617 -2.244846 0.227130
			5
			Rh -0.151864 -3.291370 0.244181
			P 0.940633 -1.727690 1.636800
			P -0.987775 -1.712529 -1.325705
			C 0.885780 -2.389019 3.322612
			C 2.695182 -1.400485 1.164678
			C -1.399002 -2.684774 -2.795923
			C -2.440422 -0.687555 -0.826773
			C 0.123968 -0.085311 1.631171
			C 0.366637 -0.560833 -1.746843
			N 0.418312 -5.238827 0.972009
			C -0.291439 -5.679488 -0.285601
			C -1.121094 -6.928913 -0.236489
			C -1.021411 -7.975500 -1.084382
			C -1.957551 -9.155253 -0.940824
			C -0.038143 -8.094276 -2.226377
			H -1.030645 -4.831128 -0.548465
			H 0.443790 -5.713529 -1.082067
			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
			H -2.545890 -9.294497 -1.857035
			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
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46

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53

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C -2.839104 -3.488066 -4.009903
C -3.846667 -4.299428 -4.545809
C -4.721407 -4.971166 -3.686514
C -4.587686 -4.839090 -2.006299
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 -4.095570
H -5.258744 -5.377419 -1.637117
H -3.458354 -3.948518 -0.708807
C -0.284600 -2.673131 0.572517
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
C 2.517029 -0.007048 -0.513993
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
H -0.469439 2.055841 3.916832
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 -3.911399
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 0.416601 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 0.358360
C -0.884175 0.803798 1.065462
C -0.181930 1.735389 -0.002825
C -0.321337 3.205661 0.320935
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 -1.232420 -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 4.586648 0.913128 -2.73847
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
H 4.332250 0.055481 -1.343505
H 4.886322 2.346615 -2.119911
H 4.308656 4.314484 -0.723666
H 3.189553 3.981384 1.461992
C 0.497427 3.455968 3.780591
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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 5.763961
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 6.591528
H -1.995382 -0.999754 5.759949
C 3.211021 -2.218559 3.925225
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 5.947888
H 2.862398 -1.838462 6.445881
H 4.962559 -3.128415 2.737492
H 5.777030 -4.041717 4.897068

H 4.460564 -3.653250 6.964457
H 2.361572 -2.353207 6.882438
C 5.015712 0.702964 3.490971
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 5.485552 -0.663788 8.260064
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
H 7.866934 -0.793968 5.883520
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 2.152425 6.920552
C 0.949747 2.733935 7.368492
C 0.909875 3.879221 8.180564
C 2.046824 4.507709 8.518560
C 3.283344 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 1.562611
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

Rh -1.614564 -0.188381 -0.230143
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P 0.088627 -1.680951 0.412883
C -1.155642 2.840573 -1.580980
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 1.387266
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 -4.821522 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 2.370827
C 1.861104 4.228252 2.012072
C 1.366937 3.608078 0.857122
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H 0.137075 2.463340 4.345860
H 1.813779 4.284509 4.166075
H 2.601429 5.006804 1.926858
H 1.733709 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 2.026299
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 -1.713058
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 9.535346 -2.301624 -1.650882
H 4.250428 -1.144235 -0.910677
C 1.721167 -1.104864 2.627263
C 2.656448 -0.445556 3.332704
C 3.442273 0.535817 2.722673
C 4.404290 1.237794 4.647198
C 5.173911 2.165213 3.873774
C 5.032484 2.443800 1.507526
C 4.122930 1.792094 0.761501
C 3.284682 0.810271 1.340537
C 3.204988 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 9.665654 3.195722 1.049042
H 4.040214 2.047050 -0.286157

TS₄₋₄₅

Rh 0.250838 -3.684156 -0.409692
P 1.880261 -2.030527 -0.078311
P -1.629753 -2.300872 1.079884
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C 2.140059 -0.889291 -1.507240
C -3.042877 -3.085403 -0.630341
C -1.952377 -1.512194 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 1.172199 -5.647643 -0.736411
C 1.388367 -5.065503 -1.990714
C 2.799994 -4.747821 -2.443013
C 0.389178 -5.120366 -3.133484
H -0.237944 -7.305627 -0.174177
H -0.986247 -5.721757 -0.780552
H 2.037078 -5.846980 -0.113028
H 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 5.066999 -7.016303 1.947450
H 1.601349 -6.672578 1.751549
H 0.368134 -6.846480 3.007594
H 0.458965 -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 1.681052
C 4.558311 -4.603997 1.201348
C 5.765855 -4.296612 0.950261
C 5.793724 -3.289910 -0.020030
H 4.624964 -2.583910 -0.333219
H 4.261711 -4.124770 1.771024
H 4.532060 -5.393068 2.347571
H 6.659797 -8.464415 1.192052
H 7.723994 -3.066475 -0.534920
H 6.649350 -1.837388 -1.106187
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C 1.545043 -0.182518 -3.756380
C 2.412859 0.905375 -3.656379
C 3.140703 1.101556 -2.482585
C 2.998317 -2.017692 -1.408063
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H 3.546223 0.396123 -0.491652
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C -3.956188 -4.118012 -2.625984
C -5.118991 -4.443038 -1.920300
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H -2.012573 -3.191074 -2.503764
H -8.363573 -4.389135 -3.673959
H -5.927125 -4.965180 -2.420759
H -6.139555 -4.373962 -0.020

