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Unravelling the mechanism of organocatalyzed aminolytic kinetic resolution of α-nitroepoxides: A theoretical study

– Electronic Supporting Information –

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Table S1. Relative energy (kcal/mol) of the statistically accessible transition states.

Transit. State	Rel. Energy[a]
TS-*RS*	0.0
TS-*RS*1	2.7
TS-*RS2*	0.1
TS-*SR*	2.5
TS-*SR*1	3.1
TS-*SR*2	2.9

[a] Energy is referred to TS-*RS*; it includes the electronic component evaluated at the (PCM)M06-2X/ma-TZVP-f level and the ZPVE (harmonic approximation) computed at the (PCM)M06-2X/TZVP level.

Equilibrium geometries (Cartesian coordinates, Å) and electronic energies (Hartree, include nuclear repulsion)

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Aniline; Energy = -287.575532; TZVP basis set.
N         -0.058063        2.325795        0.000000
H          0.293950        2.768523        0.835372
H          0.293950        2.768523       -0.835372
C         -0.000264        0.932977        0.000000
C         -0.006146       -1.872749        0.000000
C         -0.004659        0.220325        1.202373
C         -0.004659        0.220325       -1.202373
C         -0.004659       -1.166201       -1.196912
C         -0.004659       -1.166201        1.196912
H         -0.007192        0.761691        2.141503
H         -0.007192        0.761691       -2.141503
H         -0.005322       -1.698666       -2.140101
H         -0.005322       -1.698666        2.140101
H         -0.006159       -2.954519        0.000000


Epoxide; Energy = -628.629844; TZVP basis set.
O          1.036338        0.806459       -1.175959
C          1.407276        0.383739        0.087058
C          0.372562       -0.348847       -0.674290
C         -1.070181       -0.234659       -0.338036
C         -3.767507       -0.075084        0.317426
C         -1.763469        0.955761       -0.531159
C         -1.731296       -1.348307        0.173913
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C	-3.076053	-1.266307	0.505143
C	-3.110897	1.032591	-0.203759
H	-1.245743	1.811314	-0.946759
H	-1.192954	-2.279321	0.310393
H	-3.585881	-2.133177	0.905308
H	-3.649480	1.958426	-0.360177
H	-4.817800	-0.012655	0.571629
C	1.191852	1.259506	1.276854
H	1.939314	2.051803	1.299586
H	1.263904	0.680012	2.194051
H	0.200098	1.700079	1.203955
N	2.764321	-0.302713	0.071426
O	3.369443	-0.336119	1.119566
O	3.135526	-0.787457	-0.969449
H	0.694116	-1.270906	-1.150140

PRC, not Catalysed mechanism; Energy = -916.216551; TZVP basis set.

C	0.285479	1.878408	-0.145273
O	-0.241209	1.989578	-1.417495
C	-0.326458	0.704540	-0.785933
H	0.928283	-1.227383	3.030539
N	1.300596	-0.678746	2.268476
H	2.096875	-0.127731	2.556753
C	1.482121	-1.380214	1.072111
C	1.697918	-2.629303	-1.428863
C	0.543629	-2.336337	0.670322
C	2.543903	-1.078758	0.216184
C	2.642825	-1.694515	-1.023420
C	0.656677	-2.954241	-0.565291
H	-0.283223	-2.580921	1.326602
H	3.286628	-0.350809	0.522078
H	3.464461	-1.431343	-1.677596
H	-0.084467	-3.686635	-0.860360
H	1.776503	-3.105368	-2.397070
H	0.348855	-0.031522	-1.218358
C	-1.685239	0.246489	-0.380149
C	-4.215426	-0.642270	0.348794
C	-1.921194	-0.188739	0.920275
C	-2.717206	0.245547	-1.312474
C	-3.981021	-0.199792	-0.947390
C	-3.185896	-0.632908	1.282719
H	-1.109016	-0.167420	1.639351
H	-2.529880	0.601144	-2.318486
H	-4.783023	-0.199884	-1.674483
H	-3.370497	-0.967495	2.295849
H	-5.201356	-0.987820	0.632850
N	1.802301	1.859596	-0.164083
O	2.358962	2.022140	0.903062
O	2.356501	1.658274	-1.214112
C	-0.282448	2.670657	0.988144
H	-1.364302	2.691505	0.876973
H	0.104686	3.689101	0.968046
H	-0.020804	2.205317	1.936374

TS, not Catalysed mechanism; Energy = -916.172730; TZVP basis set.

C	-2.365615	0.175698	0.195993
O	-2.421955	0.673906	1.401483
C	-0.896740	0.183570	0.349979
H	0.153491	-0.183726	-1.960083
N	0.054664	-0.835098	-1.189326
H	-0.631874	-1.553391	-1.409825
C	1.290985	-1.322127	-0.704945
C	3.678137	-2.205356	0.411725
C	2.434828	-0.533698	-0.799977
C	1.334104	-2.542827	-0.035986
C	2.529399	-2.980756	0.515688
C	3.625093	-0.982756	-0.246710
H	2.385121	0.427163	-1.300584
H	0.435238	-3.144534	0.041704
H	2.561296	-3.933441	1.028443
H	4.513959	-0.370366	-0.327908
H	4.608477	-2.551666	0.841961
H	-0.543862	-0.566480	1.047030
C	-0.083103	1.413935	0.255660
C	1.589666	3.638988	0.111675

C	-0.153044	2.277392	-0.838716
C	0.842567	1.666318	1.264974
C	1.670311	2.778732	1.198025
C	0.678443	3.384817	-0.908348
H	-0.844894	2.078557	-1.647628
H	0.904002	0.989839	2.108684
H	2.380757	2.969263	1.991885
H	0.618023	4.049646	-1.760383
H	2.236409	4.505223	0.055474
N	-2.842130	-1.364608	0.149566
O	-2.518652	-2.029523	-0.828901
O	-3.498327	-1.779550	1.062203
C	-3.133172	0.837990	-0.928769
H	-2.922331	1.904667	-0.905897
H	-4.199088	0.700788	-0.741765
H	-2.882138	0.418209	-1.902673

CP, not Catalysed mechanism; Energy = -916.250147; TZVP basis set.

C	-0.648102	-2.243740	-0.555251
O	-0.824653	-3.166548	0.197748
C	-0.369028	-0.844748	0.015025
H	0.378569	-0.139166	-1.779454
N	0.634853	-0.162678	-0.797807
H	2.054657	-1.229890	-0.636913
C	1.104158	1.113582	-0.375800
C	2.167931	3.582644	0.376390
C	1.760393	1.914416	-1.311202
C	0.980826	1.555058	0.938189
C	1.516898	2.784256	1.304662
C	2.284891	3.140149	-0.936720
H	1.864203	1.565754	-2.332887
H	0.464249	0.959179	1.677787
H	1.414354	3.117322	2.329535
H	2.790349	3.750384	-1.674291
H	2.578939	4.539405	0.669641
H	0.054736	-1.019998	1.004293
C	-1.703661	-0.124584	0.154116
C	-4.200617	1.087698	0.422980
C	-2.086227	0.892992	-0.712798
C	-2.580241	-0.532219	1.158264
C	-3.822015	0.070701	1.292375
C	-3.330799	1.497476	-0.577601
H	-1.409973	1.239913	-1.485073
H	-2.284963	-1.329845	1.830779
H	-4.494461	-0.251825	2.076987
H	-3.615740	2.294126	-1.252847
H	-5.168170	1.561185	0.529210
N	2.629879	-1.960988	0.978109
O	2.759632	-1.883594	-0.375887
O	3.407476	-2.697360	1.452568
C	-0.736836	-2.385125	-2.051425
H	-1.319699	-1.568179	-2.483706
H	-1.194008	-3.339362	-2.298357
H	0.268775	-2.354661	-2.479474

Most stable aniline:epoxide binary complex; Energy = -916.219000; TZVP basis set.

C	-0.343375	-2.088062	0.285458
O	0.325850	-2.710368	-0.747387
C	0.331099	-1.281854	-0.754043
H	-3.279393	0.003052	-0.338302
N	-2.677362	0.525093	-0.960622
H	-3.143470	0.773726	-1.820295
C	-1.939776	1.544494	-0.364581
C	-0.328708	3.521472	0.805815
C	-1.575739	1.460315	0.984269
C	-1.483108	2.630211	-1.118603
C	-0.688844	3.606547	-0.534301
C	-0.782131	2.442643	1.557279
H	-1.927678	0.621974	1.574552
H	-1.756001	2.703549	-2.165075
H	-0.348574	4.440923	-1.135227
H	-0.512473	2.360931	2.603038
H	0.290593	4.284515	1.258071
H	-0.319580	-0.839782	-1.504841
C	1.628096	-0.607008	-0.482986

C	4.029191	0.695098	0.040478
C	1.665488	0.782485	-0.408255
C	2.795365	-1.344042	-0.304818
C	3.993498	-0.691386	-0.045581
C	2.863327	1.429834	-0.140739
H	0.757611	1.356171	-0.547521
H	2.759847	-2.423793	-0.378199
H	4.900818	-1.266938	0.086656
H	2.881696	2.510530	-0.075762
H	4.964118	1.201325	0.244710
N	-1.845400	-2.164383	0.101950
O	-2.522854	-1.773654	1.034371
O	-2.275008	-2.565396	-0.946908
C	0.093338	-2.259560	1.704134
H	1.179704	-2.216382	1.734643
H	-0.241840	-3.222209	2.089835
H	-0.316267	-1.464344	2.322659

Catalyst, conformer 1; Energy = -1821.419884; 6-31G(d) basis set.

C	3.837375	0.581700	0.201048
C	4.613279	-1.681083	-0.647491
C	5.897799	0.390821	-1.250253
C	5.488684	-1.008858	-1.702848
C	4.670884	1.238333	-0.907270
C	3.399554	-0.818635	-0.288039
H	5.203108	-1.851143	0.265188
H	6.543941	0.316204	-0.365384
H	4.928801	-0.937486	-2.644574
H	4.052226	1.357864	-1.807761
H	2.788866	-0.671002	-1.190918
H	4.497991	0.445532	1.075184
H	4.262453	-2.657914	-0.996242
H	6.481679	0.890035	-2.029943
H	6.371042	-1.624743	-1.902651
H	4.988594	2.237616	-0.597001
N	2.647725	1.367250	0.618188
N	2.588003	-1.566724	0.675564
H	3.035798	-2.352272	1.132086
C	2.430681	1.265622	2.065065
H	3.206130	1.810820	2.626920
H	2.443888	0.220559	2.377451
H	1.454442	1.691538	2.318155
C	2.635517	2.778812	0.237487
H	2.709737	2.894370	-0.844280
H	3.441272	3.356878	0.716819
H	1.682833	3.210505	0.559118
C	1.233011	-1.615351	0.744031
S	0.468726	-2.864071	1.573705
N	0.624075	-0.554910	0.141169
H	1.238256	0.278760	0.065140
C	-0.746538	-0.286866	0.033095
C	-3.445112	0.437307	-0.260909
C	-1.713180	-1.267246	-0.205956
C	-1.135241	1.054177	0.100522
C	-2.469835	1.405015	-0.048645
C	-3.045296	-0.891862	-0.338952
H	-1.426825	-2.307708	-0.285970
H	-0.387209	1.821903	0.278778
H	-4.488420	0.711890	-0.367775
C	-4.080627	-1.966560	-0.525197
C	-2.855291	2.856412	-0.032956
F	-5.175643	-1.498501	-1.142320
F	-4.083472	3.038232	0.469398
F	-2.001611	3.589571	0.698040
F	-2.856346	3.380467	-1.269271
F	-3.608903	-2.986793	-1.254948
F	-4.478559	-2.474844	0.649940

Catalyst, conformer 2; Energy = -1821.419838; 6-31G(d) basis set.

C	3.837876	0.587310	0.187677
C	4.617591	-1.694556	-0.605069
C	5.909627	0.361779	-1.242621
C	5.502275	-1.046906	-1.668013
C	4.681035	1.217798	-0.928549
C	3.402384	-0.823220	-0.272993

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H           5.200424       -1.845223        0.315523
H           6.548347        0.305609       -0.351054
H           4.950142       -0.995521       -2.615600
H           4.069903        1.317217       -1.836590
H           2.797077       -0.695329       -1.182486
H           4.491187        0.470222        1.069928
H           4.268102       -2.678463       -0.934795
H           6.500690        0.843320       -2.028006
H           6.385372       -1.668214       -1.846760
H           4.997028        2.223734       -0.638665
N           2.646042        1.383177        0.577354
N           2.584702       -1.548999        0.702415
H           3.029653       -2.323635        1.179929
C           2.636738        2.784968        0.162054
H           2.717448        2.874383       -0.921707
H           3.439379        3.374694        0.632383
H           1.682004        3.224647        0.466257
C           2.418244        1.316489        2.024526
H           3.190341        1.873600        2.579250
H           2.426900        0.279022        2.361728
H           1.440890        1.749850        2.259914
C           1.229500       -1.595681        0.765334
S           0.461321       -2.825635        1.619742
N           0.622925       -0.549412        0.136074
H           1.237058        0.282695        0.043452
C          -0.747823       -0.284410        0.019625
C          -3.444878        0.431159       -0.312860
C          -1.712952       -1.271170       -0.202446
C          -1.137825        1.056769        0.051327
C          -2.472282        1.403445       -0.114689
C          -3.043432       -0.899866       -0.355634
H          -1.424460       -2.312581       -0.259568
H          -0.389223        1.830423        0.200911
H          -4.485182        0.703172       -0.448788
C          -4.075559       -1.978574       -0.536643
C          -2.862526        2.850753       -0.020867
F          -5.163625       -1.521675       -1.173942
F          -4.000624        3.104365       -0.679425
F          -3.049570        3.231728        1.252331
F          -1.910777        3.651229       -0.527565
F          -3.595091       -3.010431       -1.243904
F          -4.486742       -2.467811        0.642173

Catalyst, conformer 3; Energy = -1821.413796; 6-31G(d) basis set.
C          -4.646333       -0.082922        0.177417
C          -2.860857        0.175048        1.912124
C          -5.118909        1.255550        2.260011
C          -3.617700        1.348252        2.539943
C          -5.396696        1.124109        0.759003
C          -3.133485        0.109312        0.401264
H          -3.190827       -0.772491        2.356154
H          -5.527342        0.376735        2.776809
H          -3.229356        2.290880        2.129933
H          -5.077816        2.040309        0.243970
H          -2.839993        1.071984       -0.055125
H          -4.929464       -0.968574        0.766755
H          -1.788646        0.257835        2.115925
H          -5.636361        2.131074        2.665131
H          -3.430761        1.373994        3.618024
H          -6.471724        1.011987        0.580429
N          -4.934744       -0.436790       -1.210967
N          -2.445306       -0.985793       -0.265841
H          -3.047400       -1.592625       -0.816174
C          -6.271848       -0.981994       -1.385475
H          -7.070052       -0.230267       -1.266191
H          -6.439459       -1.783549       -0.660304
H          -6.357188       -1.405295       -2.390480
C          -4.673462        0.623230       -2.173622
H          -3.640128        0.971423       -2.087014
H          -5.348835        1.487892       -2.063226
H          -4.802397        0.220139       -3.181912
C          -1.127008       -1.134300       -0.489336
S          -0.535082       -2.469815       -1.328049
N          -0.346128       -0.115138       -0.005500
H          -0.822828        0.750022        0.218060
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C	1.058213	-0.015639	-0.031837
C	3.842304	0.310099	0.011755
C	1.882350	-1.092505	0.303036
C	1.627202	1.222398	-0.326067
C	3.009137	1.377554	-0.294239
C	3.260095	-0.918676	0.307666
H	1.446060	-2.049942	0.558058
H	0.993325	2.062880	-0.593603
H	4.919261	0.432386	0.026201
C	4.136600	-2.101880	0.613168
C	3.594122	2.738528	-0.544685
F	5.328646	-1.722513	1.096562
F	4.858398	2.666015	-0.978177
F	2.886085	3.420859	-1.457197
F	3.601502	3.481874	0.574259
F	3.570962	-2.912557	1.518179
F	4.371533	-2.837310	-0.482209

Catalyst, conformer 4; Energy = -1821.413686; 6-31G(d) basis set.

C	-3.408276	-0.086818	1.247205
C	-3.064687	1.434981	-0.764650
C	-4.881438	1.956076	0.889299
C	-4.461947	2.024319	-0.579365
C	-4.809239	0.519812	1.411614
C	-2.992126	-0.002440	-0.235797
H	-2.329418	2.048572	-0.221566
H	-4.213832	2.593315	1.485744
H	-5.175932	1.455014	-1.189485
H	-5.537743	-0.095505	0.866532
H	-3.653358	-0.637885	-0.832776
H	-2.713860	0.545628	1.823340
H	-2.772070	1.432853	-1.821114
H	-5.894553	2.350804	1.018062
H	-4.484477	3.057044	-0.941809
H	-5.076292	0.468357	2.471230
N	-3.349981	-1.417663	1.848917
N	-1.642669	-0.526169	-0.413091
H	-0.960307	-0.234749	0.279079
C	-3.945435	-2.477590	1.051898
H	-3.337799	-2.757929	0.173343
H	-4.938294	-2.182804	0.701104
H	-4.064349	-3.367451	1.678857
C	-2.055925	-1.826993	2.364450
H	-1.596634	-1.000871	2.916634
H	-1.350140	-2.168919	1.587084
H	-2.196804	-2.658570	3.064061
C	-1.212281	-1.260881	-1.449044
S	-2.204814	-1.948116	-2.621050
N	0.144560	-1.481326	-1.500567
H	0.418444	-2.182924	-2.177404
C	1.168860	-0.725350	-0.899442
C	3.276467	0.736887	0.241814
C	1.071663	0.662792	-0.760991
C	2.334488	-1.374576	-0.484907
C	3.376067	-0.639692	0.066826
C	2.114018	1.372566	-0.177101
H	0.193368	1.188441	-1.123090
H	2.420408	-2.451057	-0.596637
H	4.087823	1.299761	0.689513
C	1.995528	2.869111	-0.076626
C	4.602781	-1.361239	0.555707
F	2.772059	3.362952	0.895003
F	5.685419	-0.575017	0.512521
F	4.456955	-1.764678	1.826440
F	4.857060	-2.452734	-0.177616
F	2.356553	3.467181	-1.219849
F	0.731772	3.242190	0.178383

Catalyst, conformer 5; Energy = -1821.412910; 6-31G(d) basis set.

C	-3.136841	0.059908	1.160353
C	-3.510674	-0.102226	-1.341660
C	-3.061538	2.152663	-0.270132
C	-2.919856	1.296541	-1.531517
C	-2.464613	1.427705	0.937434
C	-2.944081	-0.807980	-0.103976

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H          -3.328580       -0.728441       -2.220821
H          -2.560791        3.116698       -0.409054
H          -3.402419        1.787969       -2.382565
H          -2.525511        2.036265        1.843190
H          -3.425592       -1.780489        0.015357
H          -2.638076       -0.453772        2.009317
H          -4.595271       -0.025660       -1.204006
H          -4.123187        2.353621       -0.083383
H          -1.854187        1.215828       -1.788344
H          -1.387769        1.288847        0.765340
N          -4.567119        0.213624        1.444164
N          -1.513403       -1.086082       -0.243496
H          -0.882243       -0.531265        0.321454
C          -5.211712       -1.067001        1.714254
H          -4.701334       -1.637452        2.511654
H          -5.254318       -1.687507        0.817015
H          -6.241816       -0.885372        2.029997
C          -4.805788        1.120783        2.559860
H          -4.542345        2.146780        2.294833
H          -4.243658        0.836462        3.468490
H          -5.871019        1.109941        2.801995
C          -0.986091       -2.118313       -0.917959
S          -1.876878       -3.331171       -1.666561
N           0.389531       -2.167078       -0.956598
H           0.758557       -3.042456       -1.305927
C           1.304325       -1.162043       -0.597557
C           3.162383        0.818229        0.125859
C           1.048324        0.184950       -0.870387
C           2.512711       -1.516204        0.009297
C           3.429240       -0.529489        0.349860
C           1.962144        1.157600       -0.485570
H           0.141954        0.470527       -1.393395
H           2.728290       -2.559531        0.218034
H           3.874558        1.582080        0.417960
C           1.648692        2.594330       -0.803596
C           4.699384       -0.919745        1.056252
F           2.007484        2.913597       -2.053637
F           5.700295       -0.078653        0.766996
F           4.541456       -0.902679        2.388030
F           5.091075       -2.155529        0.720249
F           0.330084        2.835911       -0.700327
F           2.283571        3.434482        0.021407

Catalyst, conformer 6; Energy = -1821.416543; 6-31G(d) basis set.
C           3.359816        0.330027        0.211045
C           3.900314       -1.626667       -1.342040
C           5.739004       -0.110419       -0.538899
C           5.230080       -0.962506       -1.701770
C           4.707212        0.959014       -0.176008
C           2.861231       -0.575977       -0.931124
H           4.048364       -2.323396       -0.511929
H           5.922698       -0.755636        0.330639
H           5.101205       -0.323248       -2.586966
H           4.570295        1.620455       -1.042672
H           2.676915        0.059905       -1.807016
H           3.525519       -0.319494        1.078135
H           3.505535       -2.201792       -2.186711
H           6.693398        0.361097       -0.796368
H           5.963779       -1.730183       -1.968588
H           5.067031        1.585041        0.649282
N           2.313571        1.283817        0.603235
N           1.547325       -1.156506       -0.631563
H           0.782103       -0.783605       -1.180159
C           2.431405        1.706801        1.990630
H           3.330933        2.315963        2.187550
H           2.454853        0.826913        2.639848
H           1.554482        2.306814        2.254628
C           2.191751        2.438239       -0.276137
H           2.075682        2.118614       -1.317071
H           3.055256        3.121563       -0.219564
H           1.298326        3.002725       -0.000215
C           1.194503       -1.903391        0.424623
S           2.229800       -2.727416        1.465633
N          -0.165088       -2.032497        0.614815
H          -0.407790       -2.758963        1.277346
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C	-1.170291	-1.093996	0.310307
C	-3.261016	0.708149	-0.185548
C	-0.916821	0.281031	0.293460
C	-2.468736	-1.563486	0.086306
C	-3.498049	-0.663167	-0.147351
C	-1.966615	1.158429	0.035691
H	0.089073	0.657301	0.497670
H	-2.663352	-2.631250	0.091213
H	-4.067471	1.406151	-0.379539
C	-1.661245	2.629143	-0.013561
C	-4.904345	-1.167012	-0.319936
F	-2.768422	3.377728	0.029677
F	-5.586356	-0.423208	-1.201721
F	-4.931238	-2.435736	-0.748584
F	-5.582683	-1.125798	0.836685
F	-0.878059	3.003131	1.012743
F	-1.001407	2.954406	-1.138042

Catalyst, conformer 7; Energy = -1821.415755; 6-31G(d) basis set.

C	4.671061	-0.593239	0.444612
C	3.994243	-0.316591	-1.952042
C	6.434288	-0.169699	-1.300784
C	5.354148	0.307432	-2.275382
C	6.021762	0.076437	0.154799
C	3.611799	-0.005569	-0.503303
H	4.036094	-1.406816	-2.078456
H	6.601424	-1.245764	-1.446830
H	5.266932	1.400728	-2.214331
H	5.943606	1.156896	0.334695
H	3.572024	1.087108	-0.389118
H	4.768730	-1.660654	0.189329
H	3.220622	0.067508	-2.621748
H	7.386039	0.329541	-1.510612
H	5.639210	0.070549	-3.305467
H	6.787016	-0.311525	0.836270
N	4.200005	-0.573953	1.833137
N	2.318946	-0.555271	-0.119122
H	2.372125	-1.093275	0.746320
C	5.024830	-1.384869	2.715163
H	6.021440	-0.951057	2.900272
H	5.157301	-2.381079	2.282673
H	4.522201	-1.491928	3.681255
C	4.010177	0.761553	2.383971
H	3.331404	1.342641	1.752922
H	4.953038	1.321427	2.496481
H	3.553154	0.671271	3.373771
C	1.131821	0.006433	-0.428001
S	0.961618	1.366049	-1.396111
N	0.078452	-0.684995	0.132733
H	0.289674	-1.634611	0.417744
C	-1.292634	-0.383051	0.075928
C	-4.057209	0.098493	0.060299
C	-1.778402	0.915181	0.247998
C	-2.193368	-1.437734	-0.083946
C	-3.561007	-1.191439	-0.081926
C	-3.149758	1.139008	0.223978
H	-1.090659	1.736537	0.402242
H	-1.825634	-2.450312	-0.222453
H	-5.124470	0.287552	0.048938
C	-3.648312	2.552258	0.347074
C	-4.516502	-2.346135	-0.184800
F	-4.921027	2.596156	0.766105
F	-5.668300	-1.987428	-0.766145
F	-3.998440	-3.358312	-0.895265
F	-4.825188	-2.837148	1.026272
F	-2.911053	3.259542	1.215611
F	-3.597170	3.196878	-0.827153

Catalyst, conformer 8; Energy = -1821.410111; 6-31G(d) basis set.

