catalysts

MDPI

Supplementary Materials

Mechanistic Details of the Sharpless Epoxidation of Allylic Alcohols—A combined URVA and Local Mode Study

1. Movies from IRC calculations

Table S1. Movie files of the investigate reactions.

Reaction	File Name
R0	R0-mov.mpg
R1	R1-mov.mpg
R2	R2-mov.mpg
R3	R3-mov.mpg
R4	R4-mov.mpg

Table S2. Cartesian coordinates from end-points of IRC Reactant - R0.

O	-0.89795	-0.18016	-0.90955
H	2.73199	1.13512	-1.24249
C	2.07832	1.53890	-0.46371
H	2.56168	2.42261	-0.03064
C	1.77905	0.51687	0.59392
H	1.14806	1.87755	-0.93446
C	2.18497	-0.75682	0.57807
H	1.16406	0.85931	1.42656
H	2.80223	-1.14778	-0.22768
H	1.93158	-1.44636	1.37794
O	-1.77268	0.00192	0.23973
H	-2.31244	-2.01776	0.24948
H	-0.07140	-0.43469	-0.45545
C	-2.75268	-1.01647	0.15326
H	-3.31406	-0.95422	-0.78634
H	-3.42642	-0.82846	0.99555
TS - R0			
O	0.07586	-0.41914	-0.00965
H	-1.48327	1.44542	1.18038
C	-1.59663	1.39811	0.09377
H	-2.58559	1.78533	-0.17031
C	-1.45034	-0.02217	-0.39383
H	-0.83490	2.03308	-0.36485
C	-1.98003	-1.09937	0.35170
H	-1.50229	-0.11554	-1.47964
H	-2.12376	-1.00326	1.42154
H	-2.11248	-2.07945	-0.09237
O	1.91001	-0.08986	-0.66992
H	2.65924	-0.70587	1.18647
H	0.35145	-1.14137	-0.59730
C	2.64575	0.14008	0.47416
H	2.33481	1.04440	1.02915
H	3.69738	0.30938	0.16864
Product - R0			
O	0.77619	-0.66694	-0.36371
H	3.01680	0.72660	-0.87509

C	2.15298	1.38818	-0.76628
H	2.47190	2.29871	-0.24745
C	1.05041	0.70819	0.00020
H	1.81039	1.67317	-1.76625
C	1.30563	-0.38257	0.94967
H	0.13852	1.28420	0.15766
H	2.32599	-0.72828	1.10952
H	0.61052	-0.55575	1.76882
O	-1.86220	-0.42045	0.53642
H	-3.25269	-1.50145	-0.60985
H	-1.09122	-0.73801	0.03327
C	-3.00140	-0.47545	-0.29905
H	-2.89671	0.13693	-1.20858
H	-3.84862	-0.08320	0.27157
Reactant - R1			
Ti	-0.18094	1.19313	-0.34195
Ti	0.84864	-1.97070	0.00244
H	-2.29469	-1.65488	0.78534
H	2.87631	1.32133	0.38237
C	-2.13049	-1.12770	-0.16210
C	2.75861	0.28873	0.02414
C	-2.70825	-2.03463	-1.25294
C	3.70166	0.01544	-1.16832
O	-0.76076	-0.82244	-0.29507
O	1.44282	0.03200	-0.36860
C	-2.91719	0.24296	-0.16517
C	3.01558	-0.75783	1.16060
C	-3.84614	0.32414	1.06803
C	2.02549	-0.45172	2.30172
H	-3.55519	0.28524	-1.05918
H	4.06232	-0.75615	1.49978
O	-2.00618	1.29311	-0.19724
O	2.62914	-1.98248	0.63844
O	-3.66698	1.10959	1.98754
O	0.88540	-0.92618	2.19745
N	-4.86356	-0.57617	1.00705
N	2.40520	0.32511	3.33070
O	0.27321	2.44355	-1.67145
O	-0.00392	-3.34699	0.80949
H	-0.09780	-3.46924	1.76197
O	-3.91386	-2.30364	-1.21229
O	3.40151	-0.73241	-2.08875
N	-1.88112	-2.45453	-2.23265
N	4.92038	0.62369	-1.08337
O	-0.18992	1.32147	-2.49422
O	1.09260	-2.53550	-1.70016
H	1.83823	-2.05273	-2.11543
C	-1.33579	1.75263	-3.24643
H	-1.01903	2.50569	-3.97155
H	-2.10496	2.14592	-2.57860
H	-1.68580	0.85144	-3.75677
O	0.38811	2.23083	1.00601
C	0.73857	3.53241	1.41068
H	1.61558	3.46207	2.07653
C	-0.36125	4.27780	2.11966
H	1.06223	4.11043	0.52951
C	-1.59771	3.83165	2.33822