H -3.882654 -0.457180 4.229372
H -3.537380 -0.699092 1.794399
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C 0.703153 0.432302 3.667383
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C -1.153830 1.500491 2.528010
C -0.046395 0.621318 2.478737
C 0.328433 -0.067100 1.290568
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H 2.408570 -0.532745 4.565399
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H -1.016374 2.446713 5.750250
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C 1.018102 3.540431 -0.891517
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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 1.272263
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C -7.140240 -1.274293 -0.585263
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H -8.106281 -0.951220 -0.350217
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H -3.676275 1.925719 -1.976805
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 1.082870
C -3.278811 -2.320495 2.135090
C -3.251279 -3.151467 2.780879
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C -2.817821 -4.885018 1.141941
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H -2.142016 -1.323937 2.505810
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H -4.210649 -5.080653 2.773950
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H -1.400662 -4.385067 -0.388814
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C 1.207077 -3.490168 -3.728921
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H 0.181270 -1.887211 -4.730389
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C -0.516626 5.593031 -1.080736
C -0.072494 4.545306 -1.003801
H -0.981057 1.911623 2.930192
H -1.765831 3.761926 -4.410045
H -1.463622 6.115774 -3.683941
H -0.407245 6.624504 -1.497565
H 0.354289 4.767072 -0.041483
C 0.484877 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
H -0.407176 1.539780 2.463366
H 0.640196 2.316854 4.562348
H 2.711619 3.682027 4.498905

H 3.726652 4.266294 2.311332
H 2.693215 3.485111 0.207264
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C 1.884293 -1.504917 3.484831
C 2.952323 -0.681877 3.114087
C 3.942531 -0.339880 4.049497
C 4.982931 0.426980 3.682776
C 5.099107 0.892316 2.365729
C 4.170935 0.586254 1.441949
C 3.052365 -0.209839 1.780432
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
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H 5.948624 1.508244 2.091403
H 4.293354 0.974880 0.440059
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C 4.744556 -2.764764 -1.618538
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H -3.516260 -1.835505 4.972418
H -4.957256 -3.464452 3.919755
H -5.064414 -3.651999 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 3.835859 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 5.429108 -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 2.385652 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
H -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 -4.926144 -4.664853
H 2.544604 -5.677417 -2.631945
H 1.268130 -4.436810 -0.905878
C 0.579437 -2.401465 1.987298
C 2.284450 -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 2.949097
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 -3.625250 5.574100 -3.170926
C -5.501260 1.287437 -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 -4.366679
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 0.037705 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 -0.515916 -0.616272
C 3.964260 0.839790 -0.234883
C 3.533311 1.868923 -1.084330
C 3.375040 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 3.723776 0.800226 -2.998018
H 5.270085 3.808286 -0.884826
C 4.329852 3.861923 0.924882
H 3.507443 3.320364 -0.543800
C 8.241041 -1.298646 1.646668
H 5.351425 -0.361997 1.840621
H 5.433381 -2.114453 2.037783
H 3.865933 -1.290068 2.184210
C 4.689433 -2.892677 -0.268012
H 5.505262 -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 3.357681 3.451542
C 2.289821 4.742877 3.327116
C 1.452463 5.278261 3.242845
C 0.750098 4.420336 1.686661
H 1.844884 1.438100 2.664813
H 3.097938 2.947069 4.208182
H 2.837419 5.405386 1.988414
H 1.358816 6.355574 2.276277
H 0.137704 4.835140 0.706030
C -0.649811 2.651084 -2.117995
C -1.411172 3.313025 -3.068721
C -2.460751 4.149838 -2.705846
C -2.749784 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 1.564473 -2.579112 -2.985708
C 2.219168 -3.511148 -3.800318
C 2.490940 -4.789686 -3.307570
C -1.115333 -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
C 2.346232 -6.125928 -1.621505
H 1.218168 -4.459626 -0.185947
C 0.619614 -1.956779 2.181159
C 0.306102 -2.509340 3.427324
C -0.611687 -3.556006 2.523207
C -1.216700 -4.502626 3.366469
C -0.912401 -3.496673 1.118657
H 1.321713 -1.136103 2.119311
H 0.775351 -2.118844 4.319973
H -0.857071 -3.980843 4.490521