C	3.844888	0.329041	0.140782
C	3.446210	-1.621559	-1.465459
C	5.721712	-0.564425	-1.327340
C	4.708717	-1.249636	-2.244048
C	5.107542	0.670214	-0.666012
C	2.841300	-0.379783	-0.798047

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H          3.688024       -2.360561       -0.695221
H          6.039448       -1.271698       -0.549317
H          4.448028       -0.570902       -3.068682
H          4.860832        1.407153       -1.444167
H          2.602596        0.334455       -1.597842
H          4.131129       -0.381853        0.923073
H          2.695983       -2.069993       -2.127092
H          6.618771       -0.282931       -1.889023
H          5.141852       -2.147661       -2.696674
H          5.818640        1.150441        0.012717
N          3.339551        1.520718        0.819178
N          1.532481       -0.643772       -0.179871
H          0.743709       -0.272267       -0.696148
C          2.595644        2.450627       -0.002682
H          1.571983        2.109970       -0.252852
H          3.123625        2.646442       -0.940505
H          2.497862        3.403441        0.528186
C          2.696789        1.301792        2.100487
H          3.278384        0.590331        2.691927
H          1.665743        0.911667        2.029548
H          2.653568        2.252195        2.644999
C          1.241613       -1.461847        0.842915
S          2.339782       -2.384157        1.725842
N         -0.088496       -1.536186        1.190742
H         -0.288762       -2.283964        1.843117
C         -1.180433       -0.811077        0.675284
C         -3.399160        0.594880       -0.315553
C         -1.130926        0.577669        0.535904
C         -2.354421       -1.491682        0.338136
C         -3.450635       -0.784992       -0.138344
C         -2.229678        1.260799        0.024970
H         -0.243354        1.124743        0.842001
H         -2.397918       -2.572139        0.436092
H         -4.249722        1.135243       -0.714510
C         -2.128476        2.755686       -0.108743
C         -4.721693       -1.530019       -0.445348
F         -3.153573        3.267495       -0.797428
F         -5.464546       -0.886039       -1.353963
F         -4.468561       -2.757840       -0.917604
F         -5.476132       -1.678859        0.652419
F         -2.105743        3.352455        1.090353
F         -0.995405        3.106670       -0.738760

Catalyst, conformer 9; Energy = -1821.407354; 6-31G(d) basis set.
C         -3.424342        0.092829        0.915272
C         -3.530747        1.604622       -1.163907
C         -4.421437        2.434699        1.033052
C         -4.590696        2.472883       -0.485161
C         -4.489561        0.998141        1.555129
C         -3.586138        0.163354       -0.627255
H         -2.546221        2.061515       -0.987809
H         -3.450132        2.874873        1.299345
H         -5.588142        2.096765       -0.749859
H         -5.488615        0.591391        1.347964
H         -4.599474       -0.200271       -0.837825
H         -2.450567        0.511831        1.201524
H         -3.669586        1.580521       -2.249493
H         -5.188446        3.045827        1.519413
H         -4.526848        3.499307       -0.859619
H         -4.350085        0.963036        2.639377
N         -3.472221       -1.243974        1.494954
N         -2.728392       -0.763854       -1.374265
H         -3.194544       -1.437097       -1.968081
C         -4.552592       -2.091123        1.027314
H         -4.391958       -2.482166        0.005864
H         -5.505189       -1.554618        1.048741
H         -4.642358       -2.953138        1.695921
C         -2.216250       -1.977493        1.536956
H         -1.402321       -1.305987        1.827341
H         -1.947401       -2.464410        0.584290
H         -2.292754       -2.762436        2.297618
C         -1.387310       -0.895311       -1.402740
S         -0.672045       -2.132495       -2.292696
N         -0.695907        0.030611       -0.671339
H         -1.207044        0.856534       -0.391318
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C	0.686051	0.078216	-0.403557
C	3.402746	0.298651	0.244355
C	1.421623	-1.064744	-0.083934
C	1.304264	1.328358	-0.377805
C	2.650436	1.429697	-0.047218
C	2.771501	-0.940112	0.221109
H	0.941734	-2.035445	-0.072747
H	0.738537	2.220855	-0.628401
H	4.455524	0.380411	0.491010
C	3.568691	-2.183872	0.503301
C	3.291165	2.785544	0.048091
F	4.613180	-1.928379	1.304691
F	4.581236	2.747355	-0.307911
F	2.675808	3.683552	-0.734037
F	3.244776	3.262400	1.302404
F	2.820933	-3.123831	1.097400
F	4.058492	-2.722531	-0.621835

Catalyst, conformer 10; Energy = -1821.405867; 6-31G(d) basis set.

C	-3.096485	0.041277	1.254772
C	-3.469435	0.264252	-1.305324
C	-3.175939	2.366917	0.044652
C	-2.865773	1.667681	-1.277347
C	-2.690290	1.531376	1.235561
C	-2.961429	-0.611562	-0.150555
H	-3.240626	-0.248459	-2.245598
H	-2.683195	3.344991	0.079601
H	-3.244209	2.253696	-2.121073
H	-3.005112	1.973257	2.186398
H	-3.491428	-1.569808	-0.161779
H	-2.357981	-0.466592	1.889862
H	-4.560956	0.337592	-1.241769
H	-4.251861	2.562399	0.105490
H	-1.776084	1.609233	-1.405754
H	-1.590470	1.576989	1.223215
N	-4.360633	-0.206486	1.946263
N	-1.538860	-0.914397	-0.346142
H	-0.885998	-0.412695	0.245337
C	-5.578927	0.234447	1.289119
H	-5.846055	-0.366734	0.402187
H	-5.499074	1.280766	0.991776
H	-6.406901	0.153146	2.000887
C	-4.498214	-1.586064	2.383273
H	-3.608304	-1.890129	2.942281
H	-4.650976	-2.303307	1.557682
H	-5.362478	-1.662053	3.050641
C	-1.047036	-1.875973	-1.140156
S	-1.985838	-2.973635	-2.002982
N	0.325132	-1.960811	-1.209884
H	0.660120	-2.804899	-1.656934
C	1.276762	-1.044931	-0.728279
C	3.193049	0.761431	0.251483
C	1.082401	0.333550	-0.855872
C	2.452659	-1.515265	-0.138594
C	3.402036	-0.611926	0.325459
C	2.022319	1.217562	-0.342225
H	0.201061	0.712042	-1.363156
H	2.613716	-2.583630	-0.029678
H	3.921223	1.456874	0.652135
C	1.760948	2.691995	-0.486572
C	4.686428	-1.145870	0.899966
F	2.085348	3.133705	-1.708563
F	5.284122	-0.251151	1.695390
F	4.477939	-2.258854	1.616807
F	5.556309	-1.462059	-0.069967
F	0.458323	2.971537	-0.304048
F	2.460302	3.409482	0.399062

Catalyst, conformer 11; Energy = -1821.401022; 6-31G(d) basis set.

C	4.634791	0.198872	0.544939
C	3.087206	-0.362792	-1.464959
C	5.292312	-1.545481	-1.302378
C	3.813621	-1.692863	-1.656708
C	5.469459	-1.032734	0.132422
C	3.179474	0.126435	-0.008925

H	2.033552	-0.461092	-1.749320
H	5.803645	-2.509389	-1.396025
H	3.698638	-2.032259	-2.690832
H	6.518381	-0.801971	0.344383
H	2.759516	1.139808	0.074296
H	4.531472	0.150481	1.636617
H	3.525509	0.394763	-2.124636
H	5.766477	-0.874805	-2.027261
H	3.349315	-2.456932	-1.018886
H	5.195358	-1.856973	0.805194
N	5.326548	1.466237	0.323311
N	2.422645	-0.758909	0.882499
H	2.942335	-1.410773	1.457213
C	5.563890	1.873327	-1.049458
H	4.649205	2.188720	-1.583075
H	6.039497	1.069432	-1.612746
H	6.248882	2.727277	-1.046293
C	4.767196	2.564507	1.090729
H	4.638562	2.264036	2.134636
H	3.793884	2.926687	0.711923
H	5.461536	3.410010	1.061172
C	1.087606	-0.927908	0.965893
S	0.434021	-2.119560	1.960609
N	0.352468	-0.048910	0.217790
H	0.849255	0.745955	-0.165562
C	-1.050834	0.034749	0.106810
C	-3.814330	0.318678	-0.252595
C	-1.851573	-1.096600	-0.064460
C	-1.630900	1.302306	0.083905
C	-3.002563	1.434774	-0.101408
C	-3.221607	-0.939844	-0.228272
H	-1.405398	-2.082372	-0.076635
H	-1.013398	2.186898	0.210261
H	-4.883264	0.427023	-0.401795
C	-4.093450	-2.159140	-0.350133
C	-3.624934	2.802255	-0.074813
F	-5.139026	-1.935256	-1.160514
F	-4.045722	3.128620	1.156065
F	-2.756853	3.750288	-0.457183
F	-4.689863	2.874392	-0.884718
F	-3.419429	-3.208376	-0.837291
F	-4.592565	-2.524304	0.839074

Catalyst, conformer 12; Energy = -1821.404482; 6-31G(d) basis set.

C	-3.089570	-0.009656	1.191811
C	-3.448322	-0.157331	-1.379355
C	-3.282859	2.108767	-0.294203
C	-2.940472	1.276110	-1.528965
C	-2.683445	1.465692	0.957491
C	-2.927476	-0.841316	-0.102123
H	-3.151646	-0.774012	-2.233985
H	-2.891732	3.126496	-0.402094
H	-3.365932	1.725079	-2.432199
H	-2.914706	2.054007	1.851460
H	-3.419905	-1.809005	0.037765
H	-2.360399	-0.419762	1.906004
H	-4.542007	-0.144125	-1.367320
H	-4.371658	2.197091	-0.197718
H	-1.849980	1.279166	-1.665445
H	-1.586620	1.508221	0.858258
N	-4.377704	-0.263489	1.842335
N	-1.490468	-1.104460	-0.250242
H	-0.865562	-0.510054	0.282048
C	-4.509718	0.432557	3.108115
H	-4.737726	1.507964	3.004622
H	-3.582816	0.334670	3.682811
H	-5.319447	-0.024712	3.685614
C	-5.599293	-0.167433	1.063857
H	-5.581473	-0.867618	0.226443
H	-5.822694	0.842512	0.679522
H	-6.432254	-0.462719	1.709836
C	-0.950880	-2.128544	-0.926083
S	-1.830245	-3.359819	-1.659017
N	0.424752	-2.156811	-0.981131
H	0.802243	-3.031381	-1.323446

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C          1.328313       -1.147339       -0.606489
C          3.148116        0.848864        0.163739
C          1.071004        0.196093       -0.895172
C          2.519322       -1.490408        0.039083
C          3.419912       -0.495426        0.399350
C          1.964280        1.177492       -0.485193
H          0.178207        0.470033       -1.447598
H          2.727637       -2.529992        0.272982
H          3.839026        1.619169        0.486691
C          1.641959        2.611735       -0.805144
C          4.722564       -0.888634        1.042307
F          2.280094        3.458063        0.010600
F          5.212121        0.095189        1.807085
F          4.583293       -1.976019        1.812103
F          5.652277       -1.175572        0.120271
F          1.986475        2.927337       -2.060090
F          0.323147        2.847895       -0.690509

Catalyst, conformer 13; Energy = -1821.410107; 6-31G(d) basis set.
C          4.737687       -0.220857        0.730819
C          4.033944       -1.489066       -1.365541
C          6.473417       -1.131869       -0.893199
C          5.411151       -1.256374       -1.984988
C          6.116930       -0.013607        0.088141
C          3.675994       -0.374965       -0.375666
H          4.028390       -2.451154       -0.832351
H          6.545944       -2.084390       -0.349648
H          5.389192       -0.333361       -2.579662
H          6.126286        0.945530       -0.447065
H          3.590463        0.568722       -0.923230
H          4.779961       -1.170757        1.287836
H          3.254254       -1.536665       -2.133687
H          7.457995       -0.943042       -1.333584
H          5.655244       -2.072590       -2.672640
H          6.856002        0.062312        0.891153
N          4.472493        0.827090        1.718045
N          2.369743       -0.623014        0.223843
H          2.363602       -1.268030        1.007137
C          4.048871        2.099821        1.157256
H          3.018488        2.079977        0.758883
H          4.720835        2.409224        0.352289
H          4.093887        2.863862        1.940088
C          3.621171        0.452266        2.832925
H          3.917975       -0.530099        3.214326
H          2.544571        0.429733        2.587722
H          3.753991        1.178162        3.642813
C          1.192373       -0.145660       -0.221013
S          1.050832        0.912303       -1.518395
N          0.119679       -0.619452        0.502300
H          0.293380       -1.433464        1.080965
C         -1.246352       -0.349835        0.283097
C         -3.994233        0.104179       -0.036632
C         -1.724497        0.952531        0.115266
C         -2.143839       -1.415022        0.306397
C         -3.507395       -1.180570        0.155817
C         -3.086522        1.159623       -0.056051
H         -1.037371        1.788826        0.124551
H         -1.779353       -2.431348        0.427851
H         -5.055797        0.283327       -0.162743
C         -3.584594        2.557670       -0.298309
C         -4.449144       -2.347828        0.242480
F         -4.853515        2.706914        0.109460
F         -5.653028       -2.060246       -0.264983
F         -3.970433       -3.413608       -0.416825
F         -4.633964       -2.733718        1.515529
F         -2.840642        3.465677        0.348131
F         -3.550021        2.874245       -1.600289

Catalyst, conformer 14; Energy = -1821.415613; 6-31G(d) basis set.
C          4.674781       -0.561017        0.474336
C          3.985912       -0.454839       -1.933478
C          6.428976       -0.267894       -1.306077
C          5.345259        0.141619       -2.306709
C          6.025345        0.082954        0.130242
C          3.611223       -0.042148       -0.508162
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H          4.024696       -1.551319       -1.984225
H          6.591983       -1.352300       -1.375283
H          5.260858        1.236673       -2.323202
H          5.951056        1.173633        0.234881
H          3.572275        1.055748       -0.472507
H          4.769867       -1.644237        0.297089
H          3.209469       -0.116062       -2.624254
H          7.381022        0.211842       -1.556149
H          5.625072       -0.168408       -3.318661
H          6.793394       -0.258581        0.833274
N          4.211143       -0.439153        1.860002
N          2.320386       -0.562805       -0.080029
H          2.377691       -1.037011        0.821826
C          5.037167       -1.187787        2.794470
H          6.035180       -0.744388        2.946019
H          5.166381       -2.212188        2.432410
H          4.536651       -1.226017        3.766893
C          4.031043        0.934293        2.312396
H          3.346354        1.469137        1.647604
H          4.976640        1.497495        2.371777
H          3.585008        0.919283        3.311235
C          1.132121       -0.019781       -0.418539
S          0.958101        1.277972       -1.466557
N          0.081159       -0.675436        0.187097
H          0.293100       -1.607351        0.524849
C         -1.290532       -0.377859        0.117427
C         -4.056650        0.092904        0.108341
C         -1.778704        0.925802        0.219620
C         -2.189418       -1.443366        0.025487
C         -3.556746       -1.202211        0.027940
C         -3.152242        1.143309        0.201433
H         -1.093138        1.757253        0.322397
H         -1.818947       -2.461402       -0.048042
H         -5.125099        0.277165        0.114177
C         -3.651961        2.559917        0.270103
C         -4.518153       -2.347741       -0.118460
F         -3.572126        3.169629       -0.920806
F         -3.959773       -3.515927        0.229222
F         -5.607984       -2.175726        0.642355
F         -4.943057       -2.474846       -1.384522
F         -4.933323        2.617950        0.659004
F         -2.932902        3.292066        1.133755

Catalyst, conformer 15; Energy = -1821.419814; 6-31G(d) basis set.
C         -3.901494       -0.476224       -1.312382
C         -3.082531       -0.612557       -0.026847
C         -3.136296        0.718436        0.748730
C         -4.588780        1.021963        1.136587
C         -5.460651        1.124203       -0.119288
C         -5.356702       -0.143864       -0.970551
H          3.968279        1.522051       -0.079648
H          2.583152       -2.531370        0.274944
H          0.023172        0.482661       -1.421107
H          0.540640       -3.086440       -0.888994
H         -1.077707       -0.304465        0.325209
H         -3.515207       -1.425865        0.574857
H         -3.840855       -1.403387       -1.886619
H         -3.461906        0.324997       -1.922062
H         -5.794469       -0.987556       -0.419782
H         -5.938322       -0.033128       -1.891405
N         -2.142751        0.736137        1.825945
N         -1.672692       -0.894314       -0.261947
H         -6.502624        1.312355        0.159990
C         -1.173128       -2.070404       -0.669513
H         -5.130947        1.986635       -0.714616
H         -4.971910        0.220670        1.782652
H         -4.636082        1.953139        1.712776
C         -1.814134        2.081536        2.271080
H         -2.807474        1.497368        0.042781
H         -3.331507        0.228432        3.535691
H         -2.681344       -1.142593        2.600030
C          1.161705       -1.139297       -0.561453
S         -2.082351       -3.431061       -1.057517
N          0.199450       -2.145242       -0.739015
H         -1.604124       -0.178575        3.620663
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C          0.954273        0.185834       -0.950764
C          1.959856        1.129277       -0.753587
C          3.188470        0.781386       -0.215797
C          3.398334       -0.551786        0.133871
C          2.403711       -1.502896       -0.021849
C          1.664775        2.550797       -1.144864
H         -0.984414        2.028702        2.982267
H         -2.653866        2.593634        2.769579
H         -1.493491        2.683457        1.416067
C          4.719843       -0.932903        0.742082
C         -2.467928       -0.128953        2.951503
F          5.740586       -0.404161        0.053797
F          4.893961       -2.259885        0.776526
F          4.824857       -0.482124        2.001275
F          2.733039        3.343346       -1.012224
F          1.249885        2.633068       -2.416750
F          0.682629        3.066744       -0.385917

Catalyst, conformer 1; Energy = -1821.970630; TZVP basis set.
C          3.834651        0.571996        0.197631
C          4.599831       -1.687216       -0.655737
C          5.893603        0.374722       -1.248932
C          5.476207       -1.017534       -1.707943
C          4.673139        1.226134       -0.903831
C          3.391935       -0.821827       -0.296162
H          5.187428       -1.859969        0.253643
H          6.536419        0.290646       -0.366773
H          4.917660       -0.938257       -2.645849
H          4.058405        1.352913       -1.801553
H          2.784119       -0.669845       -1.195537
H          4.486495        0.431117        1.072914
H          4.245224       -2.658589       -1.005073
H          6.479115        0.872490       -2.023457
H          6.351916       -1.636273       -1.909226
H          4.995503        2.218188       -0.588411
N          2.648646        1.366021        0.608570
N          2.578046       -1.569758        0.664740
H          3.024332       -2.343332        1.137149
C          2.419882        1.264141        2.053572
H          3.197836        1.795528        2.618528
H          2.413413        0.222459        2.366624
H          1.451778        1.702970        2.301364
C          2.650054        2.777964        0.230029
H          2.729306        2.896839       -0.847767
H          3.456541        3.345179        0.713562
H          1.702992        3.216901        0.547108
C          1.229052       -1.595206        0.753254
S          0.455171       -2.810268        1.628270
N          0.623004       -0.543194        0.136436
H          1.238065        0.286863        0.052936
C         -0.745713       -0.277525        0.032762
C         -3.442848        0.430210       -0.260880
C         -1.705293       -1.260959       -0.199407
C         -1.139939        1.058265        0.093713
C         -2.473825        1.399145       -0.052216
C         -3.035050       -0.893331       -0.335024
H         -1.411974       -2.297481       -0.271841
H         -0.394973        1.826722        0.264392
H         -4.484552        0.699131       -0.367814
C         -4.059891       -1.978254       -0.533300
C         -2.862566        2.851427       -0.034379
F         -5.190152       -1.507793       -1.075409
F         -4.120076        3.031380        0.381638
F         -2.067759        3.572926        0.768569
F         -2.774265        3.403223       -1.256027
F         -3.608063       -2.949683       -1.336673
F         -4.396911       -2.560532        0.626308

Catalyst, conformer 2, SA; Energy = -1821.970681; TZVP basis set.
C          3.841192        0.573440        0.181603
C          4.602870       -1.702545       -0.629462
C          5.899966        0.345919       -1.260828
C          5.480253       -1.053933       -1.693941
C          4.680953        1.205642       -0.931513
C          3.396336       -0.828609       -0.286122
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H           5.190298       -1.859067        0.282975
H           6.542756        0.277096       -0.377331
H           4.921873       -0.991165       -2.633200
H           4.066596        1.317029       -1.831515
H           2.788538       -0.692587       -1.188043
H           4.492485        0.448005        1.059656
H           4.246793       -2.679786       -0.960448
H           6.486255        0.828216       -2.044498
H           6.354970       -1.677707       -1.883707
H           5.005054        2.202737       -0.634351
N           2.656350        1.376975        0.577252
N           2.581309       -1.556748        0.688765
H           3.026682       -2.320599        1.177572
C           2.660513        2.781436        0.171856
H           2.739642        2.879649       -0.907999
H           3.468258        3.356164        0.644338
H           1.714481        3.228133        0.480604
C           2.427341        1.303241        2.023909
H           3.205807        1.844569        2.578661
H           2.419632        0.267876        2.357171
H           1.459702        1.747766        2.263323
C           1.232559       -1.577717        0.778665
S           0.456829       -2.773069        1.679153
N           0.627007       -0.538223        0.140394
H           1.241432        0.290535        0.041403
C          -0.743019       -0.276808        0.036060
C          -3.443560        0.408397       -0.268506
C          -1.696006       -1.272203       -0.194967
C          -1.146837        1.052410        0.091079
C          -2.486331        1.383328       -0.061350
C          -3.024273       -0.916296       -0.335504
H          -1.392697       -2.305501       -0.261188
H          -0.409118        1.829080        0.259783
H          -4.487694        0.667290       -0.381961
C          -4.069147       -1.978487       -0.548783
C          -2.866007        2.837339       -0.023440
F          -4.915773       -1.644154       -1.534953
F          -4.186723        3.017448        0.053923
F          -2.313723        3.466792        1.024956
F          -2.442291        3.487070       -1.120396
F          -3.537753       -3.161574       -0.866621
F          -4.817570       -2.162245        0.549191