H	-0.06339	5.27217	2.45726
H	-1.94396	2.85514	2.01353
H	-2.31885	4.45721	2.85720
H	-4.86132	-1.29367	0.28345
H	-5.45853	-0.67176	1.81611
H	-0.86941	-2.35566	-2.18051
H	-2.26230	-3.12185	-2.88862
H	5.07306	1.40885	-0.46992
H	5.54630	0.51415	-1.86882
H	3.34681	0.67198	3.41802
H	1.71840	0.58980	4.02339
TS - R1			
Ti	-0.18327	1.16071	-0.34025
Ti	0.68082	-2.04276	0.16432
H	-2.36282	-1.48788	1.10080
H	2.93130	1.10565	0.37566
C	-2.23751	-1.03403	0.11059
C	2.72855	0.07223	0.05917
C	-2.92673	-1.97971	-0.87720
C	3.62493	-0.31045	-1.14108
O	-0.86687	-0.81124	-0.13133
O	1.39191	-0.10689	-0.29404
C	-2.95034	0.37318	0.06251
C	2.94938	-0.94507	1.22844
C	-3.81920	0.59960	1.32222
C	2.01332	-0.53843	2.38350
H	-3.62516	0.40104	-0.80505
H	4.00316	-0.99890	1.54163
O	-1.98197	1.36053	-0.07748
O	2.47296	-2.15920	0.75929
O	-3.59274	1.48118	2.13717
O	0.84464	-0.94391	2.32970
N	-4.85064	-0.28394	1.40205
N	2.47472	0.24135	3.37727
O	0.08238	2.74896	-1.43466
O	-0.23561	-3.32653	1.05471
H	-0.29839	-3.39208	2.01538
O	-4.13659	-2.19233	-0.74074
O	3.25273	-1.06323	-2.03005
N	-2.18634	-2.49609	-1.88048
N	4.88787	0.20728	-1.09998
O	-0.06579	1.18488	-2.31078
O	0.82740	-2.69576	-1.51834
H	1.58351	-2.27612	-1.97963
C	-1.14453	1.31735	-3.22204
H	-0.83262	1.93147	-4.07252
H	-2.02142	1.76365	-2.74291
H	-1.39672	0.30958	-3.57565
O	0.52425	2.13068	1.06589
C	1.17550	3.37207	1.07264
H	1.02477	3.84931	2.05500
C	0.67090	4.28555	-0.01821
H	2.26435	3.24421	0.95208
C	-0.64451	4.36660	-0.35761