H -1.937217 -4.854126 2.434639
H -1.401167 -3.875305 2.260113
C -1.299139 1.179666 0.834372
C -2.109360 0.452637 3.652199
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 1.969809 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 2.213139 -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 0.226560 1.066598
C -0.686684 0.898524 2.848028
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 0.666472
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 -0.222328 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 2.080244
H -2.734911 2.718667 -1.107484
H -1.599006 2.665978 2.479813
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 3.338853 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 -5.805996
C -2.284921 -2.262063 -7.185575
C -1.583364 -1.170428 -7.697398
C -1.052623 -0.205524 -6.835339
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 -9.005428
C -4.965694 -1.716393 -0.032445
C -5.946185 -1.123904 0.793688
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 5.451064 -1.498461
C -4.264018 5.980234 -1.713641
C -5.315780 5.130193 -2.056603
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 -5.236643
C -2.678066 2.740071 -4.976949
H 0.647265 3.507736 -5.150628
H -0.189769 5.690742 -5.673798
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 -7.505805
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 2.342723
C -0.142773 3.700513 2.015342
C -0.086488 4.968102 0.670502
C -0.793427 6.029131 3.034312
C -1.545531 5.828057 0.827680
C -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 -3.264233
C 3.985754 -3.428173 -2.104212
C 3.012852 -2.976015 -1.203315
H 2.025175 -0.165254 -2.814816
C 3.770595 -0.938980 -4.422627
H 5.010486 -3.037743 -3.958217
H 4.546727 -4.334480 -1.894495
H 2.842345 -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 3.260503
C 0.616414 -3.579006 1.42118
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 -2.457304 0.174262 3.474106
C -2.615734 -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
H -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 -1.127068 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 2.352525 -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 0.717888 -4.568081 1.652137
C 0.706292 -3.691544 0.564607
H 1.629678 -0.829255 2.142384
H 1.642638 -2.369473 0.472497
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 0.267129
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 -5.101188 -0.891297 -1.324584
C -4.329452 -0.832498 -0.595236
C -3.122454 -1.106637 -1.280129
C -1.852911 -1.048950 -0.639626
H 0.024436 -1.978288 -3.345542
H -2.104042 -2.057483 -4.403551
H -4.527923 -1.766824 -4.373154
H -6.538468 -1.269764 -3.090629
H -6.426602 -0.676226 -0.969760
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 -2.043250
C -1.501098 -1.290917 -0.683156
C -0.414777 1.500591 0.885777
N 4.233319 0.744344 2.084096
C 4.151076 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 2.859050 1.374125 1.276658
H 6.264474 -1.529454 0.686155
H 4.376765 1.30325 3.172222
H 5.014244 1.019333 -1.789470
H 5.835013 -0.447594 -2.357525
H 3.363462 -2.277079 -2.824773
H 4.883600 -2.779940 -2.048430
H 3.357930 -2.957974 -1.184771
C 4.107546 -0.277567 3.135277
H 4.998257 -0.240862 3.770683
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
H 5.305388 2.162106 3.249917
H 4.562578 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 1.256607 -5.558327 -1.626071
C 0.926737 -4.481101 -0.794583
H 0.458652 -2.088553 -3.143602
H 1.034096 -3.994579 -4.645569
H 1.546509 -6.212484 -3.658112
H 1.505588 -6.525820 -1.197764
H 0.947700 -4.610806 0.273467
C 0.924411 -1.782255 4.320001
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 2.761777 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 2.226164 3.219794 -2.398194
H 3.038411 5.568694 -2.467138
H 0.207900 7.253000 -0.945886
H 0.225318 6.604242

H -4.038927 3.425170 -2.737205
C -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
H -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 -1.842961 0.480312 4.899468
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 -1.411413 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
C -3.12205 -0.632824 4.62190
C 0.148564 -0.806981 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 -0.946191
H -2.891916 -5.433266 -1.121565
H -4.102406 -4.148431 -1.244880
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 9.202941 -2.727164 2.351463
H 4.026058 -0.749743 3.345853
H 6.663215 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 -2.862087
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 -2.694442 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 -2.106599
C -2.128977 2.035775 -0.213594
H -1.537471 1.020972 0.594176
H -4.112166 0.654399 2.505561
H -5.088886 2.392681 1.475583
H -4.973647 3.937693 -0.414261
H -3.813412 4.777273 -2.360659
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 -1.564826 -1.289722 -0.713011
C -0.864229 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 3.288602 1.381360 0.905607
H 3.568648 0.282981 2.258554
H 3.352660 -1.661183 0.930889
H 3.853766 0.183465 -2.874993
H 4.091530 1.231922 -1.450294
H 5.368184 0.156469 -1.963700
H 5.343068 -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 6.692422 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 1.023932 -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 3.389589
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 -2.997900
C -1.938875 1.154334 -4.048910
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 -3.768982 1.979427 -4.791398
H -4.157143 3.386125 -2.782304
H -2.554270 3.340893 -0.916609
C -2.175748 -2.190706 -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 -6.633120 0.003625 -0.508862
C -2.322268 -2.89328 -0.388709
H -1.658069 -2.834139 -2.225344
H -3.841531 -2.329114 -3.002753
H -5.877400 -0.985407 -2.901434
H -7.81705 0.758462 -1.854407
H -6.277498 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 0.084699
P 0.050475 -1.452071 0.829321
P 1.359730 1.405347 -0.795857
C -1.197731 -2.028853 2.008532
C 0.400453 -2.777847 -0.411936
C 0.969351 2.389937 -2.267365
C 2.450056 2.369623 0.344343
C 1.604189 -1.163769 1.747879
C 2.409635 0.003876 -1.350727
N -4.616392 -1.146646 -0.951457
C -3.210359 -1.166571 -0.938225
C -2.905585 -0.972605 -2.405939
C -2.933821 -1.935562 -3.348208
C -2.576987 -1.621007 -4.784253
C -3.308016 -3.373819 -3.076941
H -2.606465 -0.363507 -0.357999
H -2.799712 -2.112795 -0.564942
H -2.625485 0.036197 -2.701273
H -3.557989 -3.558640 -2.029754
H -2.494021 -0.404963 -3.369132
H -4.182789 -3.658088 -3.675980
H -4.428181 -1.830082 -5.452376
H -3.743649 -2.246911 -5.127855
H -2.292800 -0.571676 -4.911916
C -5.449906 -0.078417 -1.145184
H -5.282560 0.902669 -0.069827
H -6.503139 -0.339346 -1.012842
H -5.251856 0.023250 -2.213882
C -4.913937 -1.524042 0.787702
H -4.543784 -0.785070 1.527742
H -4.420077 -2.484938 1.016127
H -5.992019 -1.630093 0.923050
C -1.725282 -1.105495 2.911890
C -2.707754 -1.494082 3.830785