Catalyst, conformer 3; Energy = -1821.965053; TZVP basis set.
C          -4.643931       -0.114099        0.153926
C          -2.917386        0.040318        1.954498
C          -5.170382        1.125649        2.280305
C          -3.680321        1.191231        2.609812
C          -5.400117        1.069425        0.769167
C          -3.140577        0.050336        0.437049
H          -3.272696       -0.918949        2.341636
H          -5.600621        0.230200        2.740380
H          -3.273348        2.144034        2.254066
H          -5.056894        2.002783        0.311452
H          -2.825733        1.026542        0.037751
H          -4.955402       -1.022946        0.683835
H          -1.855076        0.099368        2.195547
H          -5.691157        1.983776        2.708375
H          -3.527653        1.167174        3.689830
H          -6.466127        0.976658        0.552501
N          -4.889275       -0.386653       -1.260342
N          -2.437423       -1.016194       -0.260338
H          -3.024887       -1.593248       -0.852722
C          -6.228382       -0.895216       -1.510395
H          -7.011672       -0.134349       -1.379843
H          -6.437917       -1.727664       -0.837798
H          -6.285386       -1.262197       -2.535726
C          -4.573699        0.717717       -2.153376
H          -3.540340        1.037274       -2.015030
H          -5.234311        1.585618       -2.015377
H          -4.675834        0.375819       -3.183428
C          -1.119856       -1.127895       -0.489048
S          -0.501747       -2.389076       -1.420763
N          -0.351018       -0.139589        0.065199
H          -0.831949        0.692985        0.374351
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C          1.051120       -0.023918        0.019037
C          3.825592        0.316788        0.029217
C          1.884924       -1.106650        0.306402
C          1.604740        1.218970       -0.245277
C          2.986084        1.380996       -0.231361
C          3.253515       -0.923777        0.298119
H          1.456255       -2.071102        0.532378
H          0.960616        2.060420       -0.473067
H          4.899996        0.443754        0.032400
C          4.174113       -2.080924        0.579211
C          3.538768        2.751920       -0.507404
F          5.098368       -1.759112        1.497663
F          4.873058        2.766199       -0.539995
F          3.104048        3.233209       -1.681211
F          3.154397        3.634128        0.429639
F          3.521350       -3.153679        1.031628
F          4.843987       -2.456179       -0.519970

Catalyst, conformer 4; Energy = -1821.965115; TZVP basis set.
C         -3.168374        0.093348        1.310150
C         -3.645679        1.036271       -1.000650
C         -5.197766        1.563763        0.894875
C         -5.093272        1.312923       -0.607326
C         -4.623852        0.390190        1.686686
C         -3.081383       -0.142471       -0.207552
H         -3.031997        1.921872       -0.798221
H         -4.645020        2.475376        1.146528
H         -5.710322        0.449415       -0.876563
H         -5.232155       -0.500079        1.497947
H         -3.645464       -1.041150       -0.464154
H         -2.582687        0.992320        1.543197
H         -3.559282        0.809871       -2.065458
H         -6.236665        1.733079        1.183623
H         -5.476576        2.166382       -1.169059
H         -4.661364        0.582274        2.759421
N         -2.630351       -0.983263        2.142997
N         -1.692101       -0.394352       -0.578559
H         -0.994654        0.073804       -0.017094
C         -3.022897       -2.323412        1.741929
H         -2.519446       -2.662280        0.822172
H         -4.099322       -2.376187        1.581068
H         -2.771514       -3.021612        2.541946
C         -1.210877       -0.924034        2.441309
H         -0.914547        0.104158        2.655855
H         -0.569380       -1.318217        1.635840
H         -1.005719       -1.520832        3.332793
C         -1.285834       -1.238864       -1.529396
S         -2.319885       -2.185232       -2.466352
N          0.069782       -1.351779       -1.719296
H          0.328983       -2.126712       -2.312985
C          1.100451       -0.639578       -1.081601
C          3.199068        0.728944        0.166809
C          1.067210        0.745899       -0.971833
C          2.203738       -1.341007       -0.587889
C          3.239425       -0.653562        0.013748
C          2.104851        1.411217       -0.328895
H          0.246026        1.305632       -1.404062
H          2.234289       -2.419272       -0.675144
H          4.007043        1.255921        0.656917
C          2.008967        2.909311       -0.207771
C          4.436706       -1.391210        0.554353
F          3.045600        3.432358        0.448447
F          5.575054       -0.933909        0.016803
F          4.547026       -1.236124        1.880856
F          4.377035       -2.702223        0.309476
F          1.954131        3.497787       -1.409398
F          0.894903        3.270926        0.448191

Catalyst, conformer 5, AS; Energy = -1821.970582; TZVP basis set.
C         -3.881797       -0.260745       -1.369839
C         -3.084016       -0.543088       -0.097589
C         -3.163291        0.677144        0.832216
C         -4.624860        0.903238        1.231878
C         -5.480869        1.148418       -0.012885
C         -5.345046        0.001246       -1.013862
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H          4.000064        1.484120        0.028944
H          2.510422       -2.535181        0.200730
H          0.093561        0.577344       -1.487387
H          0.501721       -2.995820       -1.086480
H         -1.073012       -0.246659        0.262355
H         -3.519352       -1.421860        0.391341
H         -3.794528       -1.107670       -2.048850
H         -3.450545        0.615107       -1.865830
H         -5.773536       -0.909473       -0.582589
H         -5.913525        0.219282       -1.919440
N         -1.671788       -0.802863       -0.347368
N         -2.187322        0.571932        1.920216
H         -6.526034        1.282621        0.271750
C         -1.185393       -1.954355       -0.822328
H         -5.158455        2.080727       -0.488432
H         -4.998991        0.023149        1.764310
H         -4.697275        1.752239        1.914977
C         -1.965949        1.837768        2.601591
H         -2.840735        1.543337        0.239836
H         -3.375915       -0.308741        3.464469
H         -2.577007       -1.447419        2.356231
C          1.162843       -1.086148       -0.641272
S         -2.119504       -3.272331       -1.299541
N          0.183404       -2.058273       -0.886935
H         -1.628060       -0.579615        3.562938
C          0.999678        0.249708       -0.995273
C          2.016525        1.159641       -0.733639
C          3.212040        0.768172       -0.162164
C          3.377597       -0.577066        0.150690
C          2.371475       -1.496341       -0.069268
C          1.773146        2.600070       -1.098235
H         -1.111302        1.739181        3.272054
H         -2.829272        2.160997        3.200719
H         -1.739318        2.614937        1.870824
C          4.675390       -1.005508        0.783078
C         -2.468211       -0.493206        2.873110
F          0.745937        3.111594       -0.400880
F          5.729972       -0.574147        0.079031
F          4.777350       -2.333748        0.882696
F          4.806911       -0.503258        2.019462
F          2.836239        3.371184       -0.860750
F          1.459982        2.735867       -2.393833

Catalyst, conformer 6; Energy = -1821.966323; TZVP basis set.
C          3.396268        0.298461        0.213594
C          3.855572       -1.607094       -1.410266
C          5.735380       -0.127807       -0.638870
C          5.179092       -0.951204       -1.798300
C          4.724668        0.935738       -0.213535
C          2.846317       -0.555556       -0.941078
H          4.019696       -2.322513       -0.603872
H          5.947850       -0.790029        0.206529
H          5.028209       -0.295779       -2.663436
H          4.555900        1.614258       -1.056376
H          2.650490        0.111470       -1.786249
H          3.602107       -0.384032        1.040081
H          3.428439       -2.154134       -2.253307
H          6.678087        0.343639       -0.923179
H          5.892678       -1.719045       -2.102078
H          5.117519        1.538414        0.609256
N          2.377996        1.237342        0.698993
N          1.532316       -1.125638       -0.624877
H          0.767819       -0.755731       -1.170952
C          2.566703        1.582359        2.100081
H          3.486637        2.159059        2.281853
H          2.598688        0.671579        2.699017
H          1.721647        2.185581        2.437567
C          2.232654        2.437336       -0.112231
H          2.071955        2.176692       -1.159982
H          3.102822        3.106473       -0.052070
H          1.360161        2.994725        0.228410
C          1.191151       -1.863480        0.435918
S          2.239573       -2.697004        1.457257
N         -0.162629       -1.982953        0.657861
H         -0.396697       -2.707425        1.321879
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C         -1.174322       -1.061699        0.337290
C         -3.277005        0.704862       -0.200398
C         -0.935789        0.311080        0.293923
C         -2.464937       -1.547098        0.121454
C         -3.498206       -0.664626       -0.134653
C         -1.990819        1.169964        0.013829
H          0.063736        0.695819        0.497451
H         -2.645925       -2.614045        0.149065
H         -4.087572        1.388192       -0.413065
C         -1.698933        2.644620       -0.053171
C         -4.898904       -1.187620       -0.312118
F         -2.809226        3.380800       -0.138761
F         -5.582403       -0.477405       -1.217137
F         -4.911771       -2.463943       -0.711107
F         -5.594389       -1.128594        0.833351
F         -1.024061        3.063954        1.027322
F         -0.940877        2.947212       -1.119813

Catalyst, conformer 7, AA; Energy = -1821.967859; TZVP basis set.
C          4.670824       -0.533343        0.494020
C          3.976732       -0.543497       -1.910632
C          6.414777       -0.307411       -1.302223
C          5.326579        0.048146       -2.314594
C          6.011777        0.105528        0.115239
C          3.602420       -0.070902       -0.506358
H          4.027724       -1.637202       -1.910172
H          6.585016       -1.389154       -1.322616
H          5.231925        1.137156       -2.378520
H          5.926277        1.195430        0.167174
H          3.552862        1.023250       -0.518458
H          4.773580       -1.619429        0.370120
H          3.197735       -0.244747       -2.611301
H          7.358889        0.167063       -1.575973
H          5.604242       -0.303787       -3.309515
H          6.782011       -0.195046        0.828545
N          4.214883       -0.344193        1.874193
N          2.316293       -0.582002       -0.053263
H          2.377476       -1.030186        0.858398
C          5.057808       -1.028811        2.841483
H          6.045123       -0.560366        2.961504
H          5.202832       -2.065668        2.535355
H          4.565435       -1.023896        3.814881
C          4.011971        1.047703        2.252991
H          3.314488        1.531949        1.568551
H          4.945628        1.627031        2.272141
H          3.576004        1.079419        3.252081
C          1.126261       -0.067040       -0.411136
S          0.939328        1.178119       -1.520573
N          0.077361       -0.693912        0.224777
H          0.285754       -1.603577        0.613690
C         -1.290334       -0.389076        0.134481
C         -4.041266        0.124163        0.071684
C         -1.758762        0.924917        0.212458
C         -2.198565       -1.434035        0.041126
C         -3.563327       -1.170098        0.019623
C         -3.118673        1.161681        0.169235
H         -1.060081        1.741488        0.309262
H         -1.843050       -2.456105       -0.021917
H         -5.103590        0.326604        0.048051
C         -3.640995        2.572324        0.218778
C         -4.506582       -2.338090       -0.067974
F         -4.650957        2.691432        1.093917
F         -5.786339       -1.958340       -0.086592
F         -4.290381       -3.067927       -1.172280
F         -4.353777       -3.171881        0.973415
F         -2.701227        3.451920        0.575021
F         -4.119447        2.963425       -0.971400

Aniline:Catalyst, binary complex 1; Energy = -2108.920702; 6-31G(d) basis set.
C          3.749877        0.041752       -0.777463
C          3.664669        1.344595        1.384070
C          5.650643        1.595470       -0.130657
C          5.166810        1.611607        1.319119
C          5.269044        0.286508       -0.828282
C          3.312171        0.021666        0.693529
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H          3.115565        2.159589        0.890947
H          5.193430        2.435121       -0.672425
H          5.693962        0.835300        1.889677
H          5.787961       -0.552472       -0.344902
H          3.845809       -0.781103        1.212479
H          3.259307        0.903351       -1.263392
H          3.319709        1.292692        2.422063
H          6.734856        1.740238       -0.178782
H          5.400390        2.570326        1.793259
H          5.603215        0.314096       -1.870254
N          3.276625       -1.145457       -1.507576
N          1.885656       -0.256689        0.825734
H          1.280365        0.018853        0.043200
C          3.690710       -1.143061       -2.905924
H          4.758228       -1.373759       -3.046997
H          3.490642       -0.160939       -3.348632
H          3.108350       -1.892449       -3.451356
C          3.592195       -2.423649       -0.878915
H          3.143089       -2.488112        0.116538
H          4.675465       -2.607695       -0.791966
H          3.164656       -3.222551       -1.492367
C          1.354809       -0.843190        1.905290
S          2.252748       -1.595526        3.125884
N         -0.014613       -0.864014        2.003913
H         -0.340607       -1.481542        2.736689
C         -0.997687       -0.095481        1.361870
C         -3.088258        1.352297        0.166042
C         -0.759646        1.173592        0.831499
C         -2.292295       -0.625951        1.307009
C         -3.320937        0.103925        0.735666
C         -1.798687        1.861421        0.213345
H          0.221659        1.628825        0.890903
H         -2.481149       -1.622399        1.693888
H         -3.886548        1.898611       -0.324099
C         -1.478192        3.130799       -0.518471
C         -4.711722       -0.463227        0.703425
F         -2.540745        3.936266       -0.628479
F         -5.337614       -0.159771       -0.445495
F         -4.716824       -1.796810        0.827000
F         -5.468329        0.028566        1.696910
F         -0.496547        3.824733        0.072531
F         -1.060379        2.864004       -1.774277
N          0.509815       -0.038692       -1.796678
H          1.418081       -0.493383       -1.939645
H          0.346845        0.724876       -2.444120
C         -0.549122       -0.959602       -1.729519
C         -2.674828       -2.764964       -1.424092
C         -0.341223       -2.203925       -1.116629
C         -1.826412       -0.634575       -2.194471
C         -2.878012       -1.533596       -2.042195
C         -1.398223       -3.093799       -0.967738
H          0.652490       -2.453336       -0.748655
H         -1.992165        0.336002       -2.656514
H         -3.867778       -1.259798       -2.395636
H         -1.222680       -4.052347       -0.487684
H         -3.499668       -3.458191       -1.296885

Aniline:Catalyst, binary complex 2; Energy = -2108.918043; 6-31G(d) basis set.
C         -4.673442       -0.011602       -0.334491
C         -4.066342       -2.413029       -0.822710
C         -6.475385       -1.788277       -0.458801
C         -5.420687       -2.882815       -0.293100
C         -6.026973       -0.488972        0.216763
C         -3.628205       -1.118356       -0.127556
H         -4.128641       -2.230136       -1.904502
H         -6.637926       -1.601039       -1.529326
H         -5.322587       -3.135759        0.771185
H         -5.939124       -0.657415        1.298356
H         -3.522001       -1.331667        0.941355
H         -4.788355        0.131199       -1.422112
H         -3.293049       -3.170120       -0.659370
H         -7.435638       -2.112011       -0.044173
H         -5.729810       -3.796861       -0.810162
H         -6.783023        0.290187        0.072115
N         -4.202382        1.283868        0.181798
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N          -2.331897       -0.667717       -0.605696
H          -2.330776        0.028065       -1.345640
C          -5.075491        2.387408       -0.200528
H          -6.038873        2.387401        0.332768
H          -5.274851        2.342464       -1.276019
H          -4.570774        3.334131        0.018874
C          -3.952829        1.304297        1.620116
H          -3.239937        0.521537        1.896061
H          -4.869124        1.176207        2.217828
H          -3.509280        2.269816        1.883237
C          -1.138136       -1.046536       -0.112640
S          -0.978857       -2.117891        1.177926
N          -0.091342       -0.430316       -0.755728
H          -0.346808        0.415939       -1.265837
C           1.283113       -0.573614       -0.494134
C           4.052568       -0.769911       -0.080433
C           1.872980       -1.821262       -0.275625
C           2.085418        0.568902       -0.530285
C           3.456024        0.460376       -0.325528
C           3.243445       -1.901406       -0.062612
H           1.264394       -2.715947       -0.266967
H           1.639668        1.543385       -0.710361
H           5.120792       -0.847789        0.088145
C           3.874289       -3.253721        0.115482
C           4.290686        1.708585       -0.288581
F           4.999672       -3.183159        0.841962
F           5.558780        1.468380       -0.655138
F           3.809717        2.659877       -1.102419
F           4.336783        2.237108        0.945478
F           3.049387       -4.114192        0.724976
F           4.207429       -3.801947       -1.065369
N          -1.682626        2.263966       -1.204947
H          -2.531653        1.983754       -0.693732
H          -1.915920        2.894472       -1.965863
C          -0.675405        2.775403       -0.363082
C           1.467614        3.600067        1.253581
C          -0.500409        2.233121        0.917486
C           0.228145        3.741514       -0.820531
C           1.290160        4.146168       -0.015550
C           0.562006        2.644872        1.714046
H          -1.184290        1.463244        1.268179
H           0.103017        4.164424       -1.814348
H           1.991263        4.884531       -0.392457
H           0.690433        2.200454        2.696250
H           2.307515        3.903329        1.868580

Aniline:Catalyst, binary complex 3; Energy = -2108.908526; 6-31G(d) basis set.
C          -4.292370        0.176617       -0.667174
C          -3.192402       -1.139032        1.202940
C          -3.524212       -2.216925       -1.058916
C          -2.663634       -2.176524        0.209541
C          -3.693360       -0.820432       -1.667949
C          -3.357683        0.242562        0.563266
H          -2.531787       -1.064875        2.074671
H          -3.084443       -2.899970       -1.795794
H          -2.636760       -3.163337        0.683666
H          -4.287877       -0.859641       -2.584581
H          -3.759786        0.941590        1.295908
H          -4.306143        1.182703       -1.130241
H          -4.180320       -1.449427        1.559315
H          -4.513307       -2.617198       -0.803864
H          -1.622111       -1.936301       -0.047647
H          -2.718105       -0.418927       -1.969129
N          -5.645820       -0.205504       -0.245075
N          -2.053794        0.794378        0.198518
H          -1.366869        0.183001       -0.254205
C          -6.245744        0.822521        0.600654
H          -6.251022        1.814782        0.115482
H          -5.718492        0.912145        1.552372
H          -7.277626        0.541042        0.826029
C          -6.523632       -0.456719       -1.381166
H          -6.219260       -1.355554       -1.922262
H          -6.552650        0.389018       -2.092783
H          -7.538628       -0.624708       -1.012169
C          -1.728074        2.087112        0.336065
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S	-2.814833	3.329831	0.668207
N	-0.394214	2.388116	0.162784
H	-0.222267	3.384242	0.103773
C	0.729467	1.586029	0.432693
C	3.065584	0.092618	0.931380
C	0.679981	0.434764	1.224968
C	1.960296	1.994319	-0.086437
C	3.107307	1.255458	0.173812
C	1.835990	-0.301629	1.443578
H	-0.253317	0.105109	1.665901
H	2.013224	2.879178	-0.714975
H	3.954897	-0.505289	1.088075
C	1.724993	-1.537993	2.290688
C	4.398050	1.723022	-0.435005
F	0.623653	-2.245832	1.981612
F	4.240324	2.022911	-1.737202
F	4.852548	2.835711	0.160779
F	5.363343	0.800181	-0.349615
F	2.781446	-2.346870	2.148148
F	1.629237	-1.234401	3.594730
N	-0.152148	-0.734308	-1.869986
H	-0.229144	-0.014443	-2.584605
H	-0.810697	-1.475277	-2.099487
C	1.170089	-1.240151	-1.780330
C	3.778894	-2.227514	-1.511024
C	2.245264	-0.560988	-2.357202
C	1.409886	-2.420881	-1.068514
C	2.705075	-2.907831	-0.937627
C	3.540223	-1.055414	-2.222743
H	2.068988	0.361588	-2.905681
H	0.577185	-2.946175	-0.607722
H	2.875741	-3.821160	-0.375901
H	4.365764	-0.511781	-2.672265
H	4.789064	-2.609650	-1.405928

Aniline:Catalyst, binary complex 4; Energy = -2108.909837; 6-31G(d) basis set.

C	-3.880287	0.168722	1.054114
C	-3.252100	1.236578	-1.168931
C	-5.097558	2.237253	0.212987
C	-4.578404	1.993794	-1.203712
C	-5.217602	0.920990	0.981628
C	-3.365746	-0.076721	-0.383050
H	-2.475363	1.862018	-0.701598
H	-4.403891	2.905416	0.743141
H	-5.314183	1.400517	-1.762722
H	-5.966307	0.284332	0.490634
H	-4.068287	-0.739383	-0.897981
H	-3.167192	0.841736	1.555247
H	-2.910326	1.002499	-2.184500
H	-6.066717	2.746141	0.184316
H	-4.456402	2.939763	-1.741331
H	-5.564456	1.089586	2.005458
N	-4.006628	-1.010635	1.907579
N	-2.072501	-0.753746	-0.395540
H	-1.331629	-0.280787	0.134892
C	-4.615112	-2.169239	1.271698
H	-3.951899	-2.678071	0.553408
H	-5.525744	-1.875642	0.741804
H	-4.899509	-2.888191	2.047121
C	-2.811497	-1.377072	2.641083
H	-2.468681	-0.523655	3.238806
H	-1.978803	-1.734317	2.009830
H	-3.059961	-2.179479	3.343624
C	-1.747952	-1.766123	-1.210971
S	-2.836082	-2.681149	-2.118421
N	-0.409743	-2.094309	-1.259809
H	-0.236435	-2.968913	-1.739983
C	0.693551	-1.230016	-1.120554
C	2.956959	0.414431	-0.870179
C	0.603555	0.138668	-1.386683
C	1.925218	-1.773273	-0.751809
C	3.042197	-0.952602	-0.644191
C	1.724266	0.942243	-1.234657
H	-0.337270	0.578836	-1.701035
H	1.999703	-2.833977	-0.528954

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H          3.819624        1.055586       -0.736267
C          1.565394        2.415023       -1.481269
C          4.351096       -1.577938       -0.252415
F          1.454868        2.697262       -2.786709
F          5.265744       -0.664284        0.092672
F          4.204185       -2.417691        0.786173
F          4.867479       -2.302295       -1.257590
F          0.445239        2.885761       -0.894105
F          2.594486        3.123632       -1.002874
N         -0.465934        1.079463        1.528258
H         -1.067308        0.715185        2.263480
H         -0.734923        2.043429        1.346526
C          0.901070        0.982735        1.901431
C          3.615337        0.707171        2.533951
C          1.411239       -0.256867        2.296272
C          1.756005        2.085843        1.836004
C          3.106759        1.942482        2.141407
C          2.756162       -0.387755        2.622045
H          0.748176       -1.118725        2.328343
H          1.365037        3.052708        1.530657
H          3.761446        2.806343        2.073086
H          3.140313       -1.357159        2.922695
H          4.668645        0.595755        2.769350

Aniline:Catalyst, binary complex 5; Energy = -2108.908703; 6-31G(d) basis set.
C          3.730957        0.041290       -0.671251
C          3.938971        0.767256        1.763349
C          5.334182        1.866540       -0.015483
C          4.261313        2.087775        1.068093
C          5.206026        0.473650       -0.669942
C          3.350572       -0.279534        0.781546
H          3.235517        0.904877        2.589084
H          5.248112        2.643447       -0.782909
H          4.604658        2.828284        1.796521
H          5.798670       -0.266825       -0.117756
H          3.771261       -1.251104        1.052241
H          3.140194        0.914027       -0.996106
H          4.856143        0.358758        2.203443
H          6.331495        1.968185        0.424471
H          3.345278        2.497536        0.623085
H          5.607697        0.503761       -1.686357
N          3.347241       -1.036389       -1.596082
N          1.897960       -0.391738        0.905261
H          1.326696       -0.064419        0.117363
C          3.708090       -0.730796       -2.976263
H          4.783882       -0.841946       -3.182360
H          3.419424        0.299352       -3.213172
H          3.164397       -1.404042       -3.646426
C          3.798147       -2.374725       -1.231835
H          3.334608       -2.701428       -0.297141
H          4.893459       -2.449223       -1.131957
H          3.482461       -3.067352       -2.017135
C          1.316825       -1.062358        1.908862
S          2.161086       -1.967539        3.060795
N         -0.053198       -1.030173        1.988533
H         -0.416551       -1.694570        2.660125
C         -0.998908       -0.199926        1.369124
C         -3.023209        1.369965        0.214963
C         -0.715021        1.089876        0.917265
C         -2.304772       -0.692020        1.253717
C         -3.300858        0.096733        0.703102
C         -1.721736        1.839846        0.319026
H          0.276722        1.512606        1.021552
H         -2.527473       -1.704957        1.574055
H         -3.795827        1.966926       -0.257325
C         -1.356256        3.143039       -0.327400
C         -4.704439       -0.430309        0.605486
F         -2.382455        4.001309       -0.354937
F         -5.291761       -0.049078       -0.540526
F         -4.747544       -1.767811        0.656692
F         -5.473942        0.028968        1.604808
F         -0.331383        3.746596        0.289085
F         -0.976725        2.950330       -1.608765
N          0.563951        0.013528       -1.744552
H          1.464893       -0.446331       -1.915432
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H          0.420897        0.821211       -2.341452
C         -0.510253       -0.891968       -1.754673
C         -2.663435       -2.683426       -1.604702
C         -0.330712       -2.173923       -1.214655
C         -1.772426       -0.521966       -2.226310
C         -2.837939       -1.414288       -2.151112
C         -1.401031       -3.057083       -1.142758
H          0.653247       -2.459641       -0.845954
H         -1.916363        0.475663       -2.634792
H         -3.815821       -1.106370       -2.509391
H         -1.247609       -4.045144       -0.718273
H         -3.499363       -3.371955       -1.538943