H	1.39973	4.89805	-0.54337
H	-1.41359	3.83085	0.18948
H	-0.97033	5.03509	-1.14642
H	-4.91536	-1.05636	0.74046
H	-5.42974	-0.26440	2.22747
H	-1.17053	-2.44220	-1.89853
H	-2.63780	-3.18606	-2.46430
H	5.11917	0.98717	-0.50515
H	5.49075	0.02129	-1.88882
H	3.43569	0.53982	3.41824
H	1.82464	0.58100	4.07223
Product - R1			
Ti	-0.14939	1.06874	-0.41259
Ti	0.86534	-2.09863	-0.03491
H	-2.22004	-1.74375	0.80727
H	2.90849	1.15300	0.44094
C	-2.10218	-1.23159	-0.15486
C	2.79097	0.12678	0.06416
C	-2.72096	-2.15732	-1.20510
C	3.74594	-0.13238	-1.12196
O	-0.73644	-0.93060	-0.35714
O	1.47792	-0.11507	-0.34226
C	-2.88209	0.13964	-0.14264
C	3.02947	-0.94005	1.18511
C	-3.79022	0.24637	1.10440
C	2.04047	-0.63775	2.32813
H	-3.52974	0.19302	-1.02877
H	4.07472	-0.95875	1.52868
O	-1.95691	1.17553	-0.18004
O	2.62987	-2.15073	0.64027
O	-3.61662	1.08407	1.97956
O	0.88777	-1.07486	2.21022
N	-4.78122	-0.68216	1.10742
N	2.44228	0.09955	3.37919
O	-1.23469	4.33741	-0.16845
O	-0.02442	-3.45391	0.77114
H	-0.11887	-3.56498	1.72501
O	-3.92451	-2.42458	-1.11540
O	3.44933	-0.85719	-2.06162
N	-1.92696	-2.60163	-2.19933
N	4.96976	0.46169	-1.01004
O	0.08327	1.78424	-2.02409
O	1.11428	-2.66810	-1.73332
H	1.86800	-2.19618	-2.14467
C	-0.67647	2.50222	-2.97878
H	-0.16740	3.44306	-3.21426
H	-1.67292	2.72897	-2.58582
H	-0.76382	1.90574	-3.89436
O	0.48773	2.20607	0.85755
C	0.79820	3.55499	1.07210
H	1.23696	3.66928	2.07591
C	-0.39061	4.49174	0.96960
H	1.55597	3.88849	0.34324
C	-1.78794	4.07329	1.14475
H	-0.12498	5.52867	1.19940
H	-2.04614	3.03436	1.33258
H	-2.51290	4.81455	1.48051

H	-4.79802	-1.41201	0.39587
H	-5.38272	-0.73600	1.91518
H	-0.91808	-2.48011	-2.19462
H	-2.32911	-3.26905	-2.84191
H	5.12885	1.22323	-0.36930
H	5.60812	0.35812	-1.78608
H	3.39632	0.40564	3.48221
H	1.76770	0.34886	4.08895
Reactant - R2			
Ti	0.29535	0.97325	0.70677
Ti	-0.91487	-1.82482	-0.64310
H	2.20573	-1.26766	-1.49853
H	-2.80243	1.43065	0.29420
C	2.12159	-1.15428	-0.41107
C	-2.71061	0.33505	0.27450
C	2.72205	-2.42886	0.18882
C	-3.55795	-0.30544	1.39601
O	0.77694	-0.89423	-0.07361
O	-1.38089	-0.06971	0.42388
C	2.97569	0.08524	0.07469
C	-3.11694	-0.26165	-1.11438
C	3.81358	0.64128	-1.09921
C	-2.22918	0.40335	-2.18547
H	3.67832	-0.24641	0.85098
H	-4.18974	-0.13630	-1.32350
O	2.12073	1.04420	0.60616
O	-2.73732	-1.59463	-1.07869
O	3.59941	1.72799	-1.62004
O	-1.10826	-0.08775	-2.37567
N	4.79430	-0.21813	-1.48069
N	-2.68427	1.48020	-2.84998
O	-0.10692	1.71668	2.38139
O	-0.17506	-2.82060	-1.96068
H	-0.16977	-2.58160	-2.89562
O	3.90829	-2.67974	-0.05285
O	-3.23932	-1.35035	1.94664
N	1.94263	-3.18546	0.98615
N	-4.72248	0.34929	1.67569
O	0.30348	0.39389	2.86799
O	-1.05735	-2.96521	0.75456
H	-1.74999	-2.65267	1.37420
C	1.44977	0.57271	3.70928
H	2.25890	1.06011	3.16003
H	1.73712	-0.44101	4.00215
H	1.16607	1.15611	4.58890
O	-0.12457	2.33247	-0.38193
C	0.58469	3.30717	-1.12756
H	1.65371	3.04847	-1.13354
C	0.37923	4.70415	-0.61240
H	0.24109	3.25022	-2.17295
C	-0.32328	5.04534	0.46751
H	0.88072	5.47103	-1.20391
H	-0.81649	4.29708	1.08019
H	-0.40889	6.08167	0.77951
H	-4.85048	1.31588	1.41875
H	-5.27390	-0.00479	2.44489
H	-3.59897	1.86509	-2.67672