C -3.174095 -2.812275 3.826185
C 2.670787 -3.734390 2.902856
C -1.6900082 -3.334132 1.986059
H -1.354426 -0.092555 2.090779
H -3.109817 -0.778934 4.542878
H -3.937361 -3.118421 4.533145
H -3.051359 -4.752028 2.89614
H -1.333272 -4.035894 1.254157
C 0.169027 -2.538729 -1.773796
C 0.483101 -3.510165 -2.729544
C 1.038679 -4.728092 -2.337891
C 1.287340 -4.969665 -0.986718
C 0.981308 -3.998056 -0.028324
H -0.227366 -1.584909 -2.091123
H 0.303167 -3.308586 -3.776251
H 1.287192 -5.479019 -3.108108
H 1.735760 -5.904314 -0.678134
H 1.203980 -4.185819 1.014230
C 0.136486 1.823676 3.234716
C -0.218023 2.548649 -4.378572
C 0.252354 3.855527 -4.536611
C 1.066933 4.437198 -3.562408
C 1.419583 3.701361 -2.423691
H -0.226366 0.817109 -3.092868
H -0.858998 2.104605 -5.134961
H -0.022643 4.241138 -5.421176
H 1.415495 5.458985 -3.684663
H 2.015544 4.163438 -1.656803
C 2.079199 2.540919 1.686012
C 2.926537 3.206643 7.877649
C 4.158287 3.697477 2.144025
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H 3.718933	-5.407821	-2.814217	H -4.827875	0.143994	-0.420477	H -0.735804	-5.460679	-2.081616	H 3.393100	-0.439399	4.585706
H 3.912394	-5.014304	-0.385643	H -3.884310	-2.150920	-2.321805	H 0.254805	-5.771285	0.171221	H 5.639561	0.219766	3.886251
H 3.180532	-2.953805	0.596011	H -4.279926	1.731167	-2.417489	H 0.375614	-3.879863	1.752519	H 7.246804	0.621009	2.127112
N -2.103532	3.282365	0.647243	H -5.924028	1.090668	-2.355369	C -1.232596	1.911644	-2.856680	H 6.594638	0.426951	-0.245462
N -1.985618	3.526253	1.125019	H -5.223974	1.569839	-3.905739	C -1.819062	2.588319	-3.933837	H 4.349602	-0.141496	-0.869010
H -0.936100	3.482473	2.144639	H -3.399041	-0.133638	-5.026310	C -1.276085	3.800915	-4.367471	C 1.158008	-0.365197	-2.817879
H -2.527786	2.744203	2.654824	H -5.071909	-0.655068	-5.193151	C -0.156438	4.339876	-3.727462	C 1.571523	-1.539729	-3.323209
H -2.397216	4.514018	2.382419	H -3.846775	-1.794019	-4.602110	C 0.428481	3.652471	-2.656868	C 2.160691	-2.498993	-2.495022
C -1.399966	4.382352	-0.079210	C -4.214053	-3.080753	0.195571	H -1.648493	0.978049	-2.507753	C 2.580143	-3.730420	-3.024284
H -1.562419	4.265247	-1.152558	H -4.275939	-3.683625	1.085943	H -2.692798	2.181118	-4.432096	C 3.166065	-4.642742	-2.231341
H -0.331613	4.335447	0.130451	H -2.389127	0.445145	0.050618	H -1.730251	4.330407	-5.197869	C 3.704740	-4.380682	-0.869847
H -1.785554	5.365146	0.226414	H -4.020908	-3.533043	-0.761668	H 0.250420	5.292255	-4.056093	C 2.982466	-3.213337	-0.326413
C -3.547797	3.312650	0.260221	H -4.817169	-1.240273	1.641133	H 1.265644	4.090486	-2.143434	C 2.355431	-2.222035	-1.117733
H -4.072905	2.531487	0.808347	H -4.034646	-0.550516	1.967972	C 2.127476	2.864867	1.142685	C 1.925420	-0.975728	-0.579316
H -3.631349	3.123564	-0.811219	H -4.896959	-2.066541	2.344687	C 3.261360	3.509887	1.647193	H 0.730585	0.345808	-3.501476
H -3.991870	4.293057	0.489726	H -5.772463	-0.716608	1.586946	C 4.364722	3.739290	0.824562	H 1.447432	-1.741632	-4.382888
411			C -1.335872	-0.427129	4.133847	C 4.333659	3.317685	-0.505047	H 2.436370	-3.951903	-4.075212
Rh -1.280696	1.106889	0.918191	C -2.040889	-0.647071	5.323602	C 3.206504	2.662117	-1.010759	C 3.886857	-5.591851	-2.646686
P -0.445415	-1.039077	1.585528	C -2.721510	-1.853889	5.509374	H 1.286392	2.671887	1.794574	H 3.846123	-5.131893	-0.248660
P 0.605380	1.531301	-0.822664	C -2.708281	-2.830654	4.509277	H 3.284823	3.823409	2.682002	H 3.149105	-3.058945	0.730770
C -1.283316	-1.416640	3.147891	C -1.996558	-2.602099	3.325207	H 5.245601	4.236149	1.218849	N -2.231216	3.112525	1.026314
C -0.602642	-2.479329	0.232232	H -0.817607	0.506806	3.977385	H 5.190378	3.482307	-1.144646	C -1.920864	3.563841	2.429156
C -0.093224	2.427435	-2.435894	H -2.066921	0.114004	6.098583	H 3.202872	2.317520	-2.036969	H -0.838977	3.634909	2.557399
C 2.083939	2.444446	-0.194147	H -3.274538	-2.028348	6.425890	C 1.810933	-0.793474	3.243120	H -2.321693	2.837653	3.136016
C 1.348294	-0.842729	1.913379	H -3.264047	-3.754622	4.644151	C 3.081720	-0.475756	3.545831	H -2.366395	5.459518	2.617500
C 1.281688	-0.052381	-1.448637	H -2.040802	-3.330786	2.534717	C 4.004009	-0.199714	2.531912	C -1.726258	4.144607	0.066519
N -4.469754	-1.764405	0.287835	C -1.335872	-0.427129	4.133847	C 5.328696	0.140669	2.851123	H -2.030071	3.870786	-0.944602
C -4.449421	-0.823871	-0.713413	C -1.194576	-3.381663	-1.749344	C 6.224001	0.361603	1.874101	H -0.638150	4.198640	0.119414
C -4.245307	-1.152366	-2.092863	C -0.699979	-4.632186	-1.381656	C 5.854133	0.249628	0.526834	H -2.146977	5.129636	3.303591
C -4.464282	-0.313999	-3.144026	C -0.145867	-4.808342	-0.114367	C 4.594972	-0.073173	1.821262	C -3.719793	2.998766	0.853596
C -4.179603	-0.752389	-4.559213	C -0.084973	-3.737849	0.783330	C 3.612143	-0.300335	1.172811	H -4.112563	2.301196	1.591680
C -5.000967	1.087321	-2.590369	H -1.515658	-1.344221	-1.157593	C 2.269274	-0.640718	0.848526	H -3.927140	2.616641	-0.146501
H -2.397749	0.783861	1.958136	H -1.611292	-3.233296	-2.373498	H 1.146688	-1.018406	4.057005	H 4.192110	3.981673	0.979757