Aniline:Catalyst, binary complex 6; Energy = -2108.905085; 6-31G(d) basis set.
C         -3.877894       -0.543146       -1.117815
C         -3.638632        0.856822        0.976432
C         -3.551793       -1.670893        1.133894
C         -3.075249       -0.345790        1.735818
C         -3.240251       -1.724669       -0.363039
C         -3.343283        0.780870       -0.526457
H         -3.236576        1.794845        1.371126
H         -3.069335       -2.512972        1.641410
H         -3.366325       -0.283125        2.790590
H         -3.556287       -2.674078       -0.802911
H         -3.790270        1.640476       -1.031115
H         -3.573760       -0.590750       -2.185366
H         -4.728461        0.886991        1.089352
H         -4.634071       -1.770282        1.281545
H         -1.975992       -0.314828        1.718294
H         -2.150446       -1.703387       -0.498191
N         -5.340544       -0.575329       -1.018531
N         -1.906519        0.848861       -0.801141
H         -1.474460        0.028580       -1.209365
C         -5.963240        0.517412       -1.757840
H         -5.616291        0.572427       -2.805957
H         -5.771416        1.479636       -1.278679
H         -7.045662        0.369828       -1.763618
C         -5.888718       -1.847302       -1.471674
H         -5.621335       -2.654472       -0.786664
H         -5.550152       -2.121375       -2.488024
H         -6.978904       -1.777500       -1.483911
C         -1.162474        1.963743       -0.747926
S         -1.770992        3.505490       -0.453145
N          0.178773        1.804063       -0.994789
H          0.677153        2.686139       -1.017506
C          0.985694        0.661690       -0.865868
C          2.750083       -1.516142       -0.619985
C          0.617175       -0.469229       -0.129011
C          2.251053        0.700270       -1.458353
C          3.119780       -0.373769       -1.320506
C          1.492257       -1.541313       -0.028862
H         -0.306880       -0.494656        0.434504
H          2.553609        1.576780       -2.023435
H          3.425135       -2.361099       -0.535397
C          1.114769       -2.725866        0.814521
C          4.508197       -0.261178       -1.882893
F         -0.196623       -2.769305        1.080658
F          4.536666        0.487229       -2.994367
F          5.342617        0.316976       -1.002212
F          5.023830       -1.459823       -2.183360
F          1.445182       -3.879053        0.214213
F          1.763603       -2.715432        1.995673
N          0.416899       -0.280539        3.066062
H          0.949691       -1.014893        3.516124
H         -0.373365        0.001302        3.634245
C          1.184571        0.780798        2.577449
C          2.665077        2.835551        1.361401
C          2.538621        0.592846        2.262309
C          0.585358        2.011344        2.285508
C          1.326536        3.030351        1.694010
C          3.263386        1.607172        1.650914
H          3.002485       -0.369328        2.465034
H         -0.470498        2.162860        2.501784
H          0.834614        3.973077        1.470096
H          4.302009        1.430673        1.385626
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H          3.237788        3.629135        0.891895

Aniline:Catalyst, binary complex 7; Energy = -2108.905106; 6-31G(d) basis set.
C          1.346273        2.654316        0.848456
C          0.103781        3.082240       -1.302859
C          0.035943        4.808592        0.516216
C         -0.737570        4.166554       -0.632953
C          0.487916        3.743310        1.516052
C          0.547957        2.006401       -0.297642
H          1.004270        3.526064       -1.748655
H          0.916622        5.328003        0.114340
H         -1.664500        3.722032       -0.244707
H         -0.398995        3.277475        1.966580
H         -0.352679        1.542992        0.125989
H          2.217904        3.144303        0.384973
H         -0.454862        2.604959       -2.113699
H         -0.575200        5.562660        1.023015
H         -1.031587        4.919228       -1.371669
H          1.053352        4.207318        2.331285
N          1.902829        1.660773        1.778941
N          1.373950        0.987395       -0.954799
H          2.386296        1.042476       -0.794630
C          2.891692        2.239711        2.679894
H          2.457940        2.910231        3.439543
H          3.631655        2.806892        2.104758
H          3.408817        1.432221        3.209598
C          0.902358        0.926163        2.541206
H          0.150550        0.504497        1.871413
H          0.386533        1.545509        3.293604
H          1.385803        0.095403        3.065643
C          1.046636        0.320628       -2.078272
S          2.165240       -0.151520       -3.232207
N         -0.298190        0.052632       -2.273699
H         -0.499269       -0.264719       -3.215035
C         -1.205749       -0.370790       -1.283384
C         -3.068065       -1.235481        0.628973
C         -0.768585       -0.986559       -0.104860
C         -2.572032       -0.207647       -1.507791
C         -3.488255       -0.653194       -0.558923
C         -1.699509       -1.387382        0.841967
H          0.292932       -1.150055        0.055001
H         -2.916525        0.262711       -2.424009
H         -3.786371       -1.574375        1.367898
C         -1.239080       -1.971767        2.148504
C         -4.954659       -0.427216       -0.803879
F         -1.919641       -3.080332        2.463466
F         -5.711588       -1.298686       -0.125485
F         -5.330387        0.803752       -0.422813
F         -5.260020       -0.544066       -2.103453
F          0.066561       -2.281663        2.135524
F         -1.423687       -1.101616        3.157224
N          4.109278        0.393363       -0.014720
H          3.739088        0.746499        0.863689
H          5.056719        0.705883       -0.192013
C          3.917777       -0.988485       -0.171510
C          3.407904       -3.714463       -0.593794
C          2.870499       -1.627314        0.503172
C          4.712078       -1.729118       -1.052220
C          4.456320       -3.079719       -1.256988
C          2.619128       -2.979068        0.287607
H          2.259699       -1.048916        1.193659
H          5.515648       -1.233411       -1.590464
H          5.079632       -3.639560       -1.948133
H          1.800744       -3.458063        0.816666
H          3.209179       -4.767856       -0.761372

Aniline:Catalyst, binary complex 8; Energy = -2108.905185; 6-31G(d) basis set.
C          1.348420        2.658207        0.840858
C          0.097536        3.079757       -1.307045
C          0.032290        4.809258        0.508941
C         -0.743962        4.163278       -0.636102
C          0.490546        3.747140        1.509339
C          0.546864        2.006853       -0.301070
H          0.995530        3.524629       -1.756781
H          0.910283        5.329817        0.102709
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H	-1.668292	3.716936	-0.243597
H	-0.393443	3.280612	1.964890
H	-0.352036	1.544095	0.127006
H	2.217797	3.148686	0.373690
H	-0.462963	2.599864	-2.115074
H	-0.578574	5.563008	1.016559
H	-1.042816	4.913821	-1.375029
H	1.058461	4.214452	2.320908
N	1.909610	1.667292	1.771477
N	1.370936	0.986308	-0.958362
H	2.383553	1.040847	-0.800491
C	2.895018	2.250860	2.673299
H	2.457093	2.917619	3.433810
H	3.631553	2.823121	2.098827
H	3.416863	1.445654	3.201789
C	0.912795	0.926109	2.531880
H	0.166102	0.498759	1.860080
H	0.390291	1.541679	3.282789
H	1.400828	0.099036	3.057889
C	1.041333	0.318516	-2.080905
S	2.158346	-0.156533	-3.235214
N	-0.303867	0.052206	-2.274089
H	-0.507209	-0.269628	-3.213381
C	-1.210276	-0.362533	-1.278422
C	-3.064438	-1.188905	0.657498
C	-0.770461	-0.991866	-0.107885
C	-2.575071	-0.166801	-1.483378
C	-3.488283	-0.596171	-0.523422
C	-1.696602	-1.372529	0.851364
H	0.289900	-1.174496	0.038940
H	-2.919872	0.328740	-2.386201
H	-3.779065	-1.500927	1.411572
C	-1.232769	-1.962607	2.154069
C	-4.957911	-0.436574	-0.798801
F	-1.922430	-3.064475	2.472958
F	-5.679510	-0.446065	0.329243
F	-5.216753	0.712990	-1.439315
F	-5.419678	-1.428151	-1.574578
F	0.069322	-2.285844	2.130972
F	-1.401607	-1.091722	3.164897
N	4.106982	0.389660	-0.018403
H	3.729086	0.745812	0.855723
H	5.055061	0.703024	-0.190498
C	3.917472	-0.992393	-0.173212
C	3.412813	-3.720300	-0.591198
C	2.867554	-1.630970	0.497773
C	4.717162	-1.734576	-1.047845
C	4.463896	-3.085973	-1.250533
C	2.618834	-2.983536	0.284371
H	2.252651	-1.052013	1.184057
H	5.523135	-1.239436	-1.583003
H	5.091506	-3.646892	-1.936905
H	1.798562	-3.462257	0.810781
H	3.216191	-4.774356	-0.757040

Aniline:Catalyst, binary complex 9; Energy = -2108.906228; 6-31G(d) basis set.

C	4.461101	0.671075	0.290285
C	4.528689	-1.288789	-1.325685
C	5.428410	-1.561875	1.017770
C	4.766245	-2.264763	-0.169225
C	4.603586	-0.342202	1.434657
C	3.763122	-0.032268	-0.900576
H	3.996471	-1.777661	-2.149213
H	5.534862	-2.254781	1.859749
H	5.377815	-3.105268	-0.513997
H	5.017747	0.134155	2.327559
H	3.697221	0.650912	-1.747260
H	3.801616	1.493998	0.626257
H	5.498004	-0.953235	-1.708894
H	6.436934	-1.242200	0.728203
H	3.810081	-2.696878	0.162053
H	3.591532	-0.666838	1.712387
N	5.758230	1.209257	-0.143918
N	2.384332	-0.364544	-0.557731
H	2.188285	-1.285256	-0.161277

C	5.583542	2.326092	-1.068561
H	5.008679	3.154821	-0.618516
H	5.067848	2.015630	-1.978659
H	6.567397	2.704457	-1.359594
C	6.574602	1.660874	0.975735
H	6.895642	0.820045	1.594720
H	6.048872	2.390486	1.619128
H	7.473954	2.142792	0.583046
C	1.343676	0.479390	-0.685279
S	1.481872	2.049394	-1.280270
N	0.156963	-0.102696	-0.307276
H	0.183163	-1.109792	-0.176721
C	-1.129271	0.455208	-0.246945
C	-3.763164	1.395140	-0.018799
C	-1.371469	1.762941	0.184062
C	-2.207018	-0.380663	-0.549629
C	-3.508420	0.090743	-0.423111
C	-2.681012	2.216897	0.278453
H	-0.545071	2.410304	0.444579
H	-2.024811	-1.401089	-0.878761
H	-4.779755	1.762544	0.069504
C	-2.941594	3.639673	0.686600
C	-4.663460	-0.837228	-0.665649
F	-3.093398	4.441540	-0.377534
F	-5.725957	-0.187570	-1.160906
F	-4.353387	-1.820934	-1.521295
F	-5.071172	-1.425173	0.475706
F	-4.066297	3.742464	1.412695
F	-1.939854	4.141941	1.420287
N	1.210838	-3.008250	0.743101
H	1.546165	-2.897785	1.696791
H	1.739198	-3.757066	0.302952
C	-0.186077	-3.257594	0.697605
C	-2.955185	-3.641020	0.529431
C	-1.033785	-2.708498	1.664945
C	-0.735127	-3.975985	-0.369783
C	-2.110956	-4.169916	-0.444784
C	-2.409643	-2.903149	1.576933
H	-0.612044	-2.127733	2.481756
H	-0.079534	-4.387738	-1.132866
H	-2.524531	-4.735059	-1.274465
H	-3.060532	-2.463795	2.326574
H	-4.027849	-3.779583	0.458774

Aniline:Catalyst, binary complex 10; Energy = -2108.905681; 6-31G(d) basis set.

C	3.828680	-0.303321	0.896013
C	3.487724	-0.607504	-1.602804
C	5.231313	-1.974844	-0.454842
C	4.850318	-1.275274	-1.756226
C	5.200358	-0.976029	0.698899
C	3.422546	0.376397	-0.421701
H	2.718025	-1.379111	-1.443822
H	4.524169	-2.793149	-0.258825
H	5.604932	-0.514553	-1.995855
H	5.927993	-0.174932	0.516563
H	4.095233	1.219390	-0.608389
H	3.082550	-1.102176	1.087454
H	3.211139	-0.056138	-2.508718
H	6.226077	-2.425713	-0.531675
H	4.827691	-1.980663	-2.593271
H	5.501473	-1.462789	1.631501
N	3.929618	0.592821	2.057103
N	2.060766	0.907941	-0.374994
H	1.358969	0.309783	0.078014
C	3.140505	1.813137	2.086332
H	2.049798	1.645191	2.173719
H	3.325803	2.424286	1.200481
H	3.455147	2.390677	2.961419
C	3.774456	-0.132785	3.302700
H	4.414647	-1.017509	3.323931
H	2.732733	-0.470074	3.480409
H	4.058910	0.508945	4.141646
C	1.682935	2.054939	-0.948994
S	2.736828	3.223192	-1.562078
N	0.330568	2.307527	-0.988987

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H          0.113522        3.256725       -1.266304
C         -0.737865        1.393680       -0.972625
C         -2.937763       -0.355538       -0.935499
C         -0.602053        0.079198       -1.425328
C         -1.986620        1.835020       -0.530504
C         -3.071239        0.965934       -0.530565
C         -1.689435       -0.781108       -1.373864
H          0.349812       -0.277426       -1.803450
H         -2.100120        2.850968       -0.163057
H         -3.773069       -1.043015       -0.879239
C         -1.471405       -2.202430       -1.807876
C         -4.400041        1.483465       -0.057104
F         -2.445543       -3.017419       -1.385827
F         -5.251986        0.494498        0.237636
F         -4.267151        2.246041        1.041011
F         -4.987959        2.251644       -0.987718
F         -1.402503       -2.316611       -3.141384
F         -0.306934       -2.679708       -1.322382
N          0.512454       -1.052318        1.419351
H          1.061531       -0.643426        2.173220
H          0.906713       -1.963706        1.198863
C         -0.858360       -1.146685        1.769818
C         -3.593822       -1.253887        2.362441
C         -1.504740       -0.036806        2.320935
C         -1.588201       -2.313053        1.525973
C         -2.949103       -2.359732        1.814911
C         -2.860694       -0.096538        2.621763
H         -0.939421        0.875143        2.499785
H         -1.092840       -3.178322        1.092961
H         -3.504267       -3.269490        1.606424
H         -3.351393        0.774560        3.044395
H         -4.655142       -1.289760        2.584622

Aniline:Catalyst, binary complex 11; Energy = -2108.906110; 6-31G(d) basis set.
C          3.939738       -0.283283       -0.711789
C          3.352662        1.593193        0.904015
C          5.256080        1.925596       -0.667446
C          4.722209        2.237743        0.728036
C          5.302841        0.414351       -0.877903
C          3.361583        0.072692        0.666833
H          2.648959        2.046374        0.188813
H          4.602843        2.388817       -1.420209
H          5.415296        1.842183        1.482001
H          5.983119       -0.039065       -0.145650
H          3.960876       -0.413785        1.443460
H          3.239032        0.131231       -1.467892
H          2.952006        1.769972        1.908800
H          6.254938        2.351343       -0.807962
H          4.649820        3.317817        0.891860
H          5.709406        0.180306       -1.866598
N          4.146230       -1.721670       -0.937617
N          1.985117       -0.395546        0.811986
H          1.383925       -0.346947       -0.024659
C          3.343692       -2.683643       -0.201462
H          2.278713       -2.701340       -0.500345
H          3.394786       -2.505966        0.874849
H          3.756709       -3.679060       -0.394668
C          4.144572       -2.047047       -2.349622
H          4.798078       -1.373317       -2.908472
H          3.135213       -1.988031       -2.806125
H          4.510621       -3.067904       -2.493929
C          1.452923       -0.827949        1.956437
S          2.323115       -1.258839        3.332867
N          0.076065       -0.970154        1.961074
H         -0.251945       -1.495393        2.762658
C         -0.886438       -0.157290        1.341016
C         -2.936548        1.383938        0.179619
C         -0.598000        1.077224        0.759163
C         -2.213893       -0.607728        1.351679
C         -3.217364        0.163923        0.791910
C         -1.619418        1.814226        0.166520
H          0.410520        1.472610        0.763687
H         -2.448468       -1.574353        1.786154
H         -3.720775        1.963352       -0.295006
C         -1.232301        3.044220       -0.599734
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C	-4.643182	-0.308172	0.842293
F	-2.271561	3.852955	-0.828799
F	-5.280530	-0.079492	-0.317162
F	-4.734956	-1.618430	1.103888
F	-5.337737	0.336075	1.793879
F	-0.286562	3.755332	0.029191
F	-0.718464	2.710568	-1.804496
N	0.528861	-0.608699	-1.785324
H	1.231362	-1.253663	-2.143192
H	0.564147	0.242962	-2.341026
C	-0.767815	-1.189560	-1.799058
C	-3.332436	-2.307927	-1.698750
C	-0.966209	-2.448099	-1.220289
C	-1.857702	-0.499356	-2.329858
C	-3.131696	-1.057972	-2.276801
C	-2.240244	-3.002106	-1.178622
H	-0.119926	-2.977656	-0.788998
H	-1.708162	0.484085	-2.768408
H	-3.973436	-0.504106	-2.681235
H	-2.382160	-3.978128	-0.724106
H	-4.329270	-2.733359	-1.646155

Aniline:Catalyst, binary complex 12; Energy = -2108.904403; 6-31G(d) basis set.

C	-3.717939	-0.171390	0.281580
C	-3.996676	-2.695996	0.140804
C	-5.988339	-1.238053	0.624780
C	-5.336237	-2.597726	0.872337
C	-5.049793	-0.106561	1.050644
C	-3.068324	-1.542704	0.548181
H	-4.155839	-2.657562	-0.941143
H	-6.218972	-1.135430	-0.443988
H	-5.178941	-2.731286	1.952029
H	-4.864045	-0.187446	2.130716
H	-2.907335	-1.627078	1.630648
H	-3.943712	-0.122722	-0.789433
H	-3.496760	-3.644499	0.365640
H	-6.937206	-1.162851	1.166111
H	-5.995440	-3.408323	0.545238
H	-5.526701	0.864532	0.879767
N	-2.788389	0.939604	0.542608
N	-1.722288	-1.673415	-0.018159
H	-0.999813	-1.932951	0.642739
C	-3.301401	2.205263	0.023534
H	-4.166997	2.587230	0.587825
H	-3.593902	2.076657	-1.023176
H	-2.507918	2.959216	0.068179
C	-2.411692	1.089006	1.943608
H	-1.915858	0.185372	2.312221
H	-3.266302	1.314375	2.600852
H	-1.699441	1.913783	2.033035
C	-1.338152	-1.563510	-1.297915
S	-2.357557	-1.379294	-2.630458
N	0.014647	-1.657172	-1.515718
H	0.250284	-1.682992	-2.500442
C	1.070471	-1.338428	-0.639808
C	3.271209	-0.718408	0.989473
C	0.933533	-0.418975	0.408613
C	2.311280	-1.933827	-0.869716
C	3.399294	-1.610087	-0.065918
C	2.027889	-0.132837	1.213091
H	-0.016682	0.077373	0.575868
H	2.420573	-2.657340	-1.672193
H	4.115706	-0.489519	1.629857
C	1.900693	0.858328	2.337161
C	4.731628	-2.235499	-0.374375
F	2.412805	2.052509	2.015345
F	5.573666	-2.152938	0.662741
F	4.600649	-3.532163	-0.692532
F	5.322467	-1.637391	-1.418990
F	0.618767	1.056786	2.688349
F	2.554025	0.435785	3.429221
N	-0.630280	1.408992	-1.679218
H	-1.294806	1.143145	-0.950331
H	-1.022657	1.273055	-2.603635
C	0.049939	2.600805	-1.471437

C	1.547059	4.947127	-1.021544
C	0.341061	3.031968	-0.167409
C	0.524560	3.367872	-2.546594
C	1.261085	4.523918	-2.318654
C	1.080353	4.188642	0.049600
H	-0.008321	2.442233	0.677073
H	0.308700	3.047131	-3.562724
H	1.613903	5.101827	-3.168408
H	1.299755	4.489898	1.070003
H	2.123399	5.849963	-0.849024

Aniline:Catalyst, binary complex 13; Energy = -2108.901756; 6-31G(d) basis set.

C	-4.189509	0.114336	-0.882903
C	-3.189061	-1.173337	1.130710
C	-3.332961	-2.367601	-1.075717
C	-2.509744	-2.179021	0.202159
C	-3.680921	-1.039473	-1.772036
C	-3.392645	0.186030	0.450018
H	-2.603053	-1.029412	2.046227
H	-2.792584	-3.008507	-1.784151
H	-2.386932	-3.138850	0.714948
H	-4.418846	-1.205290	-2.563975
H	-3.907394	0.869132	1.130279
H	-3.942283	1.046659	-1.406277
H	-4.163935	-1.566975	1.437786
H	-4.244873	-2.916066	-0.817159
H	-1.493950	-1.834803	-0.034719
H	-2.777863	-0.667865	-2.272765
N	-5.646808	0.153618	-0.768500
N	-2.075458	0.779982	0.209194
H	-1.368270	0.205567	-0.260415
C	-6.310029	-0.956859	-0.112201
H	-6.175105	-0.973520	0.984124
H	-5.967248	-1.908444	-0.522207
H	-7.386082	-0.882436	-0.303583
C	-6.141919	1.418619	-0.251043
H	-5.645051	2.249702	-0.758172
H	-5.984252	1.547634	0.834197
H	-7.218865	1.482637	-0.440744
C	-1.774708	2.070264	0.404693
S	-2.889253	3.289504	0.731151
N	-0.438601	2.391524	0.299382
H	-0.272669	3.390124	0.285610
C	0.685659	1.579021	0.530965
C	3.020580	0.060082	0.957150
C	0.633478	0.384994	1.258159
C	1.918845	2.015166	0.041038
C	3.064962	1.262998	0.265543
C	1.788146	-0.363243	1.439572
H	-0.301905	0.031638	1.675747
H	1.975024	2.933285	-0.537624
H	3.910139	-0.544508	1.084182
C	1.672066	-1.647428	2.211977
C	4.357138	1.762652	-0.314398
F	0.567863	-2.332037	1.860712
F	4.208889	2.101324	-1.608378
F	4.792758	2.861509	0.319759
F	5.331226	0.847895	-0.247714
F	2.724743	-2.451356	2.021807
F	1.576882	-1.421867	3.531670
N	-0.154998	-0.645430	-1.899914
H	-0.246453	0.091824	-2.594780
H	-0.806146	-1.388724	-2.141127
C	1.172508	-1.138451	-1.830638
C	3.792848	-2.105707	-1.602118
C	2.240200	-0.419106	-2.371329
C	1.425827	-2.348137	-1.174114
C	2.726808	-2.824433	-1.062401
C	3.540551	-0.903956	-2.257753
H	2.053921	0.526282	-2.875615
H	0.599043	-2.904956	-0.739697
H	2.907135	-3.760288	-0.542502
H	4.360022	-0.327743	-2.676847
H	4.807583	-2.479690	-1.512989

Aniline:Catalyst, binary complex 14; Energy = -2108.903184; 6-31G(d) basis set.