H	-2.06419	1.96496	-3.48318
H	0.93898	-3.04363	1.07648
H	2.33436	-4.06006	1.30585
H	4.81212	-1.16328	-1.09955
H	5.32545	0.00585	-2.30866
TS - R2			
Ti	-0.17232	1.12375	-0.42410
Ti	0.70636	-2.04925	0.17185
H	-2.35912	-1.43659	1.06886
H	2.90024	1.14821	0.46739
C	-2.22277	-1.05211	0.05117
C	2.72875	0.11401	0.13300
C	-2.90071	-2.06329	-0.87535
C	3.66442	-0.24259	-1.04450
O	-0.85028	-0.84194	-0.18950
O	1.40511	-0.08473	-0.25916
C	-2.94481	0.34569	-0.10213
C	2.92737	-0.91365	1.29752
C	-3.79481	0.66286	1.14965
C	1.94402	-0.53730	2.42389
H	-3.63381	0.29893	-0.95719
H	3.97029	-0.95100	1.64691
O	-1.98912	1.32487	-0.33617
O	2.49013	-2.13093	0.80022
O	-3.55871	1.60229	1.89745
O	0.79235	-0.98368	2.33513
N	-4.82125	-0.21368	1.30953
N	2.34932	0.25197	3.43396
O	0.28373	2.75067	-1.38085
O	-0.20950	-3.35436	1.02889
H	-0.28665	-3.42499	1.98826
O	-4.10549	-2.28791	-0.71352
O	3.32889	-0.99404	-1.94853
N	-2.15734	-2.61724	-1.85436
N	4.91669	0.29596	-0.96301
O	-0.01014	1.26294	-2.39951
O	0.91251	-2.69473	-1.50532
H	1.67061	-2.26615	-1.95351
C	-1.02184	1.60492	-3.32723
H	-1.90787	2.00582	-2.82449
H	-1.29267	0.68481	-3.86253
H	-0.63851	2.33439	-4.04814
O	0.25704	2.00899	1.15079
C	-0.36166	3.25966	1.38679
H	-1.44909	3.12766	1.46287
C	-0.02562	4.21741	0.26838
H	-0.00399	3.66604	2.34750
C	1.19024	4.22141	-0.34840
H	-0.80637	4.88771	-0.08305
H	2.01333	3.63540	0.04309
H	1.41160	4.91399	-1.15139
H	5.11791	1.07450	-0.35560
H	5.54493	0.12647	-1.73561
H	3.28438	0.62424	3.47350
H	1.65841	0.59921	4.08433
H	-1.14680	-2.51878	-1.89792
H	-2.59494	-3.33901	-2.40895