3.3 Simple molecules (B3LYP+D3/BS2 level)

N,N,3-trimethylbut-2-en-1-amine (Reactant)	C -2.956892	-0.231040	3.349733	C -0.372419	2.465302	2.951019	H 1.018192	0.694934	0.946928			
N -1.784101	-0.372984	0.116110	C -3.839810	0.833127	3.153341	C -1.044442	3.443943	3.730610	H -1.244859	-1.592889	-1.209283	
C -0.688743	-0.085139	-0.818263	C -4.044054	1.346559	1.870000	C -1.851327	4.386235	3.135237	H 1.029368	-1.603135	-1.096096	
C 0.611315	-0.681709	-0.350531	C -3.356693	0.806666	0.784462	C -2.019027	4.386370	1.729509	H 3.001002	1.651614	-0.253551	
C 1.776705	-0.062004	-0.110648	H -1.571574	-1.597340	2.413956	C -1.386228	3.447021	0.947153	H 2.786500	0.458064	-1.548868	
C 2.988354	-0.842688	0.342669	H -2.793416	-0.627206	3.447640	C -0.544835	2.456177	1.527937	H 1.550724	1.695119	-1.282953	
C 2.019621	1.420634	-0.260522	H -4.365077	1.266258	3.999354	C 0.104785	1.444934	0.744574	H 3.117963	-0.422266	0.262841	
H -0.597287	1.000972	-1.010685	H -4.721546	2.180923	1.717334	H 1.743943	-0.185009	3.269051	H 3.280174	-0.163676	1.499958	
H -0.957600	-0.546037	-1.779678	H -3.493720	1.230397	-0.206632	H 0.619960	1.519259	4.625424	C -0.057044	-1.440769	1.681804	
H 0.557611	-1.758459	-0.181717	C 2.276232	-2.630690	2.550911	H -0.905521	3.436521	4.808517	C 3.043011	-0.456008	1.952545	
H 2.413318	1.838637	0.076359	C 3.154541	-3.385376	3.327325	H -2.358155	5.132817	3.739518	H -0.306047	-0.853743	1.225548	
H 2.781254	1.611756	-1.029509	C 4.521305	-3.383504	3.035819	H -2.655499	5.133889	1.264841	H -3.827328	0.307457	1.130946	
H 1.122966	1.983305	-0.529312	C 5.006395	-2.626050	1.967253	H -1.531927	3.456562	-0.126517	H -3.309606	-1.275363	-0.480439	
H 3.819856	-0.725023	-0.366785	C 4.134140	-1.865814	1.187038	(E)-N,N,3-trimethylbut-1-en-1-amine (Product)	C -1.413187	1.334011	0.499711			
H 3.352913	-0.473080	1.311597	H 1.212896	-2.635453	2.780182	N -1.944311	0.134999	-0.265488	H -1.126566	1.170031	1.552920	
H 2.776383	-1.911898	0.443271	H 2.772022	-3.976661	4.154038	C -0.628603	-0.292086	-0.450723	H -0.587616	1.831853	0.014500	
C -3.077514	-0.052548	-0.469499	H 5.205400	-3.974971	3.637144	C 0.485484	0.177647	0.136357	H -2.275955	2.010491	0.489924	
H -3.221273	-0.624741	-1.393117	H 6.067710	-2.627120	1.736944	C 1.876969	-0.282307	-0.223997	tetrahydrofuran (THF)	O -0.000001	1.251576	-0.000003
H -3.877047	-0.327527	0.227710	H 2.273929	-0.781839	-2.265515	C 2.699972	0.866970	-0.837951	C -1.164210	0.429942	-0.134350	
H -3.193839	1.023962	-0.711615	C 2.956894	-0.231046	-3.349733	C 2.599147	-0.864965	1.005500	C -0.732301	-0.996037	0.231788	
C -1.601478	0.312181	1.389305	C 3.839842	0.833092	-3.153341	H 1.794753	-1.078526	-0.978859	C 0.732304	-0.996034	-0.231790	