C	-3.864772	-0.514514	-1.153712
C	-3.603176	0.823256	0.977116
C	-3.480466	-1.707290	1.055270
C	-3.009391	-0.394463	1.686960
C	-3.200868	-1.712487	-0.449185
C	-3.330765	0.795592	-0.532172
H	-3.208306	1.753611	1.395660
H	-2.980189	-2.559198	1.527923
H	-3.270601	-0.366853	2.751004
H	-3.519127	-2.651256	-0.909470
H	-3.792821	1.666209	-1.003549
H	-3.581949	-0.526739	-2.228121
H	-4.690868	0.830759	1.110209
H	-4.558053	-1.821919	1.222989
H	-1.911122	-0.342126	1.633768
H	-2.114801	-1.677664	-0.609458
N	-5.324238	-0.564059	-1.024236
N	-1.897907	0.883522	-0.821940
H	-1.472524	0.094817	-1.294898
C	-5.973535	0.547677	-1.710826
H	-5.652287	0.641514	-2.764229
H	-5.778738	1.494684	-1.203398
H	-7.054400	0.390149	-1.696000
C	-5.871596	-1.824944	-1.509061
H	-5.582151	-2.653268	-0.859174
H	-5.554435	-2.059731	-2.541869
H	-6.962256	-1.764650	-1.493777
C	-1.161200	2.002322	-0.728284
S	-1.779836	3.525968	-0.379191
N	0.181920	1.857966	-0.982455
H	0.673618	2.744174	-0.984422
C	0.997816	0.721067	-0.878611
C	2.777524	-1.454603	-0.685030
C	0.629220	-0.440215	-0.191419
C	2.273263	0.788731	-1.447807
C	3.148075	-0.283199	-1.335372
C	1.509416	-1.510695	-0.119906
H	-0.318243	-0.500222	0.327018
H	2.578948	1.687034	-1.975994
H	3.458995	-2.296032	-0.619697
C	1.122219	-2.726569	0.670571
C	4.545021	-0.137704	-1.869944
F	-0.187766	-2.749067	0.962428
F	4.581406	0.637413	-2.962270
F	5.353594	0.430926	-0.960202
F	5.082037	-1.321824	-2.188907
F	1.417835	-3.859652	0.025385
F	1.782003	-2.774358	1.848423
N	0.467618	-0.418657	3.385286
C	1.134478	0.609121	2.725619
C	2.521094	2.706850	1.463418
C	2.487062	0.464051	2.374577
C	0.487208	1.815865	2.429140
C	1.183322	2.856471	1.819693
C	3.162818	1.497297	1.740849
H	2.991037	-0.476151	2.583595
H	-0.564042	1.941009	2.681780
H	0.655058	3.780303	1.599920
H	4.199346	1.351514	1.449048
H	3.058268	3.517174	0.980341
H	0.821527	-1.350980	3.215853
H	-0.542821	-0.373701	3.360435

Aniline:Catalyst, binary complex 15; Energy = -2108.918098; 6-31G(d) basis set.

C	-4.674192	-0.015694	-0.334731
C	-4.061975	-2.417168	-0.814192
C	-6.472036	-1.796951	-0.449237
C	-5.414339	-2.888143	-0.280567
C	-6.025675	-0.494032	0.220604
C	-3.625556	-1.118809	-0.124701
H	-4.126700	-2.238182	-1.896496
H	-6.636456	-1.614344	-1.520276
H	-5.314014	-3.136372	0.784625
H	-5.935644	-0.658331	1.302655

H	-3.516597	-1.327589	0.944940
H	-4.790923	0.121597	-1.422826
H	-3.286680	-3.171886	-0.649681
H	-7.430931	-2.121359	-0.031998
H	-5.721902	-3.805134	-0.793330
H	-6.783757	0.282886	0.074376
N	-4.206143	1.283592	0.174599
N	-2.331733	-0.665939	-0.607437
H	-2.334524	0.031269	-1.345956
C	-5.079457	2.383578	-0.217379
H	-6.045195	2.384643	0.311642
H	-5.273891	2.332689	-1.293497
H	-4.577417	3.332357	-0.000695
C	-3.961320	1.313347	1.613533
H	-3.251553	0.530496	1.897005
H	-4.879997	1.191654	2.208873
H	-3.516037	2.279442	1.871647
C	-1.135292	-1.043948	-0.120475
S	-0.967181	-2.120098	1.164866
N	-0.092344	-0.422710	-0.764722
H	-0.350282	0.427094	-1.267788
C	1.282709	-0.569302	-0.507602
C	4.055194	-0.777402	-0.126437
C	1.873043	-1.823008	-0.323368
C	2.084947	0.572733	-0.524100
C	3.457901	0.458601	-0.334850
C	3.245000	-1.909258	-0.126042
H	1.265129	-2.717928	-0.343819
H	1.639067	1.550538	-0.684182
H	5.127215	-0.861582	0.012991
C	3.870142	-3.253835	0.118585
C	4.293662	1.705893	-0.290619
F	3.164568	-4.243609	-0.445206
F	4.334207	2.231176	0.944922
F	5.562964	1.466464	-0.652948
F	3.816137	2.659942	-1.103584
F	5.117593	-3.313487	-0.374559
F	3.957711	-3.529780	1.428646
C	1.462344	3.602067	1.267275
C	-0.677177	2.779255	-0.354936
C	1.286792	4.150739	-0.001046
C	0.556648	2.645204	1.724088
C	-0.503924	2.234093	0.924670
C	0.226483	3.746961	-0.808705
H	1.987909	4.890489	-0.375197
H	0.102875	4.171700	-1.801931
N	-1.682258	2.269090	-1.200082
H	-2.532110	1.986076	-0.691890
H	-1.914637	2.901228	-1.959915
H	2.300812	3.904766	1.884520
H	-1.187471	1.462475	1.272262
H	0.683808	2.198751	2.705521

Aniline:Catalyst, binary complex 16; Energy = -2108.911083; 6-31G(d) basis set.

C	4.364363	-0.730901	-0.073044
C	3.635199	-2.762210	1.232920
C	6.062917	-2.468068	0.635328
C	4.940529	-3.476419	0.882680
C	5.669187	-1.453686	-0.443662
C	3.252670	-1.772078	0.127832
H	3.746803	-2.213391	2.178181
H	6.279425	-1.931935	1.569669
H	4.787954	-4.081380	-0.021341
H	5.538896	-1.974145	-1.401734
H	3.109370	-2.341572	-0.798218
H	4.525435	-0.233457	0.898284
H	2.814770	-3.474944	1.358183
H	6.985030	-2.981396	0.343908
H	5.217235	-4.168498	1.684419
H	6.472808	-0.722240	-0.579903
N	3.943475	0.339799	-0.994471
N	2.004383	-1.086284	0.412484
H	2.087116	-0.150216	0.793796
C	4.933711	1.406134	-1.100320
H	5.814178	1.124777	-1.698354

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H          5.273694        1.693840       -0.100531
H          4.470327        2.280918       -1.569262
C          3.550180       -0.130333       -2.320915
H          2.694287       -0.808652       -2.248352
H          4.363802       -0.638262       -2.861005
H          3.244365        0.734806       -2.918183
C          0.768673       -1.518297        0.086840
S          0.473075       -3.052959       -0.534044
N         -0.166197       -0.532550        0.284253
H          0.231879        0.414060        0.219240
C         -1.555135       -0.555711        0.146942
C         -4.352437       -0.343563       -0.072401
C         -2.359735       -1.687085        0.317466
C         -2.163704        0.679371       -0.109631
C         -3.541997        0.776474       -0.218408
C         -3.739860       -1.561560        0.200235
H         -1.915140       -2.647464        0.539246
H         -1.546932        1.567973       -0.215274
H         -5.430583       -0.267561       -0.161268
C         -4.598377       -2.789357        0.329629
C         -4.168845        2.123314       -0.440736
F         -4.014757       -3.732673        1.080008
F         -3.335069        2.962625       -1.077425
F         -5.288116        2.033009       -1.171551
F         -4.503870        2.711958        0.717378
F         -5.783262       -2.501264        0.889982
F         -4.858939       -3.339948       -0.865769
C          0.398072        5.218559        0.557892
C          2.385838        3.308065        0.914666
C          1.430582        5.460624        1.461229
C          0.352313        4.031470       -0.165993
C          1.350387        3.066801        0.005855
C          2.422438        4.497321        1.634324
H          1.461484        6.387551        2.023871
H          3.233465        4.671602        2.335123
N          1.284356        1.829849       -0.668490
H          0.824094        1.895742       -1.572833
H          2.202044        1.376814       -0.771645
H          3.159045        2.554223        1.050341
H         -0.459673        3.848442       -0.866745
H         -0.382198        5.959466        0.412679

Aniline:Catalyst, binary complex 17; Energy = -2108.907926; 6-31G(d) basis set.
C          4.540798        0.053825       -0.214901
C          4.241288       -1.327798        1.860675
C          6.541998       -1.041691        0.855304
C          5.616565       -1.965475        1.650890
C          5.901306       -0.611567       -0.469425
C          3.629134       -0.948654        0.510166
H          4.330476       -0.421294        2.474380
H          6.757861       -0.145353        1.453033
H          5.491839       -2.911688        1.107277
H          5.765816       -1.490265       -1.114088
H          3.537707       -1.865430       -0.088675
H          4.709098        0.895653        0.477457
H          3.566239       -2.014901        2.378492
H          7.501874       -1.533089        0.665287
H          6.065973       -2.213495        2.617877
H          6.562871        0.081634       -1.000860
N          3.861485        0.640130       -1.375230
N          2.306096       -0.353705        0.630110
H          2.242548        0.578819        0.223755
C          4.604899        1.743686       -1.964380
H          5.489700        1.419700       -2.536471
H          4.939299        2.426249       -1.176160
H          3.948139        2.299491       -2.642026
C          3.469507       -0.322700       -2.396421
H          2.805074       -1.082191       -1.973567
H          4.326451       -0.828100       -2.870873
H          2.919125        0.205450       -3.181579
C          1.160034       -1.055599        0.737316
S          1.109842       -2.725588        0.908332
N          0.058781       -0.231277        0.717823
H          0.266549        0.762497        0.780553
C         -1.301631       -0.502839        0.541923
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C	-4.068308	-0.734237	0.044398
C	-1.825130	-1.682739	0.003959
C	-2.178414	0.544934	0.852064
C	-3.531704	0.434008	0.576041
C	-3.196330	-1.782260	-0.218225
H	-1.173034	-2.508801	-0.246039
H	-1.787903	1.464340	1.279274
H	-5.128119	-0.821425	-0.163244
C	-3.724004	-3.083027	-0.759313
C	-4.390865	1.650781	0.749291
F	-3.722967	-4.042342	0.176127
F	-4.281382	2.462766	-0.329561
F	-5.685421	1.349625	0.877375
F	-4.026363	2.383547	1.808700
F	-4.981726	-2.963823	-1.207175
F	-2.972722	-3.530436	-1.776473
C	-0.997561	3.566752	-0.085365
C	1.723683	3.012908	-0.134010
C	-0.145101	4.159789	0.839303
C	-0.499113	2.675091	-1.049902
C	0.879913	2.405446	-1.062118
C	1.222208	3.888411	0.827612
H	-0.558514	4.839541	1.578394
H	1.884442	4.352282	1.550400
N	-1.351392	2.108203	-1.989324
H	-1.040753	1.226704	-2.378807
H	-2.325718	2.074997	-1.712385
H	2.786302	2.785169	-0.171487
H	1.294535	1.714930	-1.794898
H	-2.063963	3.778208	-0.062222

Aniline:Catalyst, binary complex 18; Energy = -2108.898198; 6-31G(d) basis set.

C	3.842636	-1.877836	0.663212
C	3.294192	-2.445901	-1.711860
C	5.707568	-2.149280	-1.005824
C	4.697289	-2.016090	-2.149013
C	5.239500	-1.398962	0.246805
C	2.869138	-1.615105	-0.500107
H	3.288195	-3.509265	-1.436439
H	5.831799	-3.212806	-0.758889
H	4.658483	-0.968059	-2.478377
H	5.201797	-0.320579	0.040153
H	2.912458	-0.553259	-0.783467
H	3.886580	-2.969617	0.802934
H	2.575248	-2.306187	-2.522519
H	6.689820	-1.780906	-1.320243
H	5.019871	-2.606484	-3.012691
H	5.950472	-1.549336	1.067386
N	3.309080	-1.349368	1.922851
N	1.521992	-1.899655	-0.019724
H	1.516621	-2.032951	0.993469
C	3.993353	-1.883705	3.089405
H	5.027376	-1.514632	3.194306
H	4.020027	-2.976163	3.035043
H	3.443885	-1.596410	3.991271
C	3.249429	0.106816	1.978224
H	2.721752	0.509425	1.106855
H	4.245028	0.576826	2.020138
H	2.698399	0.403701	2.876619
C	0.407643	-1.377959	-0.567245
S	0.362013	-0.569831	-2.037092
N	-0.712713	-1.613657	0.204672
H	-0.656773	-2.382118	0.862688
C	-1.961425	-0.982680	0.094764
C	-4.465905	0.279425	0.040570
C	-2.051025	0.394813	-0.126207
C	-3.124339	-1.721434	0.298927
C	-4.362370	-1.084517	0.276219
C	-3.294447	1.005716	-0.161298
H	-1.144804	0.973920	-0.253635
H	-3.065548	-2.791157	0.476410
H	-5.433065	0.769426	0.029847
C	-3.372656	2.479010	-0.446450
C	-5.607086	-1.908944	0.447004
F	-3.476320	2.728288	-1.757077

F	-5.412864	-2.922153	1.305231
F	-6.629283	-1.175956	0.907010
F	-6.000635	-2.452487	-0.713965
F	-4.431106	3.043982	0.148982
F	-2.273433	3.126367	-0.013146
N	0.741745	3.869045	1.264629
H	-0.151862	3.462261	1.019456
H	0.841052	3.988326	2.264418
C	1.844624	3.312658	0.622033
C	4.092311	2.321708	-0.755076
C	3.138333	3.496692	1.135032
C	1.694363	2.614950	-0.584727
C	2.807819	2.128756	-1.261923
C	4.244509	3.008786	0.448993
H	3.267873	4.037877	2.069039
H	0.700381	2.465688	-1.000519
H	2.658295	1.585267	-2.190695
H	5.236354	3.166895	0.863864
H	4.959388	1.949185	-1.291993

Aniline:Catalyst, binary complex 19; Energy = -2108.910153; 6-31G(d) basis set.

C	-4.657326	0.071416	0.028357
C	-4.023359	-1.110059	-2.086743
C	-6.456004	-0.925052	-1.432932
C	-5.401746	-1.771230	-2.149713
C	-6.033860	-0.609817	0.006405
C	-3.628005	-0.863242	-0.627486
H	-4.038963	-0.146969	-2.614719
H	-6.592519	0.018682	-1.978888
H	-5.343582	-2.759966	-1.674540
H	-5.993599	-1.540696	0.587940
H	-3.621209	-1.833732	-0.111107
H	-4.721465	0.969858	-0.607540
H	-3.267377	-1.739239	-2.562834
H	-7.424953	-1.435367	-1.435932
H	-5.690790	-1.938631	-3.192361
H	-6.778274	0.037512	0.483416
N	-4.182083	0.557220	1.327011
N	-2.312090	-0.257815	-0.487705
H	-2.310174	0.600799	0.063448
C	-5.005906	1.628818	1.862427
H	-5.987766	1.286616	2.229287
H	-5.173565	2.386087	1.089668
H	-4.483485	2.104484	2.699498
C	-3.966493	-0.484465	2.321374
H	-3.256817	-1.227760	1.946747
H	-4.893762	-0.998404	2.623203
H	-3.531470	-0.030440	3.217724
C	-1.145401	-0.924523	-0.593607
S	-1.033602	-2.555505	-0.989748
N	-0.065864	-0.107422	-0.363482
H	-0.261676	0.891712	-0.338446
C	1.298051	-0.422857	-0.309377
C	4.077867	-0.807416	-0.094812
C	1.803394	-1.599734	0.252041
C	2.190447	0.545558	-0.771613
C	3.560172	0.358317	-0.642645
C	3.179488	-1.779014	0.336284
H	1.128103	-2.364143	0.613957
H	1.809104	1.453894	-1.229336
H	5.147711	-0.958931	-0.010287
C	3.703226	-3.025404	0.994768
C	4.458394	1.484068	-1.056301
F	2.925327	-4.085290	0.745610
F	4.407160	2.496127	-0.155287
F	5.736271	1.116012	-1.157559
F	4.086070	2.019312	-2.228414
F	4.943634	-3.321427	0.580884
F	3.759150	-2.886246	2.329983
N	1.645464	4.022343	-0.610948
H	2.601191	3.713820	-0.485650
H	1.405933	4.212135	-1.574646
C	0.679495	3.402842	0.164629
C	-1.285588	2.222303	1.805959
C	-0.678912	3.465337	-0.187006

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C          1.037908        2.723404        1.342374
C          0.065413        2.144985        2.147620
C         -1.645625        2.889486        0.635527
H         -0.971215        3.984721       -1.095834
H          2.089613        2.647836        1.607369
H          0.369163        1.615943        3.045838
H         -2.694186        2.951879        0.352349
H         -2.046631        1.757393        2.423356

Aniline:Catalyst, binary complex 20; Energy = -2108.917314; 6-31G(d) basis set.
C         -3.816333       -0.040449       -0.674361
C         -3.303891       -2.426717       -1.266252
C         -5.573679       -1.453120       -1.802359
C         -4.796723       -2.719672       -1.436508
C         -5.321478       -0.329509       -0.790511
C         -3.104283       -1.325268       -0.221584
H         -2.870073       -2.094195       -2.219157
H         -5.257319       -1.111836       -2.797723
H         -5.188314       -3.127004       -0.494619
H         -5.716794       -0.622076        0.191650
H         -3.532286       -1.678429        0.725520
H         -3.448117        0.189961       -1.687817
H         -2.762492       -3.321037       -0.946000
H         -6.645713       -1.666809       -1.866886
H         -4.942957       -3.491004       -2.199526
H         -5.855277        0.576608       -1.096762
N         -3.421314        1.109981        0.145922
N         -1.703305       -1.009222        0.022968
H         -1.420750       -0.095495       -0.314953
C         -3.767468        0.991663        1.556036
H         -3.324385        0.087062        1.985190
H         -4.854342        0.971361        1.740021
H         -3.352934        1.854573        2.087419
C         -3.904003        2.370204       -0.400035
H         -3.621528        2.444999       -1.454761
H         -3.434770        3.197522        0.137173
H         -4.997389        2.488307       -0.321392
C         -0.908989       -1.648142        0.891638
S         -1.321901       -3.131889        1.605970
N          0.289178       -1.065841        1.189618
H          0.950465       -1.676014        1.682785
C          0.760734        0.185444        0.743790
C          1.762099        2.672580       -0.093082
C         -0.034760        1.333612        0.834097
C          2.063428        0.291726        0.252843
C          2.551223        1.530254       -0.148815
C          0.466097        2.553858        0.398762
H         -1.039007        1.277525        1.243850
H          2.694573       -0.589850        0.184790
H          2.150003        3.632621       -0.413975
C         -0.431842        3.757828        0.423504
C          3.949601        1.592194       -0.699262
F         -1.113692        3.884329       -0.726788
F          4.816200        0.939196        0.087889
F          4.023571        1.026620       -1.913462
F          4.382302        2.854627       -0.820758
F         -1.342200        3.681494        1.408105
F          0.259292        4.891494        0.596162
N          2.153764       -3.269160        1.947128
H          1.331603       -3.864068        1.873444
H          2.736237       -3.532030        2.733971
C          2.842431       -3.061185        0.743917
C          4.101030       -2.305020       -1.647584
C          4.168565       -2.611690        0.751869
C          2.160213       -3.155668       -0.476508
C          2.789645       -2.777838       -1.657833
C          4.787050       -2.235266       -0.436518
H          4.699462       -2.528872        1.696886
H          1.128952       -3.502898       -0.482231
H          2.244042       -2.845605       -2.594341
H          5.808502       -1.868181       -0.410305
H          4.581497       -1.993990       -2.569001

Aniline:Catalyst, binary complex 21; Energy = -2108.921266; 6-31G(d) basis set.
C          3.547587        0.584604        0.448850
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C          4.001031       -1.890222        0.600438
C          5.752447       -0.244242        1.363166
C          5.499187       -1.625001        0.755036
C          5.057501        0.858042        0.556636
C          3.345311       -0.780214       -0.227578
H          3.519537       -1.925997        1.588764
H          5.368233       -0.227994        2.392844
H          5.973469       -1.679784       -0.234089
H          5.494238        0.905953       -0.450062
H          3.818509       -0.776748       -1.216760
H          3.158587        0.498830        1.476753
H          3.817230       -2.849009        0.106337
H          6.827254       -0.043732        1.424264
H          5.959182       -2.405248        1.370305
H          5.229523        1.831071        1.029052
N          2.735786        1.629207       -0.183109
N          1.924836       -1.011303       -0.431010
H          1.304225       -0.593405        0.278801
C          2.770108        2.878918        0.560900
H          2.004887        3.552355        0.168759
H          3.742268        3.396476        0.504633
H          2.547127        2.683385        1.615622
C          3.028804        1.855794       -1.592011
H          2.900686        0.930354       -2.162593
H          2.313277        2.587715       -1.978874
H          4.044784        2.244660       -1.773538
C          1.414481       -1.726133       -1.431156
S          2.315650       -2.648297       -2.522990
N          0.039757       -1.709674       -1.546124
H         -0.309417       -2.405520       -2.192900
C         -0.862151       -0.696843       -1.184389
C         -2.803026        1.240189       -0.553981
C         -0.480662        0.626151       -0.946351
C         -2.216732       -1.042981       -1.100041
C         -3.167190       -0.080539       -0.802429
C         -1.455939        1.563205       -0.617551
H          0.562089        0.933567       -0.969974
H         -2.515374       -2.076377       -1.246725
H         -3.545463        1.983485       -0.286261
C         -0.991081        2.933590       -0.227732
C         -4.618606       -0.463408       -0.746320
F         -0.442610        2.921868        1.010305
F         -5.240295       -0.216886       -1.910771
F         -4.785697       -1.765704       -0.480060
F         -5.275038        0.231922        0.195771
F         -0.042828        3.401889       -1.054236
F         -1.984681        3.827022       -0.201640
N          0.495102       -0.051741        1.971489
H          1.175569       -0.388133        2.649628
H          0.418348        0.958985        2.054732
C         -0.764260       -0.695360        2.125973
C         -3.238485       -1.993001        2.275031
C         -1.924768        0.031671        2.390039
C         -0.845645       -2.079703        1.940289
C         -2.075622       -2.721816        2.023611
C         -3.156062       -0.616166        2.459766
H         -1.860788        1.108865        2.525006
H          0.058666       -2.638591        1.710056
H         -2.128227       -3.796356        1.875802
H         -4.054578       -0.037362        2.651379
H         -4.199615       -2.494337        2.322655

Aniline:Catalyst, binary complex 22; Energy = -2108.917440; 6-31G(d) basis set.
C         -3.595624       -0.772846       -0.437949
C         -3.816802        0.594429        1.662179
C         -5.528190       -1.174378        1.153146
C         -5.282118        0.185548        1.804674
C         -5.074204       -1.175183       -0.309235
C         -3.399735        0.615227        0.185778
H         -3.172573       -0.117079        2.197911
H         -4.968949       -1.944429        1.702192
H         -5.915039        0.942894        1.322745
H         -5.694029       -0.474145       -0.884406
H         -4.035496        1.343998       -0.333393
H         -3.001342       -1.486919        0.157061
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H	-3.643106	1.586704	2.088645
H	-6.586802	-1.447248	1.214532
H	-5.563830	0.162812	2.862269
H	-5.225281	-2.169025	-0.742691
N	-3.046843	-0.847432	-1.802098
N	-2.012564	1.039796	0.038812
H	-1.349017	0.388156	-0.384033
C	-3.564352	0.159254	-2.723901
H	-3.334733	1.164909	-2.359546
H	-4.649826	0.079261	-2.891859
H	-3.066292	0.030752	-3.690225
C	-3.156264	-2.184378	-2.375436
H	-2.511547	-2.250228	-3.258230
H	-2.814571	-2.925676	-1.646120
H	-4.180862	-2.444565	-2.682896
C	-1.607817	2.316195	0.121579
S	-2.635755	3.648350	0.231784
N	-0.249966	2.519851	0.076880
H	-0.000166	3.495879	-0.022229
C	0.801653	1.635851	0.381772
C	3.007163	-0.001273	0.997936
C	0.649805	0.531310	1.223152
C	2.069876	1.928805	-0.128992
C	3.152169	1.119172	0.187706
C	1.744219	-0.279071	1.502190
H	-0.314807	0.298517	1.659783
H	2.205096	2.789985	-0.777446
H	3.850390	-0.644961	1.217107
C	1.542700	-1.441914	2.433036
C	4.484560	1.423257	-0.435435
F	2.531563	-2.338684	2.342415
F	5.494879	0.877873	0.251919
F	4.565343	0.952412	-1.693349
F	4.705516	2.744529	-0.508060
F	1.488145	-1.038939	3.713449
F	0.386691	-2.080707	2.186183
N	-0.137940	-0.195283	-2.043389
H	0.088246	0.429039	-2.809269
H	-1.088518	-0.569002	-2.119209
C	0.855259	-1.133217	-1.749401
C	2.869663	-2.939782	-0.992300
C	2.169605	-0.962193	-2.196564
C	0.559658	-2.226833	-0.922473
C	1.558449	-3.117851	-0.551468
C	3.164708	-1.857330	-1.817803
H	2.414621	-0.108051	-2.822850
H	-0.455367	-2.351853	-0.549600
H	1.312174	-3.948916	0.103101
H	4.181012	-1.694487	-2.164693
H	3.648367	-3.633591	-0.692802

Aniline:Catalyst, binary complex 23; Energy = -2108.914924; 6-31G(d) basis set.