H	-4.89159	-1.03215	0.70626
H	-5.38889	-0.13860	2.13979
Product - R2			
Ti	0.28450	0.77341	0.79472
Ti	-0.92651	-1.97349	-0.65638
H	2.10581	-1.43849	-1.53706
H	-2.79314	1.31238	0.19814
C	2.08879	-1.30192	-0.44953
C	-2.72211	0.21515	0.17457
C	2.74218	-2.55373	0.13856
C	-3.63748	-0.41758	1.24596
O	0.75940	-1.07064	-0.03236
O	-1.40918	-0.21197	0.38426
C	2.93444	-0.03127	-0.04584
C	-3.07144	-0.36535	-1.23682
C	3.67870	0.52085	-1.28127
C	-2.12059	0.29165	-2.25698
H	3.68887	-0.31963	0.69775
H	-4.13051	-0.21938	-1.49713
O	2.07715	0.91301	0.50510
O	-2.71883	-1.70552	-1.18941
O	3.39596	1.58706	-1.81124
O	-0.99288	-0.20405	-2.38275
N	4.65956	-0.31925	-1.70515
N	-2.52773	1.37487	-2.94324
O	1.03484	4.26086	1.75539
O	-0.15684	-2.97071	-1.95701
H	-0.13162	-2.72947	-2.89108
O	3.92548	-2.77888	-0.13677
O	-3.34789	-1.45058	1.83305
N	1.99524	-3.32623	0.95202
N	-4.82290	0.23160	1.43895
O	0.14322	0.89545	2.57277
O	-1.12593	-3.11546	0.72923
H	-1.83258	-2.80609	1.33275
C	0.89321	1.40172	3.66119
H	1.86894	0.90381	3.71712
H	0.34444	1.20768	4.59010
H	1.05031	2.47887	3.54356
O	-0.23764	2.32763	-0.00084
C	0.51675	3.38796	-0.55111
H	1.51419	3.02651	-0.83699
C	0.65291	4.55432	0.40750
H	0.01393	3.75279	-1.46044
C	-0.28039	4.79282	1.51544
H	1.17308	5.41279	-0.02539
H	-1.09149	4.08698	1.68284
H	-0.44419	5.80655	1.88065
H	-4.95330	1.18556	1.14056
H	-5.42880	-0.11948	2.16714
H	-3.46289	1.73935	-2.85847
H	-1.87724	1.83488	-3.56450
H	0.99779	-3.18382	1.07799
H	2.40705	-4.18879	1.27774
H	4.73877	-1.24906	-1.29670
H	5.13554	-0.10057	-2.56721

Reactant - R3			
Ti	-0.10539	1.31133	-0.11779
Ti	0.33372	-2.00448	-0.15056
H	-2.79001	-1.18813	0.47016
H	2.81251	0.68927	1.11406
C	-2.43882	-0.58131	-0.37294
C	2.57731	-0.19833	0.50943
C	-3.05379	-1.20469	-1.63063
C	3.57406	-0.33742	-0.66174
O	-1.02657	-0.53473	-0.35485
O	1.27608	-0.13375	0.00691
C	-2.95952	0.90660	-0.23310
C	2.57043	-1.51548	1.35611
C	-4.02609	1.00671	0.88276
C	1.56428	-1.33106	2.50843
H	-3.43820	1.20533	-1.17602
H	3.57488	-1.78195	1.71765
O	-1.87731	1.74260	0.01808
O	2.02994	-2.48970	0.53110
O	-3.84719	1.63775	1.91667
O	0.37184	-1.55466	2.26006
N	-5.16019	0.32316	0.58459
N	2.00463	-0.92987	3.71371
O	0.73123	2.46143	1.11017
O	-0.82766	-3.31384	0.30569
H	-1.02716	-3.58184	1.21108
O	-4.28608	-1.25099	-1.71957
O	3.24138	-0.75428	-1.76523
N	-2.22111	-1.63157	-2.59948
N	4.86345	-0.01972	-0.35525
O	0.17766	1.53182	2.10263
O	0.64447	-2.27577	-1.91632
H	1.50324	-1.88807	-2.17945
C	-0.77504	2.24549	2.91509
H	-0.26490	3.07696	3.40864
H	-1.10408	1.50523	3.64966
H	-1.63189	2.56916	2.32340
O	0.39432	2.00599	-1.67695
C	1.30480	2.08548	-2.74593
H	1.84546	1.13169	-2.83337
C	2.29605	3.21038	-2.61094
H	0.73164	2.21970	-3.67629
C	2.37450	4.07056	-1.59608
H	2.98836	3.28800	-3.45026
H	1.69122	4.02364	-0.75406
H	3.12289	4.85735	-1.58597
H	-5.18676	-0.28459	-0.23408
H	-5.87888	0.26694	1.29015
H	-1.21425	-1.70227	-2.47704
H	-2.64481	-2.09540	-3.39040
H	5.08592	0.54036	0.45310
H	5.53906	-0.04849	-1.10587
H	2.98093	-0.75907	3.89327