H -0.633631	0.040757	1.820337	C 4.044101	1.346486	-1.869961	H -0.542283	-1.078497	-1.200978	C 1.164208	0.429945	0.134354	
H -1.635293	1.417218	1.292779	C 3.356726	0.806586	-0.784435	H 0.427680	0.946378	0.905692	H -1.528401	0.475643	-1.172940	
H -2.389174	0.008686	2.087929	H 1.571541	-1.597333	-2.413987	H 3.610008	-1.206288	0.748997	H -1.951928	0.824119	0.518757	
BINAP-Rh(I)	H 2.793406	-0.627184	-4.347647	H 2.793406	-0.627184	H 2.693399	-0.106090	1.793479	H -1.345724	-1.764120	-0.249425	
Rh -0.000031	-2.460104	-0.000022	H 4.365120	2.266229	-3.999371	H 2.043583	-1.711851	1.423199	H 1.786492	-1.145396	-1.317064	
P 1.546401	-0.952108	-0.440680	H 4.721619	2.180826	-1.717274	H 2.798649	1.695338	-0.124014	H 1.528390	0.475645	1.172947	
P -1.546374	-0.952154	0.440593	H 3.493766	1.230290	0.206669	H 3.711423	0.534753	-1.104907	H 1.951930	0.824125	-0.518746	
C -2.760540	-1.852166	-1.478764	C -1.098200	0.540590	-2.788131	C -2.150447	1.258829	-1.738715	H 1.528390	0.475645	1.172947	
C -2.466758	-0.262137	0.978029	C -0.470770	1.496195	-3.549020	C -2.968186	-0.896770	-0.348741	H 1.951930	0.824125	-0.518746	
C 2.760486	-1.852254	1.478744	C 0.372479	2.465329	-2.950995	H -3.019456	-1.529243	0.555417	trimethylamine (TMA)	N -0.000005	0.000000	-0.375237
C 2.466758	-0.262185	-0.978028	C 1.044525	3.443964	-3.730573	H -3.949395	-0.432651	-0.498371	C -1.384366	0.106386	0.061403	
C -0.912245	0.496969	-1.380088	C 1.851436	4.386226	-3.135190	H -2.766503	-1.547381	-1.206223	H -1.962631	-0.738630	-0.329195	
C 0.912255	0.496929	1.380091	C 2.019143	4.386335	-1.729462	H -1.948197	0.772858	1.774092	H -1.826696	1.029865	-0.329158	
C -2.276307	-2.630612	-2.550935	C 3.863322	3.446992	-0.947118	H -1.553966	2.015684	0.560999	H -1.494662	0.114850	1.165477	
C -3.154636	-3.385269	-3.327354	C 0.544901	2.456178	-1.527914	C -2.269275	1.447472	0.727301	C 6.600049	-1.252081	0.061408	
C -4.521401	-3.383361	-0.335850	H -0.104747	1.444946	-0.744562	(Z)-N,N,3-trimethylbut-1-en-1-amine (Product)	H -1.743956	-0.184920	-3.269056	H 0.120095	1.330400	-0.329279
C -5.006469	-2.625900	-1.067279	H -1.743956	-0.184920	-3.269056	H 0.619932	1.519335	-4.625409	H 0.021433	-0.296909	-0.329082	
H -1.341994	-1.865692	-1.187059	H 0.905599	3.436562	-4.808480	H 0.905599	3.436562	-4.808480	H 0.647950	-1.351764	1.165480	
H -1.212970	-2.635404	-2.780205	H 2.358280	5.132805	-3.739462	H 2.358280	5.132805	-3.739462	C 0.784315	1.145692	0.061406	
H -2.772133	-3.976561	-4.154070	H 2.655637	5.133830	-1.264786	H 2.655637	5.133830	-1.264786	H 0.341629	2.069014	-0.329132	
H -5.205511												