C	-3.537433	-0.893248	-0.433485
C	-4.165527	0.633277	1.464124
C	-5.705146	-1.252432	0.816300
C	-5.618463	0.164743	1.385792
C	-5.000638	-1.349675	-0.541716
C	-3.504966	0.550348	0.084971
H	-3.600439	0.000088	2.162318
H	-5.230247	-1.952797	1.517042
H	-6.182609	0.852472	0.741417
H	-5.526355	-0.719246	-1.271235
H	-4.059670	1.204446	-0.599183
H	-3.045753	-1.524406	0.325689
H	-4.103734	1.664162	1.824622
H	-6.750029	-1.564070	0.716946
H	-6.080713	0.208357	2.377088
H	-5.040277	-2.378726	-0.914901
N	-2.719876	-1.037978	-1.645418
N	-2.123093	1.011671	0.125420
H	-1.415873	0.306062	-0.055528
C	-3.157702	-0.223599	-2.776553
H	-4.147735	-0.515321	-3.160060
H	-2.430121	-0.344050	-3.585241
H	-3.181429	0.834726	-2.500265

C	-2.554984	-2.428007	-2.054623
H	-2.297391	-3.040564	-1.185185
H	-3.458518	-2.849777	-2.521918
H	-1.734282	-2.490247	-2.777720
C	-1.749052	2.299921	0.127687
S	-2.813298	3.599321	-0.009817
N	-0.402629	2.545333	0.221762
H	-0.162417	3.517087	0.070333
C	0.651861	1.666370	0.529482
C	2.842008	0.003869	1.119009
C	0.502327	0.583797	1.400584
C	1.910168	1.927332	-0.021009
C	2.987765	1.109263	0.289321
C	1.587967	-0.246914	1.655863
H	-0.449455	0.390868	1.884637
H	2.037817	2.764335	-0.702313
H	3.674543	-0.659528	1.315795
C	1.358750	-1.442953	2.536872
C	4.330324	1.451296	-0.294722
F	1.035560	-1.076821	3.786827
F	4.243326	1.724473	-1.606700
F	4.847409	2.543782	0.290178
F	5.216682	0.461508	-0.142766
F	0.337861	-2.192797	2.083916
F	2.435029	-2.232105	2.611382
N	0.115813	-0.281488	-2.386031
H	0.315204	0.672982	-2.654658
H	-0.786627	-0.414253	-1.930752
C	1.181780	-1.022562	-1.895566
C	3.329425	-2.597198	-0.981329
C	2.493661	-0.761902	-2.320300
C	0.964604	-2.083675	-1.003675
C	2.028147	-2.860385	-0.556988
C	3.550224	-1.539754	-1.863881
H	2.676045	0.061668	-3.005754
H	-0.044503	-2.275167	-0.644483
H	1.836389	-3.667210	0.144876
H	4.558146	-1.310795	-2.198371
H	4.157904	-3.202833	-0.628743

Aniline:Catalyst, binary complex 1, AS-A1; Energy = -2109.570258; TZVP basis set.

C	3.754007	0.018615	-0.768186
C	3.658645	1.465272	1.294915
C	5.647164	1.613070	-0.223095
C	5.159710	1.723930	1.218354
C	5.269976	0.262205	-0.831676
C	3.310381	0.100833	0.695192
H	3.115101	2.242495	0.745688
H	5.193456	2.412472	-0.818891
H	5.681117	0.987291	1.838158
H	5.786499	-0.539006	-0.292927
H	3.837482	-0.663039	1.269525
H	3.263520	0.838007	-1.315082
H	3.310282	1.482948	2.329258
H	6.728207	1.753920	-0.275371
H	5.392108	2.708148	1.628312
H	5.603900	0.221870	-1.869412
N	3.292812	-1.222194	-1.409926
N	1.881609	-0.166987	0.833789
H	1.288620	0.038424	0.027599
C	3.715121	-1.322782	-2.801895
H	4.778218	-1.571247	-2.915425
H	3.527852	-0.375755	-3.313108
H	3.130731	-2.100721	-3.296394
C	3.604652	-2.446603	-0.681737
H	3.136696	-2.442013	0.303618
H	4.684391	-2.608727	-0.558611
H	3.200718	-3.291628	-1.240910
C	1.341934	-0.700319	1.931246
S	2.231178	-1.363799	3.209159
N	-0.027024	-0.746801	2.008065
H	-0.350752	-1.328790	2.767569
C	-1.011131	-0.026395	1.318865
C	-3.109429	1.346879	0.065443
C	-0.784024	1.215266	0.731445

C	-2.299153	-0.567555	1.291501
C	-3.329287	0.125858	0.689098
C	-1.828238	1.868849	0.093976
H	0.189018	1.682055	0.778589
H	-2.480428	-1.537826	1.735800
H	-3.915063	1.872149	-0.430707
C	-1.538248	3.144347	-0.646562
C	-4.726051	-0.432442	0.703442
F	-2.590937	3.968052	-0.670698
F	-5.323569	-0.306548	-0.490311
F	-4.757405	-1.727246	1.031023
F	-5.503218	0.214198	1.587405
F	-0.512062	3.819471	-0.115941
F	-1.212824	2.896781	-1.929936
N	0.529104	-0.187024	-1.870538
H	1.457881	-0.614049	-1.914048
H	0.362782	0.489072	-2.602701
C	-0.496580	-1.125516	-1.705604
C	-2.549926	-2.972419	-1.244131
C	-0.249515	-2.294194	-0.976752
C	-1.781477	-0.892278	-2.197138
C	-2.794273	-1.813563	-1.971028
C	-1.269752	-3.205670	-0.751924
H	0.748344	-2.473104	-0.588810
H	-1.980238	0.013468	-2.759722
H	-3.785389	-1.619016	-2.361880
H	-1.061380	-4.105835	-0.186524
H	-3.344920	-3.684432	-1.066252

Aniline:Catalyst, binary complex 2; Energy = -2109.568581; TZVP basis set.

C	-4.671618	-0.080588	-0.411674
C	-3.991557	-2.495953	-0.624826
C	-6.417329	-1.908971	-0.345940
C	-5.334125	-2.944569	-0.055056
C	-6.010935	-0.534080	0.184834
C	-3.596800	-1.121816	-0.076961
H	-4.051034	-2.433027	-1.716883
H	-6.576223	-1.845933	-1.427782
H	-5.238526	-3.076444	1.027662
H	-5.920582	-0.583816	1.274515
H	-3.486406	-1.208287	1.006055
H	-4.779346	-0.066813	-1.504999
H	-3.201383	-3.205453	-0.375542
H	-7.367348	-2.212344	0.097474
H	-5.609824	-3.915375	-0.470145
H	-6.784433	0.201987	-0.042721
N	-4.248663	1.278532	-0.041334
N	-2.314398	-0.688507	-0.608602
H	-2.339921	-0.055574	-1.398327
C	-5.103138	2.306274	-0.623783
H	-6.105227	2.340511	-0.176330
H	-5.207450	2.135161	-1.696399
H	-4.638704	3.283087	-0.474290
C	-4.102928	1.492237	1.395238
H	-3.456437	0.730288	1.831348
H	-5.064193	1.483820	1.925678
H	-3.632554	2.463393	1.560591
C	-1.112383	-1.005820	-0.104894
S	-0.917123	-1.983677	1.253125
N	-0.079253	-0.412493	-0.789574
H	-0.339234	0.424951	-1.307160
C	1.292554	-0.549013	-0.519508
C	4.053038	-0.761263	-0.103310
C	1.875438	-1.797839	-0.315067
C	2.094787	0.588265	-0.534581
C	3.462555	0.469718	-0.337359
C	3.239641	-1.885582	-0.094304
H	1.262429	-2.686983	-0.323368
H	1.651832	1.564472	-0.694226
H	5.118699	-0.845238	0.061133
C	3.859138	-3.245221	0.079578
C	4.310248	1.711651	-0.320179
F	5.002266	-3.190837	0.774433
F	5.565845	1.463991	-0.718640
F	3.821247	2.664712	-1.123842

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F          4.397014        2.245818        0.908087
F          3.043750       -4.092555        0.715970
F          4.154265       -3.809883       -1.104388
N         -1.629145        2.309060       -1.216128
H         -2.500106        1.980291       -0.785335
H         -1.814748        2.960271       -1.967288
C         -0.678212        2.777971       -0.294599
C          1.356231        3.527199        1.478532
C         -0.571557        2.171654        0.960187
C          0.240799        3.767919       -0.648287
C          1.246920        4.137011        0.235135
C          0.437500        2.545278        1.834511
H         -1.266836        1.385637        1.234168
H          0.170462        4.239229       -1.622158
H          1.958462        4.898194       -0.059217
H          0.512958        2.052006        2.795387
H          2.150766        3.806690        2.156903

Aniline:Catalyst, binary complex 3, AA-A3; Energy = -2109.568650; TZVP basis set.
C         -4.674233       -0.082528       -0.406817
C         -3.992653       -2.495998       -0.635778
C         -6.417921       -1.912999       -0.344494
C         -5.332586       -2.949048       -0.063331
C         -6.010820       -0.540640        0.192249
C         -3.597088       -1.124496       -0.081867
H         -4.056419       -2.427099       -1.727231
H         -6.580979       -1.844241       -1.425367
H         -5.232735       -3.086626        1.018296
H         -5.916232       -0.596339        1.281279
H         -3.482515       -1.216839        1.000257
H         -4.786044       -0.062872       -1.499642
H         -3.200840       -3.206086       -0.393482
H         -7.365947       -2.219717        0.100879
H         -5.608891       -3.917886       -0.482591
H         -6.785900        0.195915       -0.028237
N         -4.251373        1.275023       -0.030571
N         -2.317115       -0.687009       -0.615971
H         -2.346096       -0.048922       -1.401418
C         -5.108741        2.304989       -0.604828
H         -6.109563        2.335570       -0.154284
H         -5.215976        2.139722       -1.678071
H         -4.645016        3.281505       -0.451253
C         -4.101665        1.481115        1.406720
H         -3.453682        0.717075        1.836913
H         -5.061451        1.469381        1.939769
H         -3.631229        2.451559        1.575986
C         -1.112920       -1.005822       -0.118638
S         -0.911085       -1.991753        1.232601
N         -0.082799       -0.407293       -0.803009
H         -0.344704        0.433600       -1.313970
C          1.289749       -0.545946       -0.536855
C          4.051359       -0.765918       -0.142391
C          1.872818       -1.800062       -0.355654
C          2.091102        0.590324       -0.537894
C          3.461380        0.468035       -0.351516
C          3.237835       -1.892238       -0.151339
H          1.259942       -2.688234       -0.384180
H          1.648114        1.568779       -0.683076
H          5.119949       -0.854305        0.002352
C          3.867206       -3.237298        0.088160
C          4.308986        1.709973       -0.326771
F          3.107748       -4.241537       -0.362150
F          4.383816        2.244376        0.902089
F          5.567945        1.463118       -0.714061
F          3.826312        2.662971       -1.134715
F          5.060805       -3.340352       -0.515090
F          4.079081       -3.461508        1.394045
C          1.351311        3.523033        1.486265
C         -0.684266        2.779341       -0.287821
C          1.240157        4.137929        0.245519
C          0.434250        2.538381        1.838915
C         -0.575305        2.167395        0.964029
C          0.233342        3.771676       -0.638335
H          1.950307        4.901447       -0.046139
H          0.161304        4.247217       -1.610018
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N         -1.636603        2.314125       -1.209877
H         -2.506546        1.983316       -0.778638
H         -1.823902        2.968824       -1.957577
H          2.146139        3.800601        2.165059
H         -1.269128        1.379087        1.235082
H          0.511482        2.040891        2.797467

Aniline:Catalyst, binary complex 4, AS-A5; Energy = -2109.567718; TZVP basis set.
C         -3.767949       -0.049354       -0.724136
C         -3.202709       -2.441432       -1.229141
C         -5.460036       -1.520739       -1.870737
C         -4.681640       -2.762467       -1.438663
C         -5.260786       -0.364704       -0.887486
C         -3.057211       -1.308958       -0.213670
H         -2.745052       -2.129725       -2.173885
H         -5.114348       -1.207072       -2.861548
H         -5.097617       -3.144262       -0.500430
H         -5.686550       -0.633156        0.084581
H         -3.512494       -1.636861        0.725338
H         -3.365618        0.165790       -1.723531
H         -2.660261       -3.313759       -0.864535
H         -6.522816       -1.751204       -1.964831
H         -4.790514       -3.556368       -2.179491
H         -5.791655        0.520568       -1.241983
N         -3.426633        1.123037        0.089683
N         -1.668802       -0.970015        0.067468
H         -1.383981       -0.067265       -0.290336
C         -3.793379        1.009658        1.494555
H         -3.314598        0.139876        1.948235
H         -4.878250        0.934960        1.654931
H         -3.439451        1.898919        2.019281
C         -3.935800        2.360990       -0.482060
H         -3.650273        2.424813       -1.533152
H         -3.493710        3.207928        0.042381
H         -5.028984        2.451012       -0.410546
C         -0.901586       -1.573803        0.977819
S         -1.339872       -3.024961        1.744669
N          0.292360       -0.988475        1.277864
H          0.947176       -1.585771        1.784980
C          0.773174        0.240936        0.787431
C          1.785942        2.688568       -0.116496
C         -0.003183        1.397908        0.875483
C          2.057544        0.314161        0.257253
C          2.553404        1.537171       -0.172593
C          0.503198        2.598089        0.407583
H         -0.995994        1.357957        1.307617
H          2.662215       -0.582716        0.176689
H          2.178406        3.635524       -0.461291
C         -0.367628        3.824056        0.436096
C          3.945360        1.573421       -0.745919
F         -1.010395        3.997595       -0.729989
F          4.825974        0.963867        0.058680
F          4.008533        0.950341       -1.931044
F          4.379664        2.824274       -0.935674
F         -1.305970        3.753351        1.388873
F          0.341298        4.937130        0.654901
N          2.152913       -3.226531        2.039267
H          1.301898       -3.777974        2.053239
H          2.775287       -3.462091        2.798794
C          2.759954       -3.093365        0.785913
C          3.887097       -2.532634       -1.715135
C          4.098547       -2.708005        0.682643
C          1.995202       -3.214092       -0.377864
C          2.559375       -2.933249       -1.613863
C          4.652312       -2.430343       -0.559262
H          4.695171       -2.604797        1.581689
H          0.955169       -3.513476       -0.299276
H          1.951767       -3.024869       -2.505600
H          5.687644       -2.119258       -0.620443
H          4.319346       -2.303347       -2.679775

Aniline:Catalyst, binary complex 5, AS-A2; Energy = -2109.568983; TZVP basis set.
C          3.554329        0.627862        0.374837
C          3.944215       -1.855998        0.486351
C          5.757660       -0.267811        1.214429
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C          5.450539       -1.632522        0.600712
C          5.071210        0.859702        0.440264
C          3.300370       -0.720080       -0.309225
H          3.491479       -1.891505        1.484436
H          5.405548       -0.252529        2.251844
H          5.892071       -1.688236       -0.399638
H          5.477574        0.904888       -0.575281
H          3.746209       -0.716078       -1.306754
H          3.190833        0.543902        1.407622
H          3.723309       -2.800033       -0.013682
H          6.835520       -0.098110        1.244681
H          5.904629       -2.428986        1.192785
H          5.281216        1.818791        0.916801
N          2.755533        1.697826       -0.229281
N          1.869589       -0.910469       -0.481894
H          1.285967       -0.492886        0.246547
C          2.848527        2.942200        0.517947
H          2.095791        3.639649        0.151848
H          3.831018        3.428247        0.431931
H          2.648969        2.750079        1.574034
C          3.006116        1.917335       -1.646800
H          2.817179        1.005285       -2.215692
H          2.314836        2.681549       -2.006077
H          4.028985        2.259603       -1.860061
C          1.319145       -1.574624       -1.491254
S          2.181795       -2.485982       -2.625242
N         -0.051568       -1.523570       -1.592058
H         -0.421106       -2.193706       -2.250894
C         -0.944481       -0.546941       -1.135939
C         -2.879559        1.330061       -0.352229
C         -0.562685        0.747532       -0.787258
C         -2.298926       -0.892989       -1.094369
C         -3.243465        0.041061       -0.721377
C         -1.535708        1.653480       -0.386086
H          0.475937        1.063420       -0.809390
H         -2.598687       -1.902965       -1.343783
H         -3.622016        2.050905       -0.038246
C         -1.070498        3.009470        0.062303
C         -4.701736       -0.326370       -0.713534
F         -0.421008        2.937329        1.241807
F         -5.337521        0.148504       -1.796174
F         -4.895108       -1.649077       -0.696823
F         -5.335236        0.182368        0.353708
F         -0.214686        3.561992       -0.808544
F         -2.078259        3.870034        0.229705
N          0.583499       -0.176764        2.138808
H          1.348039       -0.592547        2.657999
H          0.408389        0.761260        2.477038
C         -0.572607       -0.989623        2.119680
C         -2.847768       -2.600144        1.936564
C         -1.831839       -0.460687        2.392084
C         -0.458883       -2.329113        1.743291
C         -1.590315       -3.126949        1.660901
C         -2.959928       -1.264987        2.302413
H         -1.923624        0.580699        2.681018
H          0.519332       -2.734505        1.506713
H         -1.488044       -4.165356        1.371265
H         -3.933326       -0.841350        2.517197
H         -3.730026       -3.222491        1.865235

Aniline:Catalyst, binary complex 6, AS-A4; Energy = -2109.567924; TZVP basis set.
C         -3.445809       -0.767243       -0.626659
C         -3.844219        0.187317        1.667160
C         -5.419392       -1.540294        0.751219
C         -5.286028       -0.311838        1.647777
C         -4.902047       -1.251949       -0.658749
C         -3.358586        0.485936        0.247579
H         -3.189406       -0.571594        2.109938
H         -4.842687       -2.365497        1.182474
H         -5.935475        0.485844        1.272577
H         -5.529059       -0.485700       -1.125405
H         -3.994660        1.269710       -0.170655
H         -2.847364       -1.550788       -0.139175
H         -3.751520        1.096700        2.263033
H         -6.458669       -1.870216        0.704685
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H         -5.616268       -0.540209        2.662371
H         -4.975340       -2.150531       -1.273755
N         -2.822200       -0.551219       -1.939373
N         -1.990242        0.985937        0.255830
H         -1.267514        0.358301       -0.077895
C         -3.381130        0.559559       -2.703754
H         -3.264847        1.496677       -2.157505
H         -4.440562        0.420572       -2.955099
H         -2.826645        0.647648       -3.640017
C         -2.771966       -1.766361       -2.743567
H         -2.058474       -1.628217       -3.558865
H         -2.427060       -2.600206       -2.130329
H         -3.742841       -2.032943       -3.180883
C         -1.648104        2.257235        0.487892
S         -2.753123        3.523545        0.653556
N         -0.308274        2.523438        0.568016
H         -0.086780        3.508484        0.566010
C          0.754968        1.615491        0.723965
C          2.923136       -0.135533        1.017164
C          0.643252        0.488429        1.531742
C          1.965687        1.882319        0.089284
C          3.031822        1.015241        0.248006
C          1.717576       -0.381298        1.648803
H         -0.278850        0.288285        2.062515
H          2.054303        2.752487       -0.549670
H          3.748080       -0.828272        1.101784
C          1.540350       -1.603044        2.508115
C          4.335279        1.350291       -0.424909
F          2.522086       -2.492176        2.342754
F          5.146739        0.293625       -0.517454
F          4.151559        1.824287       -1.666165
F          5.004212        2.300702        0.248490
F          1.506923       -1.289410        3.813099
F          0.382592       -2.230286        2.241269
N          0.061548        0.319229       -2.220207
H          0.315643        0.911440       -2.996070
H         -0.930877        0.084665       -2.179721
C          0.930023       -0.730050       -1.952682
C          2.711273       -2.791336       -1.268824
C          2.246720       -0.725059       -2.427491
C          0.519190       -1.790935       -1.135853
C          1.401362       -2.807467       -0.803249
C          3.121175       -1.746165       -2.089689
H          2.578737        0.089815       -3.060653
H         -0.500229       -1.809194       -0.762521
H          1.063807       -3.613754       -0.163339
H          4.136634       -1.718163       -2.465555
H          3.397870       -3.583905       -1.002634

RS epoxide:Catalyst, binary complex 1; Energy = -2449.836438; 6-31G(d) basis set.
N          1.269255        0.141335       -0.353421
H          0.295970       -0.114597       -0.500831
C          1.564783        1.467849       -0.583535
S          3.128148        2.056883       -0.781046
N          0.440726        2.201689       -0.679952
H         -0.413752        1.740354       -0.384075
C          2.121578       -0.961493       -0.221762
C          3.652635       -3.301376        0.075818
C          1.649386       -2.188702       -0.697305
C          3.361393       -0.912485        0.425313
C          4.109557       -2.076265        0.551411
C          2.408933       -3.341099       -0.540437
H          0.687575       -2.238231       -1.200726
H          3.728647        0.021726        0.826742
H          4.248261       -4.200416        0.187988
C          5.469989       -2.006945        1.187106
C          1.844624       -4.654243       -1.000878
F          6.434484       -1.829634        0.271536
F          5.565460       -0.996033        2.060473
F          5.762531       -3.140506        1.844740
F          1.080404       -4.511759       -2.094280
F          2.808214       -5.538118       -1.290098
F          1.068257       -5.214951       -0.058017
C          0.307453        3.655117       -0.762413
C          0.563963        5.886437        0.336115
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C          0.399757        5.729351       -2.174768
C          1.003575        6.497704       -0.997217
C          0.756604        4.242305       -2.105352
C          0.963387        4.403536        0.415721
H         -0.526864        5.982260        0.434753
H         -0.693477        5.843944       -2.155795
H          2.099073        6.459828       -1.066557
H          1.837519        4.108771       -2.212909
H          2.046423        4.337169        0.266394
H         -0.778334        3.813188       -0.697965
H          1.010221        6.434260        1.174654
H          0.746342        6.150249       -3.124484
H          0.717005        7.553967       -1.043729
H          0.273791        3.687481       -2.917081
N          0.693382        3.734079        1.686493
C          1.655250        4.082921        2.715525
H          2.667765        3.904803        2.341573
H          1.495792        3.442958        3.589779
H          1.583641        5.133014        3.053128
C         -0.666516        3.877019        2.173819
H         -0.914120        4.902051        2.502233
H         -0.808568        3.209824        3.030431
H         -1.386318        3.583021        1.402585
C         -3.960725       -0.386363       -0.781500
N         -2.552101        0.124776       -0.595580
O         -1.645405       -0.617817       -0.930987
O         -2.405693        1.224709       -0.102226
C         -4.838619       -0.110997        0.384994
C         -6.015072       -0.967100        0.692936
C         -8.191341       -2.595568        1.302164
C         -6.022307       -1.709507        1.875128
C         -7.103334       -1.030270       -0.178137
C         -8.189614       -1.844562        0.128922
C         -7.107451       -2.526202        2.175533
H         -5.179108       -1.648142        2.558400
H         -7.097730       -0.429848       -1.082972
H         -9.037872       -1.887847       -0.546704
H         -7.108916       -3.105555        3.093108
H         -9.039616       -3.229390        1.540227
C         -4.059718       -1.528425       -1.743452
H         -3.447211       -2.365908       -1.408811
H         -3.726806       -1.216214       -2.736055
H         -5.102841       -1.841909       -1.795088
H         -4.370545        0.407729        1.221083
O         -4.868691        0.657279       -0.815165