H	1.33350	-0.72631	4.44041
TS - R3			
Ti	-0.10539	1.31133	-0.11779
Ti	0.33372	-2.00448	-0.15056
H	-2.79001	-1.18813	0.47016
H	2.81251	0.68927	1.11406
C	-2.43882	-0.58131	-0.37294
C	2.57731	-0.19833	0.50943
C	-3.05379	-1.20469	-1.63063
C	3.57406	-0.33742	-0.66174
O	-1.02657	-0.53473	-0.35485
O	1.27608	-0.13375	0.00691
C	-2.95952	0.90660	-0.23310
C	2.57043	-1.51548	1.35611
C	-4.02609	1.00671	0.88276
C	1.56428	-1.33106	2.50843
H	-3.43820	1.20533	-1.17602
H	3.57488	-1.78195	1.71765
O	-1.87731	1.74260	0.01808
O	2.02994	-2.48970	0.53110
O	-3.84719	1.63775	1.91667
O	0.37184	-1.55466	2.26006
N	-5.16019	0.32316	0.58459
N	2.00463	-0.92987	3.71371
O	0.73123	2.46143	1.11017
O	-0.82766	-3.31384	0.30569
H	-1.02716	-3.58184	1.21108
O	-4.28608	-1.25099	-1.71957
O	3.24138	-0.75428	-1.76523
N	-2.22111	-1.63157	-2.59948
N	4.86345	-0.01972	-0.35525
O	0.17766	1.53182	2.10263
O	0.64447	-2.27577	-1.91632
H	1.50324	-1.88807	-2.17945
C	-0.77504	2.24549	2.91509
H	-0.26490	3.07696	3.40864
H	-1.10408	1.50523	3.64966
H	-1.63189	2.56916	2.32340
O	0.39432	2.00599	-1.67695
C	1.30480	2.08548	-2.74593
H	1.84546	1.13169	-2.83337
C	2.29605	3.21038	-2.61094
H	0.73164	2.21970	-3.67629
C	2.37450	4.07056	-1.59608
H	2.98836	3.28800	-3.45026
H	1.69122	4.02364	-0.75406
H	3.12289	4.85735	-1.58597
H	-5.18676	-0.28459	-0.23408
H	-5.87888	0.26694	1.29015
H	-1.21425	-1.70227	-2.47704
H	-2.64481	-2.09540	-3.39040
H	5.08592	0.54036	0.45310
H	5.53906	-0.04849	-1.10587
H	2.98093	-0.75907	3.89327
H	1.33350	-0.72631	4.44041
Product - R3			
Ti	-0.14828	1.15522	-0.07374

Ti	0.28440	-2.14019	-0.18220
H	-2.77055	-1.38104	0.43175
H	2.70483	0.58462	1.13453
C	-2.46868	-0.73569	-0.40123
C	2.50301	-0.33272	0.56291
C	-3.11939	-1.33102	-1.65105
C	3.59750	-0.56631	-0.50095
O	-1.05699	-0.66402	-0.44292
O	1.25872	-0.26892	-0.07117
C	-3.00702	0.73221	-0.17652
C	2.38535	-1.59132	1.48564
C	-3.96073	0.76348	1.03838
C	1.28008	-1.30900	2.52043
H	-3.57984	1.04410	-1.06017
H	3.34405	-1.85310	1.95721
O	-1.92191	1.57942	-0.00506
O	1.90124	-2.60812	0.67412
O	-3.68084	1.31577	2.09374
O	0.11105	-1.52131	2.16723
N	-5.12358	0.10223	0.79510
N	1.60441	-0.83383	3.73488
O	2.43790	4.00831	-0.52946
O	-0.90385	-3.44131	0.22954
H	-1.14519	-3.71695	1.12216
O	-4.35293	-1.36952	-1.70586
O	3.34712	-1.00000	-1.61817
N	-2.30705	-1.75397	-2.64017
N	4.86826	-0.30477	-0.07937
O	0.37261	1.86438	1.49485
O	0.68314	-2.43985	-1.92111
H	1.54968	-2.05306	-2.15843
C	-0.28247	2.57328	2.53446
H	-0.02032	3.63680	2.47642
H	0.05685	2.18857	3.50506
H	-1.36864	2.44981	2.45662
O	0.41601	2.10505	-1.49887
C	1.50953	2.47022	-2.29331
H	2.29338	1.69958	-2.24253
C	2.10006	3.81200	-1.90585
H	1.18298	2.53225	-3.34238
C	1.37313	4.79643	-1.09620
H	2.85530	4.17311	-2.60980
H	0.37761	4.54978	-0.73516
H	1.59457	5.85737	-1.20957
H	-5.21901	-0.45392	-0.05293
H	-5.76722	-0.02624	1.56117
H	-1.29938	-1.81217	-2.53433
H	-2.73926	-2.21269	-3.42906
H	5.04276	0.27345	0.72811
H	5.60940	-0.39460	-0.75997
H	2.56088	-0.66978	4.00506
H	0.86510	-0.57271	4.37229
Reactant - R4			
Ti	-0.01424	1.24203	0.03810
Ti	0.44762	-2.04657	-0.36595
H	-2.67090	-1.32032	0.43383
H	2.96762	0.52463	1.06205