C -2.268675 -4.862329 2.002780
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 H -2.065750 -1.068276 2.756778
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 C 4.774993 -2.344652 -3.159702
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 H -2.002647 -4.382388 3.964434
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 C 1.810369 5.035478 3.191927
 C 1.060659 5.363337 2.061824
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 H 2.657094 3.427717 4.358503
 H 2.191176 5.818501 3.841060
 H 0.858228 6.404071 1.825604
 H 0.006795 4.640273 0.339511
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 C -2.158809 3.779122 -2.112450
 C -1.589334 3.226818 -0.965857
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 H -0.112019 2.399035 -4.455922
 H -2.079689 3.907404 -4.262403
 H -3.035119 4.414068 -2.025946
 H -2.037117 3.422243 0.004477
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 C -1.986419 -0.741049 -3.567313
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 C -4.021408 0.641118 -3.846584
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 C -4.082976 1.108770 -1.083170
 C -3.032740 0.306853 -1.613328
 C -1.994059 -0.243796 -0.789729
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 H -1.985900 -0.948575 -4.634477
 H -3.990053 0.453232 -4.916770
 H -5.790086 1.842518 -3.934998
 H -5.842179 2.252550 -1.476526
 H -4.114892 1.304219 -0.017938
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 C -2.247791 0.457955 3.467084
 C -3.146991 -0.453109 2.862269
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C -2.593561 -1.371329 -3.071382
C -3.330164 -2.330925 -3.815371
C -4.234592 -3.160628 -3.193697
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C -3.738745 -2.140704 -1.048326
C -2.790191 -1.269344 -1.656312
C -2.008416 -0.333906 -0.897295
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H -1.530716 -0.561568 -4.772899
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H -5.157628 -3.713949 -1.310473
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P -0.293707 1.617205 -0.314617
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C -0.005581 -2.464176 1.057058
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C -4.515212 -0.383315 -1.952893
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H -1.768026 -5.388526 -4.555388
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C -2.263350 -0.324563 4.831993
C -3.311312 -1.216444 4.797743
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C -1.670302 0.278157 1.157069
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H -3.737323 -1.595268 5.722207
H -4.657326 -2.353754 5.334012
H -3.718267 -1.513248 1.427724
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P -0.100517 1.555332 0.569640
P -0.430095 -1.468792 -0.603992
C -0.724835 2.780267 1.793023
C -0.805226 2.501123 -0.709614
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C -5.737012 4.443905 -1.125376
H -2.344219 3.216914 0.632222
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C 2.822140 -2.614675 -3.742741
C 3.068999 -3.969448 -3.500032
C 2.480316 -4.594492 -2.400168
C 1.642138 -3.876985 -1.542436
H 1.823284 -0.835198 -3.067553
C 3.276179 -2.120340 -4.596992
H 3.718493 -4.532066 -4.164191
H 2.671081 -5.645775 -2.204695
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C -0.049907 -3.186998 3.094494
C -0.942627 -2.430710 2.843134
C -1.413817 -4.451282 1.546094
C -0.997171 -3.627204 0.502334
H 1.037519 -1.528394 2.249877
H 0.305218 -3.003370 4.103437
H -1.279703 -4.865638 3.657072
H -2.120414 -5.252252 1.351396
H -1.387318 -3.784770 -0.499568
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C -2.970642 -1.059549 2.942766
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C -4.685195 -2.781236 3.016587
C -4.702811 -2.816299 1.601511
C -3.874752 -1.996627 0.868375
C -2.982581 -1.091326 1.510495
C -2.087870 -0.242341 0.775203
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H -3.896042 -2.043420 -0.213798
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C -2.279676 -0.476905 -3.540424
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C -4.399477 0.802388 -3.522755
C -5.403172 1.435061 -2.825836
C -5.353297 1.493323 -1.412195
C -4.303629 0.928982 -0.723309
C -3.246441 0.268183 -1.010649
C -2.127581 -0.311302 -0.724875
H -0.462096 -1.572951 -3.430535
H -2.341163 -0.554333 -4.623018
H -4.430064 0.746323 -4.607851
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TS₄₆₋₄₇
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C -0.478268 2.392605 -1.179087
C 0.225394 -3.021020 -1.861623
C -0.417899 -2.584232 0.971808
C -0.610999 1.100634 1.445537
C -1.617802 -0.894675 -1.075214
N 5.067633 -0.872213 1.231965
C 4.195199 -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 3.672178 -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 4.024321 -0.050290 2.869903
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H 4.821405 -2.642301 2.353200
H 6.512503 -2.134599 2.097600
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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 -3.827805
C 0.204668 -5.320085 -2.634240
C -0.040536 -4.376814 -1.632067
H 0.961876 -1.580442 -3.287284
H 1.367128 -3.248717 -5.070531
H 0.893472 -5.656599 -4.649274
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H -0.426417 -4.706916 -0.673993
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C 0.169984 -3.104953 3.268674
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
H -2.856590 -4.438724 2.464390
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C -0.276250 1.358893 2.804702
C -1.008991 0.828107 3.837702
C -2.144075 0.020957 3.585239
C -2.915689 -0.529501 4.080315
C -4.044311 -1.270611 4.379574
C -4.443687 -1.491840 3.039889
C -3.707503 -0.982961 1.994406
C -2.531601 -0.213622 2.262957
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H 0.557726 2.006419 3.040817
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H -4.633268 -1.681145 5.194603
H -5.338307 -2.073055 2.835044
H -4.023779 -1.173361 0.975713
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C -3.253226 -0.445776 -2.822077
C -3.869759 0.546515 -2.023097
C -4.983758 1.293024 -2.491459
C -5.580273 2.242988 -1.694767
C -5.082334 2.484620 -0.391834
C -3.999831 1.781933 0.087131
C -3.355089 0.793352 -0.709511
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
H -6.434370 2.805940 -2.059923
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 1.520277
C 0.424294 -1.450200 1.147846
C 1.748050 0.863931 -0.932951
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C -4.537782 1.043000 0.693612
C -3.813532 0.414277 -0.760385
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C -2.693586 0.670731 -2.976702
C -3.432235 2.760921 -1.790690
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H -3.957251 -0.612647 -1.081417
H -4.233354 2.854619 -2.539123
H -2.577051 3.341075 -2.143613
H -3.777369 3.220553 -0.863280
H -1.842568 1.182658 -3.436100
H -3.540774 0.773037 -3.671824
H -2.457791 -0.392615 -0.891372
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H -6.895141 -0.892603 0.018622
H -6.302828 -1.647361 1.520322
C -6.092140 0.827251 2.124226
H -5.659627 1.810987 2.057475
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 2.12837