RS epoxide:Catalyst, binary complex 2; Energy = -2449.840503; 6-31G(d) basis set.
N          1.428966        0.436338       -0.697345
H          0.447514        0.167834       -0.683786
C          1.641559        1.794652       -0.580007
S          3.015326        2.455423        0.128699
N          0.609592        2.492516       -1.103402
H         -0.146768        1.913221       -1.454814
C          2.305765       -0.609500       -0.380911
C          3.926629       -2.835244        0.173004
C          1.768815       -1.742872        0.231901
C          3.659810       -0.596010       -0.731722
C          4.449563       -1.700699       -0.441595
C          2.577062       -2.842686        0.497433
H          0.715662       -1.763819        0.499059
H          4.082795        0.263731       -1.235117
H          4.552334       -3.696623        0.376910
C          5.913734       -1.662472       -0.780588
C          1.977668       -4.028512        1.197540
F          6.158654       -0.887261       -1.845558
F          6.646184       -1.179869        0.233771
F          6.386910       -2.888088       -1.054759
F          2.675174       -5.149141        0.968282
F          1.939015       -3.853179        2.527477
F          0.713584       -4.248446        0.800530
C          0.123746        3.805746       -0.661231
C         -0.701512        5.158674        1.310701
C          0.424505        6.304090       -0.619246
C          0.235251        6.296184        0.898855
C          1.012347        4.974573       -1.095051
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C	-0.158894	3.797430	0.854113
H	-1.685023	5.339059	0.855661
H	-0.548388	6.477102	-1.101730
H	1.211371	6.164458	1.384281
H	2.009617	4.840610	-0.668118
H	0.808219	3.645312	1.346717
H	-0.841498	3.913277	-1.177279
H	-0.849981	5.146723	2.397488
H	1.079892	7.127352	-0.921787
H	-0.167445	7.255178	1.242111
H	1.118379	4.954194	-2.185160
N	-0.991920	2.632295	1.192743
C	-0.613411	2.008018	2.450323
H	0.451023	1.755336	2.426893
H	-1.183177	1.080623	2.574549
H	-0.803736	2.647813	3.330911
C	-2.421735	2.873683	1.147620
H	-2.786221	3.549147	1.940584
H	-2.943987	1.918019	1.278851
H	-2.708170	3.297216	0.178101
C	-3.733854	0.030019	-0.405199
N	-2.292397	0.368298	-0.707443
O	-1.433950	-0.200439	-0.061734
O	-2.082204	1.168353	-1.599770
C	-3.941851	-1.398927	-0.056766
C	-5.251014	-2.073000	-0.268251
C	-7.681936	-3.365413	-0.693602
C	-5.334641	-3.117668	-1.190518
C	-6.382504	-1.682951	0.449361
C	-7.595659	-2.330725	0.235108
C	-6.550134	-3.759036	-1.405411
H	-4.448634	-3.429164	-1.737917
H	-6.299531	-0.885843	1.182234
H	-8.473011	-2.031151	0.799432
H	-6.613016	-4.569370	-2.124595
H	-8.629058	-3.869334	-0.858050
C	-4.718495	0.949695	-1.055400
H	-4.585252	0.947392	-2.137715
H	-4.591155	1.968553	-0.682416
H	-5.723327	0.600744	-0.814568
H	-3.052306	-2.027010	-0.074539
O	-3.881671	-0.358153	0.916792

RS epoxide:Catalyst, binary complex 3; Energy = -2449.840427; 6-31G(d) basis set.

N	0.946919	0.381818	-0.443332
H	0.982581	0.319157	-1.453933
C	2.182157	0.309816	0.198158
S	2.535301	1.212493	1.564363
N	2.996901	-0.542173	-0.434507
H	2.536021	-1.204735	-1.051361
C	-0.241488	0.882288	0.101492
C	-2.712054	1.765840	1.105272
C	-1.053025	1.721682	-0.660205
C	-0.666906	0.486537	1.375689
C	-1.885056	0.938629	1.862118
C	-2.280849	2.146202	-0.156703
H	-0.724498	2.045927	-1.644312
H	-0.037330	-0.164267	1.974167
H	-3.667277	2.100504	1.491635
C	-2.335733	0.461251	3.214529
C	-3.126615	3.052319	-1.005336
F	-3.329056	1.211886	3.705374
F	-2.791633	-0.805560	3.158239
F	-1.334835	0.470577	4.101472
F	-3.194659	2.604909	-2.275469
F	-4.383600	3.141221	-0.551435
F	-2.630018	4.294126	-1.062797
C	4.433043	-0.728130	-0.251286
C	6.735986	0.216445	-0.417229
C	6.293155	-1.756528	1.089512
C	7.128841	-0.491276	0.882640
C	4.795930	-1.439928	1.058379
C	5.239555	0.575319	-0.413320
H	6.959163	-0.443377	-1.267887
H	6.529667	-2.477052	0.293509

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H          6.965454        0.191310        1.727395
H          4.526431       -0.792997        1.899382
H          5.045487        1.184666        0.476261
H          4.718728       -1.400709       -1.070955
H          7.332580        1.126264       -0.553016
H          6.552602       -2.237050        2.038687
H          8.196139       -0.737276        0.872785
H          4.197622       -2.353915        1.143094
N          4.765147        1.365730       -1.547604
C          5.180947        2.754353       -1.468799
H          4.883682        3.168938       -0.501019
H          4.676729        3.325959       -2.254885
H          6.268819        2.900139       -1.595700
C          5.073699        0.802623       -2.849483
H          6.149855        0.817691       -3.096060
H          4.549410        1.377287       -3.620012
H          4.723417       -0.232543       -2.912258
C         -1.229967       -2.805994       -0.405209
N          0.257032       -2.533208       -0.385902
O          0.825272       -2.440430       -1.461986
O          0.785176       -2.399206        0.696659
C         -1.933827       -2.176187       -1.550614
C         -3.375109       -1.816186       -1.499795
C         -6.050078       -1.044540       -1.368284
C         -3.734582       -0.488239       -1.729429
C         -4.362403       -2.767798       -1.239596
C         -5.697073       -2.378910       -1.174388
C         -5.067388       -0.098494       -1.652793
H         -2.969316        0.239945       -1.977530
H         -4.081961       -3.808757       -1.106948
H         -6.464083       -3.120925       -0.976436
H         -5.333536        0.940238       -1.821858
H         -7.091953       -0.745235       -1.312097
C         -1.791888       -3.123282        0.944094
H         -1.650720       -2.286673        1.628171
H         -1.304982       -4.009317        1.357754
H         -2.860141       -3.312986        0.840096
H         -1.309247       -1.585604       -2.220419
O         -1.581394       -3.556736       -1.518618

RS epoxide:Catalyst, binary complex 4; Energy = -2449.852449; 6-31G(d) basis set.
N         -0.132777       -1.834473       -0.250089
H         -0.154872       -2.577706        0.441582
C         -1.354697       -1.479795       -0.792642
S         -1.514563       -0.701149       -2.271191
N         -2.367438       -1.880196       -0.003172
H         -2.107733       -2.088405        0.956439
C          1.159852       -1.382747       -0.551302
C          3.816905       -0.506701       -0.858745
C          2.229343       -2.223006       -0.222190
C          1.428806       -0.104665       -1.044509
C          2.746521        0.314817       -1.187299
C          3.536276       -1.780714       -0.374294
H          2.036856       -3.218363        0.166810
H          0.621306        0.560907       -1.312083
H          4.839560       -0.168058       -0.977697
C          2.986501        1.737002       -1.611523
C          4.665397       -2.667801        0.069085
F          4.236837        1.923404       -2.056580
F          2.146516        2.117134       -2.581732
F          2.803937        2.580743       -0.581179
F          4.360853       -3.966106       -0.061348
F          5.782089       -2.437267       -0.633620
F          4.964970       -2.462627        1.361653
C         -3.806175       -1.712598       -0.213101
C         -5.804967       -0.222173       -0.253485
C         -5.880616       -2.465838       -1.406692
C         -6.384739       -1.021315       -1.424463
C         -4.350271       -2.516109       -1.400393
C         -4.266673       -0.242091       -0.286104
H         -6.161851       -0.653134        0.692767
H         -6.265630       -2.970763       -0.509693
H         -6.083183       -0.545717       -2.367272
H         -3.956974       -2.100122       -2.332868
H         -3.942783        0.146990       -1.257980
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H         -4.247466       -2.155441        0.688987
H         -6.162424        0.813043       -0.288593
H         -6.265884       -3.016858       -2.270660
H         -7.479108       -0.999419       -1.392071
H         -3.994655       -3.549019       -1.323720
N         -3.596044        0.588305        0.715835
C         -3.766747        2.009951        0.459783
H         -3.514385        2.230127       -0.581937
H         -3.085719        2.579050        1.103187
H         -4.790956        2.369834        0.657111
C         -3.934990        0.282397        2.098395
H         -4.965374        0.570775        2.366520
H         -3.245361        0.818954        2.758838
H         -3.808546       -0.784359        2.302267
C          0.505986        0.486208        2.297302
N          0.064423       -0.949463        2.494853
O          0.917395       -1.815274        2.479469
O         -1.129302       -1.157233        2.621282
C         -0.486181        1.307389        1.548207
C         -0.108588        2.545772        0.815011
C          0.548131        4.851166       -0.611489
C         -0.489449        2.676206       -0.522940
C          0.568465        3.590619        1.447441
C          0.895226        4.739352        0.733127
C         -0.148286        3.819862       -1.237801
H         -1.059943        1.879163       -0.998275
H          0.817495        3.505915        2.501077
H          1.420155        5.549875        1.228848
H         -0.432351        3.905875       -2.281698
H          0.810966        5.745383       -1.167834
C          1.991590        0.668021        2.352705
H          2.242891        1.650815        1.950982
H          2.490946       -0.095744        1.754123
H          2.341398        0.592442        3.385522
H         -1.382665        0.786090        1.195062
O         -0.349889        1.341289        2.973259

RS epoxide:Catalyst, binary complex 5; Energy = -2449.838058; 6-31G(d) basis set.
N          1.263558        0.266534        0.606714
H          0.751364       -0.277008        1.297098
C          0.491042        1.106673       -0.161994
S          0.982204        1.709287       -1.644482
N         -0.720411        1.313845        0.424354
H         -0.682377        1.221792        1.436313
C          2.525393       -0.266872        0.283993
C          5.032783       -1.411286       -0.220932
C          2.722548       -1.634493        0.459168
C          3.588696        0.538855       -0.133555
C          4.821078       -0.044499       -0.391299
C          3.973709       -2.193887        0.213699
H          1.893997       -2.263253        0.774933
H          3.448138        1.606226       -0.246515
H          6.004423       -1.850799       -0.416149
C          5.949185        0.809398       -0.898534
C          4.161094       -3.662791        0.465310
F          5.811918        2.089290       -0.528381
F          7.135601        0.379379       -0.441929
F          6.018133        0.789903       -2.237906
F          5.278357       -4.133339       -0.102560
F          4.239568       -3.929578        1.778882
F          3.129954       -4.377122       -0.011038
C         -1.752731        2.284211        0.037047
C         -2.477676        4.682550       -0.009680
C         -3.546780        3.001783       -1.551638
C         -3.111058        4.459258       -1.385179
C         -2.358499        2.058632       -1.351087
C         -1.284277        3.740029        0.218910
H         -3.238093        4.499747        0.762369
H         -4.330410        2.766625       -0.817257
H         -2.380658        4.706984       -2.167323
H         -1.606866        2.246873       -2.120672
H         -0.537751        3.929152       -0.562765
H         -2.558229        2.084817        0.757626
H         -2.153075        5.723993        0.101965
H         -3.981183        2.843748       -2.544426
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H         -3.963847        5.133467       -1.519656
H         -2.675973        1.014934       -1.443421
N         -0.583608        3.901594        1.495662
C          0.307520        5.048450        1.502078
H          0.989012        4.988266        0.648512
H          0.905724        5.035842        2.418896
H         -0.221418        6.017475        1.460896
C         -1.446289        3.912502        2.666255
H         -2.067483        4.821050        2.747852
H         -0.824972        3.851860        3.565427
H         -2.113504        3.043790        2.664046
C         -2.855046       -1.194843        0.450404
N         -1.917941       -0.968723        1.606860
O         -0.859278       -1.575836        1.583037
O         -2.266181       -0.210493        2.486878
C         -4.257018       -1.437872        0.874211
C         -5.202362       -2.220226        0.033542
C         -6.967729       -3.726426       -1.508729
C         -5.683408       -3.440243        0.512484
C         -5.614210       -1.749250       -1.213704
C         -6.497236       -2.503269       -1.981441
C         -6.560705       -4.193507       -0.260413
H         -5.370290       -3.799061        1.489618
H         -5.250913       -0.788767       -1.568210
H         -6.821636       -2.132487       -2.948509
H         -6.930189       -5.142888        0.113598
H         -7.655107       -4.313076       -2.109891
C         -2.171931       -1.719543       -0.774167
H         -1.386273       -1.026641       -1.089666
H         -2.912390       -1.814845       -1.569521
H         -1.729036       -2.695961       -0.574269
H         -4.437531       -1.432120        1.949118
O         -3.800567       -0.184656        0.370643

RS epoxide:Catalyst, binary complex 6; Energy = -2449.840424; 6-31G(d) basis set.
N          1.432302        0.451612       -0.682357
H          0.455132        0.167837       -0.681588
C          1.621335        1.813056       -0.558476
S          2.974330        2.494877        0.170413
N          0.584896        2.495286       -1.092647
H         -0.159266        1.906311       -1.453709
C          2.321328       -0.583297       -0.364801
C          3.972712       -2.782596        0.201257
C          1.793317       -1.733901        0.221546
C          3.683484       -0.538572       -0.685034
C          4.486581       -1.630538       -0.390628
C          2.617521       -2.821437        0.493449
H          0.736044       -1.777473        0.468739
H          4.103120        0.340150       -1.156520
H          4.614676       -3.628508        0.422052
C          5.939882       -1.618213       -0.773695
C          2.029620       -4.022199        1.177588
F          6.709493       -2.111403        0.208800
F          6.164517       -2.381646       -1.856383
F          6.380654       -0.387899       -1.057532
F          2.744266       -5.130751        0.942394
F          1.979757       -3.860630        2.508814
F          0.771598       -4.255706        0.769485
C          0.080343        3.806248       -0.665039
C         -0.771884        5.167492        1.290213
C          0.356260        6.308119       -0.640937
C          0.157968        6.309783        0.875995
C          0.959518        4.980822       -1.103030
C         -0.214683        3.807472        0.847893
H         -1.753909        5.336731        0.827712
H         -0.615396        6.468400       -1.130268
H          1.132181        6.189758        1.368322
H          1.955813        4.860304       -0.669878
H          0.749482        3.667033        1.349487
H         -0.881914        3.898278       -1.189657
H         -0.927309        5.162335        2.376085
H          1.005658        7.135240       -0.945859
H         -0.254855        7.267864        1.209707
H          1.071511        4.953004       -2.192397
N         -1.040841        2.638139        1.187968
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C         -0.668251        2.025316        2.452832
H          0.398950        1.784032        2.441402
H         -1.229221        1.092534        2.576720
H         -0.874341        2.668090        3.327674
C         -2.472108        2.866967        1.128714
H         -2.849374        3.544023        1.914369
H         -2.987327        1.907695        1.261038
H         -2.753662        3.282552        0.154311
C         -3.732069       -0.001970       -0.413235
N         -2.293711        0.350026       -0.715065
O         -1.430392       -0.206177       -0.065025
O         -2.090520        1.147988       -1.610915
C         -3.925564       -1.429978       -0.052746
C         -5.227309       -2.119602       -0.260147
C         -7.644342       -3.440573       -0.677324
C         -5.298472       -3.174494       -1.171744
C         -6.364234       -1.733796        0.451156
C         -7.570389       -2.395739        0.241017
C         -6.507038       -3.830150       -1.382537
H         -4.408181       -3.482939       -1.713915
H         -6.290997       -0.928541        1.176136
H         -8.451833       -2.099116        0.800499
H         -6.560050       -4.648643       -2.093233
H         -8.586031       -3.955520       -0.838785
C         -4.725326        0.901090       -1.073527
H         -4.610487        1.924417       -0.708896
H         -5.726839        0.542798       -0.832569
H         -4.589103        0.891221       -2.155447
H         -3.029467       -2.048797       -0.063660
O         -3.878159       -0.380320        0.911873

RS epoxide:Catalyst, binary complex 7; Energy = -2449.853493; 6-31G(d) basis set.
N         -0.058750       -1.077833        0.582686
H         -0.240021       -0.218151        1.093615
C         -1.092749       -1.479235       -0.231684
S         -0.956762       -2.620994       -1.451526
N         -2.241934       -0.818103        0.054163
H         -2.327719       -0.438985        1.003213
C          1.311756       -1.359267        0.447573
C          4.084896       -1.769662        0.254968
C          1.812702       -2.632914        0.168151
C          2.203734       -0.307679        0.669854
C          3.571829       -0.515343        0.562312
C          3.188367       -2.816339        0.071218
H          1.137715       -3.467879        0.037661
H          1.819901        0.675546        0.922710
H          5.153996       -1.931911        0.177321
C          4.490697        0.664937        0.687183
C          3.706096       -4.183532       -0.280637
F          4.013112        1.585640        1.535804
F          5.712023        0.312280        1.104905
F          4.645947        1.282572       -0.501345
F          4.969402       -4.357661        0.134696
F          2.960173       -5.150837        0.270276
F          3.696354       -4.388088       -1.606207
C         -3.554058       -1.225403       -0.446498
C         -5.992882       -1.174263        0.120884
C         -5.249369       -1.218541       -2.292030
C         -6.323597       -0.742240       -1.311275
C         -3.855916       -0.745301       -1.869145
C         -4.606909       -0.653599        0.522919
H         -6.010230       -2.270753        0.185397
H         -5.256718       -2.316429       -2.333475
H         -6.383808        0.354102       -1.347944
H         -3.809253        0.351124       -1.889166
H         -4.606764        0.437712        0.383895
H         -3.597214       -2.324764       -0.444519
H         -6.749592       -0.796505        0.817923
H         -5.471762       -0.862840       -3.303378
H         -7.306443       -1.126017       -1.604994
H         -3.094085       -1.129087       -2.552509
N         -4.200128       -0.862556        1.914938
C         -4.922396       -0.008376        2.844139
H         -4.842324        1.031283        2.516546
H         -4.467617       -0.094450        3.835901
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H	-5.989148	-0.273592	2.938412
C	-4.226961	-2.252469	2.347373
H	-5.246057	-2.667965	2.412013
H	-3.772178	-2.322791	3.340044
H	-3.640370	-2.875181	1.665151
O	-0.235258	1.820420	0.589988
C	-0.328824	3.243300	0.486967
C	-1.136493	2.313080	-0.343823
H	-0.854942	3.696141	1.327199
N	-2.557716	2.194069	0.151651
O	-3.437889	2.399453	-0.659899
O	-2.726094	1.944803	1.329233
C	0.849212	3.987874	-0.031089
C	3.033284	5.461892	-0.941462
C	1.972740	3.332173	-0.537458
C	0.826219	5.383122	0.025485
C	1.912122	6.118035	-0.437025
C	3.064194	4.070374	-0.986034
H	1.999251	2.247046	-0.574265
H	-0.041715	5.891958	0.437060
H	1.887318	7.202127	-0.393099
H	3.941458	3.552800	-1.358358
H	3.886409	6.035255	-1.290082
C	-0.971243	1.995075	-1.795896
H	-1.616897	2.632413	-2.399927
H	-1.230744	0.946593	-1.973621
H	0.069547	2.163316	-2.075919

RS epoxide:Catalyst, binary complex 8; Energy = -2449.852518; 6-31G(d) basis set.