C	-2.34408	-0.63428	-0.35679
C	2.70291	-0.29529	0.37921
C	-2.99091	-1.13950	-1.65132
C	3.62376	-0.29380	-0.86088
O	-0.93422	-0.57544	-0.36982
O	1.37172	-0.19453	-0.03379
C	-2.87156	0.82904	-0.06654
C	2.75026	-1.69325	1.08202
C	-3.90665	0.82226	1.08276
C	1.80775	-1.63671	2.30117
H	-3.38153	1.20714	-0.96312
H	3.77442	-1.98483	1.35897
O	-1.78577	1.65118	0.22601
O	2.16967	-2.58341	0.19243
O	-3.70817	1.37304	2.15790
O	0.60548	-1.85231	2.10113
N	-5.03837	0.14636	0.76024
N	2.31456	-1.34362	3.51235
O	0.83111	2.27310	1.35927
O	-0.69143	-3.40121	0.01207
H	-0.83291	-3.75850	0.89748
O	-4.22533	-1.19159	-1.70691
O	3.25013	-0.68016	-1.96029
N	-2.18472	-1.45365	-2.68310
N	4.90443	0.11123	-0.61948
O	0.30124	1.25317	2.27411
O	0.68356	-2.13367	-2.15867
H	1.52795	-1.70129	-2.40633
C	-0.63184	1.88874	3.16820
H	-0.11271	2.67629	3.72092
H	-0.94136	1.08576	3.84304
H	-1.50320	2.26067	2.62809
O	0.41506	2.15765	-1.43240
C	-0.09223	3.12813	-2.31799
H	-0.02036	2.72900	-3.34111
C	0.63691	4.44270	-2.24184
H	-1.16177	3.28994	-2.10919
C	1.62335	4.73632	-1.39664
H	0.28611	5.18647	-2.95792
H	1.98047	4.01109	-0.67255
H	2.09465	5.71422	-1.40039
H	-5.08144	-0.38993	-0.10658
H	-5.73766	0.02384	1.47681
H	-1.17344	-1.52913	-2.59725
H	-2.62863	-1.84529	-3.50166
H	5.13387	0.65413	0.19856
H	5.52228	0.18246	-1.41588
H	3.29853	-1.17898	3.65137
H	1.68501	-1.21785	4.29189
TS - R4			
Ti	-0.09396	1.22262	-0.05889
Ti	0.45736	-2.03638	-0.47961
H	-2.59228	-1.52209	0.38181
H	2.79536	0.61771	1.12219
C	-2.35789	-0.74365	-0.35427
C	2.61988	-0.21963	0.43202
C	-3.07315	-1.15454	-1.64352