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
H 0.984866 -1.502269 -4.826386
H 2.002677 -3.760412 -4.607224
H 1.782883 -5.015300 -2.474482
H 0.549869 -4.026785 -0.573493
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C -0.131091 4.662944 -3.114346
C 0.157789 5.874244 -2.479164
C 0.539002 5.876271 -1.137451
C 0.643025 4.676153 -0.428621
H -0.283662 2.531859 -2.901137
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H 0.760715 6.813657 -0.635352
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C 0.716940 2.250815 3.926405
C 2.018417 2.727409 4.093693
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C 2.331657 2.726127 1.695799
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H 3.836900 3.335332 3.105201
H 2.969577 2.891638 0.831863
C 0.088926 -1.965603 2.431194
C 0.940458 -1.837700 3.501371
C 2.198669 -1.205694 3.360311
C 3.095073 -1.079614 4.454967
C 4.334965 -0.508263 4.286386
C 4.723925 -0.034537 3.010625
C 3.870547 -0.130095 1.935088
C 2.579316 -0.716155 2.069770
C 1.666330 -0.833010 0.964872
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C 4.631277 -1.525650 -2.969383
C 5.047553 -2.721286 -2.431158
C 5.515157 -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
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H 4.845982 -4.106534 -0.774565
H 3.174917 -2.765442 0.413347

TS₉₅₋₉₆
Rh 1.514008 1.348643 -0.255082
P -0.693470 1.754263 0.369484
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
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C 2.231980 5.007852 -0.998126
C 1.659418 6.064508 -0.125032
C 0.579431 5.629257 0.677698
C 0.079522 4.327238 0.622740
H 2.175333 3.064050 -1.570790
H 3.059310 5.367223 -1.639193
H 2.046200 7.018417 -0.077507
H 1.124118 6.351915 1.346863
H -0.761311 4.051954 1.251447
C -1.123189 1.274705 -2.934906
C -2.093298 1.469762 -3.918950
C -3.205498 2.270529 -3.653920
C -3.343447 2.886743 -2.406771
C -2.374693 2.698199 -1.424155
H -0.261780 0.641594 -3.129398
H -1.983429 0.990469 -4.887500
H -3.964756 2.145869 -4.416741
H -4.211097 3.504509 -2.196427
H -2.493267 3.170958 -0.453676
H -1.934084 -1.938635 -1.989019
C -3.225338 -1.675126 -2.375745
C -4.043248 -0.791064 -1.632635
C -3.560587 -0.464022 -2.049943
C -6.137102 0.400478 -1.313138
C -5.626060 0.969681 -0.121336
C -4.353248 0.670702 0.309295
C -3.518717 -0.212982 -0.432714
C -2.170316 -0.498683 -0.039744
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H -3.629990 -2.143415 -3.269365
H -5.743212 -0.908987 -2.964762
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H -6.245302 1.649184 0.457200
H -3.974225 1.118361 1.220678
C -0.159389 1.661811 2.306982
C -0.566163 1.173827 3.609695
C -1.545012 0.151866 3.693576
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C -2.910656 -1.367198 5.011122
C -3.442952 -1.914907 3.819878
C -3.039184 -1.445653 2.589827
C -2.873227 -0.393115 2.484609
C -1.646713 0.123655 2.198299
H 0.611099 2.421463 1.254788
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
H -3.451172 -1.880302 1.686800

3.5 Associative mechanism (B3LYP+D3/BS2 level)

291
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P 0.322059 -1.073981 -0.975492
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P 1.238468 -1.731798 -2.436002
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 3.222400 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 4.605984
H 5.301084 -0.628474 2.267480
H 3.639530 -1.187065 3.345219
H 3.964113 0.485779 3.820519
C 6.032405 0.477388 -0.708992
H 5.647227 1.341625 -1.287321
H 7.028241 0.238830 -1.096490
H 6.133338 0.773763 0.337506
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H 4.459853 -2.079346 -2.218965
H 6.034888 -1.356824 -2.608847
C 1.508640 -0.846804 -3.497758
C 2.225948 -1.271315 -4.615254
C 2.695294 -2.565649 -4.685300
C 2.443997 -3.467947 -3.632829
C 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
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H 1.546134 -3.742574 -1.701009
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C 1.049378 -3.215254 2.448700
C 0.372856 -4.416560 2.228389
C -0.311378 -4.622557 1.027721
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 -0.806886
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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
C -0.596070 4.021200 2.112405
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C -6.091791 0.194185 -0.487389
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C -2.139700 -0.752266 0.902019
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368
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P 0.291765 -1.525098 -0.717398
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