C	3.67815	-0.22736	-0.69228
O	-0.95792	-0.62659	-0.47469
O	1.34856	-0.14217	-0.13832
C	-2.91155	0.65421	0.13489
C	2.60826	-1.60238	1.16472
C	-3.81671	0.45738	1.37146
C	1.53592	-1.53425	2.26874
H	-3.52526	1.09139	-0.66490
H	3.59849	-1.87164	1.56238
O	-1.84166	1.49578	0.41649
O	2.14631	-2.51893	0.23241
O	-3.51030	0.84139	2.49281
O	0.36762	-1.77527	1.93482
N	-4.97104	-0.19359	1.06744
N	1.88646	-1.20754	3.52511
O	1.03320	2.75395	0.42451
O	-0.62547	-3.46136	-0.21165
H	-0.79941	-3.86916	0.64539
O	-4.30773	-1.22012	-1.64209
O	3.39541	-0.45087	-1.86161
N	-2.30629	-1.40482	-2.72150
N	4.95727	-0.00288	-0.27477
O	0.48941	1.69285	1.78397
O	0.79116	-2.06108	-2.25659
H	1.60228	-1.56609	-2.48457
C	-0.31333	2.43673	2.69885
H	0.28179	2.64315	3.59571
H	-1.21147	1.85556	2.93489
H	-0.62618	3.38503	2.25259
O	-0.14344	1.90210	-1.77283
C	-0.19981	3.27637	-2.05181
H	-0.13694	3.42904	-3.14142
C	0.92902	4.00184	-1.36042
H	-1.16107	3.70047	-1.72341
C	2.15380	3.43465	-1.18665
H	0.74179	5.00651	-0.98911
H	2.38943	2.47115	-1.62498
H	2.95223	3.97433	-0.69085
H	-5.08368	-0.61403	0.14554
H	-5.57416	-0.46808	1.82809
H	-1.29273	-1.39863	-2.68189
H	-2.76488	-1.73053	-3.55952
H	5.16598	0.34831	0.64619
H	5.68565	0.02066	-0.97347
H	2.83882	-0.99229	3.77240
H	1.15976	-1.05990	4.21151
Product - R4			
Ti	-0.20165	1.12602	0.14156
Ti	0.42120	-2.08459	-0.44919
H	-2.63803	-1.63350	0.35741
H	2.75476	0.59778	1.09494
C	-2.41888	-0.84912	-0.37640
C	2.56720	-0.24858	0.41874
C	-3.09082	-1.29079	-1.67819
C	3.59471	-0.26663	-0.73365
O	-1.01866	-0.67698	-0.46523
O	1.27893	-0.18845	-0.12098

C	-3.03250	0.52639	0.09682
C	2.58516	-1.62133	1.17071
C	-3.94730	0.30555	1.32282
C	1.53827	-1.54547	2.29886
H	-3.64953	0.94258	-0.71099
H	3.58711	-1.87828	1.54516
O	-1.99200	1.39987	0.38596
O	2.10540	-2.55430	0.26276
O	-3.66787	0.70767	2.44404
O	0.36001	-1.77767	1.99358
N	-5.07370	-0.38636	1.00657
N	1.92205	-1.21211	3.54359
O	2.12420	4.37056	-0.41783
O	-0.66951	-3.49497	-0.13658
H	-0.83332	-3.88696	0.72987
O	-4.32235	-1.38858	-1.70044
O	3.30816	-0.62930	-1.86659
N	-2.29760	-1.52377	-2.74267
N	4.86044	0.09470	-0.37309
O	0.33276	1.71827	1.74995
O	0.74058	-2.14637	-2.22661
H	1.57437	-1.68227	-2.44619
C	-0.31892	2.12791	2.94096
H	0.10989	1.58973	3.79633
H	-1.39242	1.91470	2.87990
H	-0.15796	3.20178	3.09394
O	0.20762	2.32624	-1.14714
C	-0.08707	3.67575	-1.40303
H	-0.60833	3.75819	-2.36876
C	1.16280	4.53157	-1.46333
H	-0.76011	4.07907	-0.63175
C	2.48726	3.97179	-1.75337
H	0.96523	5.57151	-1.73781
H	2.58016	2.89853	-1.90470
H	3.24288	4.59353	-2.23359
H	-5.16339	-0.80925	0.08389
H	-5.68323	-0.67124	1.75820
H	-1.28465	-1.54014	-2.67807
H	-2.73701	-1.88702	-3.57608
H	5.03407	0.61985	0.46999
H	5.55340	0.14416	-1.10659
H	2.88796	-1.04830	3.77811
H	1.21883	-1.09852	4.26020