N	0.517468	0.874074	-0.469758
H	0.547307	-0.122252	-0.667679
C	1.741514	1.490742	-0.431368
S	1.977977	3.148824	-0.278779
N	2.746176	0.596973	-0.566046
H	2.563214	-0.365390	-0.276325
C	-0.782954	1.368453	-0.333982
C	-3.480538	2.136481	-0.103128
C	-1.800073	0.602521	-0.918512
C	-1.126746	2.521615	0.382245
C	-2.463489	2.887990	0.476649
C	-3.129069	0.983212	-0.793155
H	-1.545968	-0.285216	-1.491729
H	-0.358281	3.122444	0.847247
H	-4.517299	2.446830	-0.027622
C	-2.846650	4.104222	1.274074
C	-4.203482	0.112732	-1.381300
F	-3.765932	4.840658	0.630745
F	-3.388025	3.761007	2.454967
F	-1.799525	4.894537	1.531326
F	-3.759372	-0.586715	-2.436286
F	-4.661273	-0.774948	-0.484934
F	-5.256456	0.835477	-1.788616
C	4.164327	0.919188	-0.537204
C	6.432796	-0.079969	-0.202585
C	6.145055	1.944545	-1.687563
C	6.965909	0.681549	-1.421047
C	4.652482	1.628156	-1.805766
C	4.941708	-0.401758	-0.382510
H	6.569420	0.531443	0.699359
H	6.293119	2.655766	-0.863583
H	6.915326	0.025833	-2.301276
H	4.470065	0.968394	-2.664990
H	4.831014	-0.941000	-1.336689
H	4.362110	1.577558	0.322019
H	7.001575	-1.004922	-0.054881
H	6.494857	2.440825	-2.598738
H	8.021610	0.933611	-1.274425
H	4.075101	2.541836	-1.960097
N	4.329246	-1.276049	0.623225
C	4.835801	-2.638876	0.553370
H	4.744986	-3.013491	-0.471505
H	4.237638	-3.275318	1.211611
H	5.890800	-2.730630	0.861589
C	4.410660	-0.761796	1.985359
H	5.445033	-0.711628	2.363189

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H          3.830554       -1.416406        2.640283
H          3.963418        0.235054        2.037483
O         -0.003413       -2.046081       -0.434264
C         -0.989112       -2.161571        0.600620
C          0.282959       -2.923275        0.610175
H         -1.020378       -1.291771        1.257580
N          1.310424       -2.335269        1.547439
O          1.946420       -3.117088        2.224431
O          1.393684       -1.124410        1.588329
C         -2.290250       -2.781982        0.235990
C         -4.750809       -3.913507       -0.405649
C         -3.246749       -2.982309        1.233791
C         -2.568100       -3.140817       -1.082430
C         -3.801953       -3.701222       -1.401458
C         -4.471753       -3.554676        0.912395
H         -3.031357       -2.687892        2.257822
H         -1.822109       -2.969358       -1.853209
H         -4.022488       -3.964972       -2.430913
H         -5.213799       -3.711861        1.688492
H         -5.712355       -4.350571       -0.655926
C          0.461080       -4.381553        0.335391
H          0.408535       -4.949943        1.264293
H          1.430310       -4.560105       -0.136613
H         -0.336455       -4.704237       -0.335515

RS epoxide:Catalyst, binary complex 9; Energy = -2449.852319; 6-31G(d) basis set.
N          0.610646        0.812373       -0.604177
H          0.632001       -0.179249       -0.825071
C          1.835655        1.419476       -0.505979
S          2.066633        3.074392       -0.315844
N          2.840858        0.524363       -0.621685
H          2.645258       -0.438036       -0.339479
C         -0.684797        1.311816       -0.431653
C         -3.369275        2.075747       -0.105097
C         -1.013203        2.372698        0.419941
C         -1.708190        0.635915       -1.109270
C         -3.031751        1.014466       -0.936181
C         -2.345584        2.740048        0.562263
H         -0.238059        2.900586        0.957376
H         -1.461690       -0.184523       -1.777173
H         -4.404133        2.380847        0.016503
C         -4.133864        0.269935       -1.635265
C         -2.724988        3.866398        1.483456
F         -4.988021        1.113470       -2.234743
F         -3.668332       -0.565780       -2.574252
F         -4.854716       -0.458614       -0.770157
F         -3.491129        3.424125        2.495541
F         -1.660223        4.469841        2.020626
F         -3.443244        4.800294        0.841428
C          4.257717        0.840633       -0.529127
C          6.504357       -0.180209       -0.111757
C          6.291310        1.866068       -1.580484
C          7.091489        0.593183       -1.297492
C          4.802609        1.563133       -1.765917
C          5.019456       -0.487048       -0.356168
H          6.609280        0.417683        0.803415
H          6.409797        2.564798       -0.741131
H          7.071839       -0.050504       -2.187735
H          4.651948        0.916868       -2.641469
H          4.943588       -1.016490       -1.319245
H          4.420778        1.487359        0.346231
H          7.059049       -1.112151        0.045898
H          6.683170        2.371887       -2.469014
H          8.142117        0.835386       -1.105191
H          4.238311        2.483213       -1.931228
N          4.356865       -1.363827        0.614302
C          4.844369       -2.733344        0.551277
H          4.796406       -3.094677       -0.481069
H          4.205142       -3.366952        1.172735
H          5.882077       -2.845743        0.908164
C          4.386356       -0.866236        1.984082
H          5.404298       -0.833678        2.406098
H          3.770611       -1.521194        2.605041
H          3.949458        0.135531        2.029678
O         -0.160539       -2.054493       -0.494617
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C         -1.113109       -2.027165        0.575435
C          0.080936       -2.907321        0.581335
H         -1.037038       -1.130648        1.191585
N          1.200313       -2.379728        1.449643
O          1.813557       -3.191679        2.111785
O          1.380297       -1.178534        1.450450
C         -2.481080       -2.535983        0.292108
C         -5.051521       -3.500690       -0.171555
C         -3.437878       -2.489872        1.308061
C         -2.816788       -3.048376       -0.961140
C         -4.103817       -3.526777       -1.190735
C         -4.718415       -2.978996        1.077199
H         -3.178366       -2.071476        2.277240
H         -2.073712       -3.056561       -1.753780
H         -4.366564       -3.913646       -2.170215
H         -5.459419       -2.944080        1.869450
H         -6.054123       -3.875080       -0.352567
C          0.113716       -4.387768        0.375693
H          0.057175       -4.902931        1.335012
H          1.037785       -4.678961       -0.129392
H         -0.741691       -4.670884       -0.238839

RS epoxide:Catalyst, binary complex 10; Energy = -2449.842324; 6-31G(d) basis set.
N          0.392130       -0.893791        0.206449
H          0.494578       -0.000823        0.687502
C          1.518325       -1.469866       -0.332711
S          1.474577       -2.690359       -1.494313
N          2.656074       -0.925494        0.121997
H          2.591408       -0.231341        0.858372
C         -0.920460       -1.398084        0.114588
C         -3.562435       -2.341242        0.049276
C         -1.193759       -2.747075        0.367471
C         -1.970628       -0.529482       -0.172408
C         -3.281137       -1.004928       -0.189795
C         -2.501956       -3.203531        0.321014
H         -0.381957       -3.426109        0.599006
H         -1.770056        0.513008       -0.400092
H         -4.582428       -2.707670        0.024911
C         -4.398298       -0.035824       -0.451328
C         -2.784735       -4.665247        0.528343
F         -5.528400       -0.654877       -0.812210
F         -4.687416        0.694808        0.645340
F         -4.081578        0.834490       -1.418960
F         -1.849465       -5.252883        1.286287
F         -3.970712       -4.856296        1.127545
F         -2.825225       -5.328790       -0.636004
C          4.004029       -1.205984       -0.359661
C          6.295681       -0.234711       -0.692822
C          6.091813       -2.565868        0.186557
C          6.907658       -1.275850        0.241092
C          4.637361       -2.274291        0.544351
C          4.826752        0.091077       -0.372541
H          6.325683       -0.602026       -1.726860
H          6.144744       -2.988701       -0.825578
H          6.915621       -0.893181        1.271248
H          4.584683       -1.917663        1.583005
H          4.774021        0.499766        0.657370
H          3.916058       -1.603475       -1.375801
H          6.877049        0.693181       -0.675077
H          6.499033       -3.318484        0.869686
H          7.950301       -1.462141       -0.037341
H          4.017704       -3.174816        0.478654
N          4.373977        1.111040       -1.332887
C          3.041126        1.035659       -1.901142
H          2.834770        0.041174       -2.303876
H          2.991338        1.745686       -2.734126
H          2.234263        1.292840       -1.190062
C          4.650700        2.449549       -0.845385
H          4.007233        2.733060        0.008263
H          4.496781        3.174093       -1.651515
H          5.692191        2.528911       -0.520515
O         -0.510198        1.817343        1.320738
C         -0.339067        2.753759        0.248808
C          0.175061        2.986608        1.619671
H          0.399344        2.434460       -0.488940
```

N	1.655838	2.731213	1.739924
O	2.336765	3.617578	2.200729
O	2.073386	1.664246	1.320773
C	-1.558323	3.430668	-0.265963
C	-3.827271	4.686279	-1.275813
C	-2.813124	3.129646	0.262207
C	-1.437540	4.354800	-1.306288
C	-2.571349	4.987505	-1.802591
C	-3.947622	3.752846	-0.250332
H	-2.900298	2.387451	1.049946
H	-0.459438	4.573411	-1.727040
H	-2.476721	5.708613	-2.608007
H	-4.924258	3.492083	0.144549
H	-4.712245	5.171443	-1.675101
C	-0.358584	3.951015	2.630959
H	0.157594	4.907588	2.547976
H	-0.221098	3.554092	3.639582
H	-1.423027	4.094559	2.441227

RS epoxide:Catalyst, binary complex 11; Energy = -2449.852380; 6-31G(d) basis set.

N	-0.508124	-0.793204	0.272683
H	-0.000669	0.052170	0.026032
C	0.272168	-1.923157	0.322542
S	-0.323245	-3.493990	0.232471
N	1.583391	-1.631749	0.425250
H	1.863606	-0.659450	0.333337
C	-1.895286	-0.706325	0.083892
C	-4.653587	-0.317563	-0.259842
C	-2.369257	0.275124	-0.788240
C	-2.806909	-1.494232	0.792756
C	-4.168669	-1.296944	0.602168
C	-3.736856	0.467912	-0.945706
H	-1.663349	0.879332	-1.352175
H	-2.449918	-2.240376	1.490655
H	-5.719653	-0.161669	-0.380033
C	-5.142800	-2.179805	1.331177
C	-4.219136	1.505088	-1.918963
F	-5.421640	-3.290749	0.633873
F	-4.665983	-2.571715	2.520825
F	-6.308564	-1.551929	1.549773
F	-5.442067	1.952859	-1.604548
F	-3.396161	2.566574	-1.956232
F	-4.285368	1.022179	-3.168659
C	2.650206	-2.612445	0.306632
C	4.993446	-3.022534	-0.424068
C	3.973533	-4.434812	1.411852
C	5.260784	-3.830978	0.849845
C	2.912681	-3.354591	1.621906
C	3.939556	-1.928788	-0.173362
H	4.643467	-3.693501	-1.220321
H	3.583674	-5.183882	0.709603
H	5.704694	-3.166451	1.604265
H	3.249731	-2.630343	2.376038
H	4.309525	-1.299564	0.654264
H	2.333853	-3.353988	-0.439373
H	5.928539	-2.571755	-0.770600
H	4.173998	-4.956321	2.353425
H	5.998318	-4.614377	0.646014
H	1.974005	-3.790541	1.973762
N	3.694731	-0.994992	-1.289582
C	4.941672	-0.409362	-1.772682
H	5.553131	-0.081212	-0.924781
H	4.715096	0.457750	-2.399582
H	5.542764	-1.113264	-2.369544
C	2.967113	-1.582645	-2.412865
H	3.508215	-2.418842	-2.884540
H	2.817721	-0.806183	-3.169564
H	1.980656	-1.930098	-2.095878
O	1.588513	1.467057	0.598886
C	1.077530	2.730340	0.153786
C	2.269269	2.080046	-0.447331
H	0.152429	2.645874	-0.417137
N	1.965399	1.407445	-1.762164
O	2.688209	1.671114	-2.697990
O	0.976605	0.697362	-1.810891

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C          1.178516        3.884745        1.083869
C          1.339082        6.086695        2.781233
C          1.809141        3.763815        2.322813
C          0.618322        5.104489        0.699977
C          0.704034        6.204621        1.546096
C          1.886694        4.866136        3.169271
H          2.218021        2.803618        2.623247
H          0.114262        5.191533       -0.259095
H          0.269414        7.151936        1.243663
H          2.369654        4.768283        4.136255
H          1.399097        6.944267        3.443765
C          3.695296        2.488716       -0.270979
H          4.034014        3.068844       -1.129126
H          4.314552        1.595174       -0.168421
H          3.777449        3.093844        0.633009

RS epoxide:Catalyst, binary complex 12; Energy = -2449.853446; 6-31G(d) basis set.
N         -0.053769       -1.084720        0.566096
H         -0.237058       -0.229686        1.084183
C         -1.086941       -1.480854       -0.251990
S         -0.946944       -2.607801       -1.485320
N         -2.238884       -0.828554        0.042925
H         -2.325878       -0.462860        0.997160
C          1.318171       -1.357315        0.422366
C          4.089346       -1.749344        0.192620
C          2.204935       -0.300857        0.635687
C          1.822791       -2.628667        0.134389
C          3.197069       -2.803390        0.020962
C          3.573660       -0.499734        0.509441
H          1.817524        0.680614        0.889801
H          1.148998       -3.463300       -0.002044
H          5.157756       -1.901878        0.085483
C          3.745552       -4.181258       -0.227895
C          4.485353        0.688290        0.611271
F          4.861534       -4.138437       -0.971033
F          4.068987       -4.793511        0.923088
F          2.865066       -4.966639       -0.858350
F          4.610244        1.302980       -0.582348
F          4.018080        1.607962        1.466638
F          5.717833        0.346739        1.004522
C         -3.549317       -1.235191       -0.462723
C         -5.987846       -1.204923        0.106612
C         -5.245481       -1.210808       -2.307231
C         -6.321490       -0.754191       -1.319128
C         -3.854315       -0.736365       -1.878242
C         -4.604349       -0.683133        0.515599
H         -5.999649       -2.302289        0.155307
H         -5.247154       -2.307980       -2.364604
H         -6.387425        0.342233       -1.340107
H         -3.813625        0.360467       -1.882870
H         -4.610141        0.410093        0.393006
H         -3.586917       -2.334641       -0.476800
H         -6.746233       -0.840910        0.809153
H         -5.470301       -0.841599       -3.313191
H         -7.302519       -1.138777       -1.617823
H         -3.090578       -1.106562       -2.567042
N         -4.195398       -0.910727        1.904124
C         -4.922860       -0.075722        2.846545
H         -4.850304        0.969317        2.534680
H         -4.466913       -0.173544        3.836659
H         -5.987699       -0.349679        2.937293
C         -4.212729       -2.307221        2.315240
H         -5.229042       -2.730357        2.374393
H         -3.756647       -2.389735        3.306360
H         -3.622687       -2.915563        1.623083
O         -0.248750        1.813185        0.600036
C         -0.350006        3.236978        0.517396
C         -1.156070        2.314231       -0.323243
H         -0.875615        3.674964        1.365811
N         -2.574827        2.181568        0.176415
O         -3.459438        2.392930       -0.628789
O         -2.737050        1.916502        1.351368
C          0.822345        3.995936        0.007720
C          2.996769        5.497300       -0.880954
C          1.944095        3.355663       -0.521867
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C          0.796317        5.389398        0.098001
C          1.877236        6.138173       -0.353796
C          3.030801        4.107334       -0.959506
H          1.973443        2.271835       -0.585118
H         -0.069992        5.885709        0.527781
H          1.850083        7.220808       -0.283311
H          3.906862        3.601235       -1.350000
H          3.846301        6.081130       -1.220795
C         -0.995342        2.015888       -1.779992
H         -1.248314        0.967807       -1.969357
H          0.042906        2.194709       -2.062798
H         -1.647889        2.656211       -2.373359

RS epoxide:Catalyst, binary complex 13; Energy = -2449.853100; 6-31G(d) basis set.
N          0.044945       -1.003388        0.493636
H         -0.159031       -0.165485        1.031400
C         -0.986099       -1.425822       -0.312494
S         -0.816651       -2.488441       -1.599083
N         -2.165641       -0.853689        0.038164
H         -2.247327       -0.541311        1.011642
C          1.419179       -1.263187        0.364158
C          4.196348       -1.663778        0.221861
C          2.301985       -0.215153        0.627286
C          1.930691       -2.529259        0.057376
C          3.305259       -2.707051       -0.018139
C          3.675892       -0.421619        0.552492
H          1.911392        0.766088        0.884707
H          1.259850       -3.360022       -0.112222
H          5.267244       -1.821512        0.161843
C          3.854158       -4.053224       -0.401590
C          4.586039        0.731096        0.865588
F          4.119446       -4.122900       -1.714706
F          5.003621       -4.313420        0.240678
F          2.998083       -5.042495       -0.117230
F          4.174542        1.857298        0.255450
F          4.613641        0.996691        2.180272
F          5.845517        0.500656        0.477474
C         -3.462307       -1.321811       -0.452107
C         -5.879425       -1.489305        0.176585
C         -5.204602       -1.336903       -2.252348
C         -6.281775       -1.000801       -1.218402
C         -3.840006       -0.782647       -1.834766
C         -4.524866       -0.888901        0.576789
H         -5.811964       -2.585651        0.175005
H         -5.130772       -2.427743       -2.359528
H         -6.423177        0.088203       -1.187247
H         -3.881483        0.313071       -1.789397
H         -4.611885        0.205335        0.505605
H         -3.428981       -2.419331       -0.517995
H         -6.642618       -1.212350        0.913045
H         -5.482571       -0.941028       -3.234612
H         -7.242052       -1.439366       -1.510149
H         -3.069841       -1.064547       -2.557870
N         -4.063211       -1.149218        1.942833
C         -4.812485       -0.399336        2.938514
H         -4.803931        0.661332        2.674612
H         -4.329108       -0.516992        3.913321
H         -5.858388       -0.735805        3.038410
C         -3.988033       -2.560565        2.292269
H         -4.976610       -3.043875        2.360143
H         -3.498654       -2.658167        3.265940
H         -3.385431       -3.103424        1.557559
O         -0.360972        1.841687        0.564585
C         -0.532932        3.259840        0.505721
C         -1.342852        2.307897       -0.298275
H         -1.024473        3.666939        1.389301
N         -2.722647        2.103287        0.278967
O         -3.661070        2.307446       -0.465347
O         -2.805108        1.793251        1.451005
C          0.572332        4.068678       -0.071522
C          2.626813        5.640826       -1.108363
C          1.682123        3.465417       -0.664554
C          0.497285        5.460740        0.009682
C          1.519185        6.244285       -0.514994
C          2.709185        4.252410       -1.177180
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H          1.749372        2.382637       -0.711328
H         -0.359456        5.928780        0.487512
H          1.455529        7.325884       -0.452080
H          3.577164        3.775934       -1.621095
H          3.428709        6.253256       -1.508304
C         -1.250654        2.039737       -1.767112
H         -1.438569        0.978789       -1.958852
H         -0.247276        2.295921       -2.109279
H         -1.982467        2.639646       -2.308187

RS epoxide:Catalyst, binary complex 14; Energy = -2449.843153; 6-31G(d) basis set.
N          0.354283       -0.726891       -1.257150
H          0.286613        0.109838       -1.826983
C          1.622090       -1.167697       -0.943794
S          1.904131       -2.698680       -0.305872
N          2.556998       -0.253273       -1.251059
H          2.225361        0.671696       -1.509822
C         -0.882209       -1.183258       -0.780786
C         -3.462622       -1.807251        0.147638
C         -1.994295       -1.010910       -1.604950
C         -1.064474       -1.680240        0.514390
C         -2.344105       -1.994340        0.953681
C         -3.268545       -1.304893       -1.131836
H         -1.862200       -0.618417       -2.610103
H         -0.213466       -1.799003        1.174666
H         -4.457380       -2.028210        0.515461
C         -2.501559       -2.542297        2.345215
C         -4.436264       -1.050882       -2.040347
F         -3.769934       -2.463244        2.771394
F         -2.137148       -3.829437        2.415361
F         -1.737406       -1.873496        3.222493
F         -4.340838        0.163887       -2.615370
F         -4.509926       -1.942682       -3.035689
F         -5.602412       -1.082941       -1.380487
C          4.006458       -0.320540       -1.047405
C          5.941615       -0.504754        0.537644
C          6.208862       -1.250491       -1.848819
C          6.621261       -1.506501       -0.398529
C          4.687980       -1.306079       -2.005043
C          4.411990       -0.590412        0.415979
H          6.282542        0.508578        0.283613
H          6.572252       -0.259884       -2.156809
H          6.330419       -2.526459       -0.113275
H          4.326955       -2.317041       -1.786852
H          4.120555       -1.620404        0.638388
H          4.348324        0.690523       -1.308835
H          6.233681       -0.688645        1.578917
H          6.676029       -1.981449       -2.517013
H          7.709698       -1.442592       -0.294014
H          4.392728       -1.066227       -3.032136
N          3.655841        0.256858        1.343665
C          3.464091       -0.380487        2.636792
H          2.990662       -1.356203        2.494010
H          2.800809        0.239880        3.249891
H          4.405213       -0.519581        3.198505
C          4.192915        1.598551        1.508279
H          5.152795        1.620114        2.051775
H          3.477503        2.203169        2.075776
H          4.338453        2.078271        0.534588
O         -0.056335        2.109331       -1.234593
C         -0.605556        3.254473       -0.552905
C          0.515551        2.467593       -0.020357
H         -0.360203        4.197965       -1.041054
N          1.868145        3.102625       -0.202554
O          2.200231        3.901822        0.645111
O          2.539796        2.756623       -1.158347
C         -1.971419        3.112834        0.027759
C         -4.504821        2.845634        1.149016
C         -2.351240        3.934123        1.090743
C         -2.859868        2.166857       -0.478662
C         -4.127187        2.033060        0.083101
C         -3.617843        3.798018        1.649813
H         -1.654057        4.670177        1.483121
H         -2.560574        1.544191       -1.314274
H         -4.818446        1.296721       -0.315546
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H         -3.911079        4.431185        2.481038
H         -5.490988        2.739206        1.589678
C          0.498556        1.539336        1.158280
H          0.629835        2.117377        2.076960
H          1.316267        0.810319        1.071463
H         -0.467991        1.030883        1.186455

RS epoxide:Catalyst, binary complex 15; Energy = -2449.842774; 6-31G(d) basis set.
N         -0.004293       -0.850693       -0.606072
H          0.043592        0.076370       -1.018385
C          1.194729       -1.425584       -0.251495
S          1.294663       -2.767525        0.762375
N          2.241191       -0.769532       -0.784485
H          2.035796        0.011316       -1.401056
C         -1.311135       -1.260005       -0.305739
C         -4.013408       -1.908370        0.110923
C         -1.722279       -2.599032       -0.318989
C         -2.255169       -0.258815       -0.084066
C         -3.594032       -0.587608        0.106306
C         -3.057591       -2.901795       -0.097375
H         -1.005074       -3.385668       -0.509391
H         -1.939596        0.781782       -0.062808
H         -5.056488       -2.161041        0.263475
C         -4.575493        0.534356        0.273688
C         -3.496386       -4.339147       -0.057108
F         -4.197507        1.385948        1.238612
F         -4.673511        1.263590       -0.857880
F         -5.803803        0.099985        0.571602
F         -2.630093       -5.148147       -0.678680
F         -3.619244       -4.779203        1.204077
F         -4.694489       -4.500309       -0.641455
C          3.670755       -1.083713       -0.684302
C          5.725340       -1.337641        0.741284
C          5.514198       -2.679653       -1.365375
C          6.031741       -2.678793        0.073196
C          4.011685       -2.400721       -1.396085
C          4.215200       -1.046837        0.756540
H          6.251521       -0.545289        0.191398
H          6.046562       -1.908224       -1.939609
H          5.547124       -3.489114        0.634117
H          3.476025       -3.216149       -0.899731
H          3.724648       -1.856754        1.303191
H          4.152821       -0.267491       -1.238703
H          6.107035       -1.319004        1.769517
H          5.721245       -3.638600       -1.851874
H          7.109518       -2.872610        0.094531
H          3.645503       -2.346907       -2.427266
N          3.833218        0.199634        1.432205
C          3.687113        0.025021        2.868808
H          2.971632       -0.777382        3.068827
H          3.297756        0.951162        3.306486
H          4.638607       -0.211018        3.377930
C          4.700624        1.330863        1.142870
H          5.699365        1.244318        1.603205
H          4.236770        2.245620        1.527095
H          4.831219        1.452257        0.062113
O          0.404098        1.974076       -1.307318
C          0.280386        3.409541       -1.217321
C          1.254532        2.639177       -0.431532
H          0.654603        3.908470       -2.111796
N          2.661175        2.734486       -0.957293
O          3.338145        3.616861       -0.475534
O          3.021096        1.941890       -1.807399
C         -0.935389        3.981250       -0.572304
C         -3.166454        5.136381        0.624307
C         -0.784875        5.098693        0.251138
C         -2.201619        3.443232       -0.799676
C         -3.316468        4.021646       -0.196125
C         -1.901026        5.675976        0.847376
H          0.206627        5.510543        0.424004
H         -2.318954        2.580776       -1.450905
H         -4.298059        3.594317       -0.365470
H         -1.782571        6.542136        1.490626
H         -4.036802        5.584359        1.093104
C          1.218202        2.325836        1.034038
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H          1.694365        3.131130        1.598187
H          1.757742        1.385145        1.212837
H          0.175836        2.233753        1.345511

RS epoxide:Catalyst, binary complex 16; Energy = -2449.844831; 6-31G(d) basis set.
N         -1.788996       -0.572451       -0.796451
C         -1.425311        0.126617       -1.875557
S         -2.462414        0.887078       -2.969295
C         -3.149252       -0.957481       -0.392365
C         -4.028733        0.229018        0.041361
C         -5.415581       -0.330313        0.399748
C         -6.145588       -0.898958       -0.835795
C         -5.170581       -1.252276       -1.968034
C         -3.866684       -1.855084       -1.440698
N         -3.379933        1.011689        1.100744
C         -3.511546        0.443653        2.436955
N         -0.074670        0.266743       -2.092149
C          1.025234       -0.339719       -1.471520
C          1.033867       -1.684158       -1.087989
C          2.205424       -2.243973       -0.587715
C          3.377022       -1.505889       -0.469711
C          3.349042       -0.165415       -0.843520
C          2.190579        0.422484       -1.328302
C          2.168842       -3.659752       -0.085081
F          1.315683       -4.417121       -0.784292
C          4.560436        0.696144       -0.621684
F          5.695728       -0.000514       -0.747283
C         -3.818366        2.400297        1.101163
F          3.373897       -4.239079       -0.136044
F          1.766263       -3.696591        1.197717
F          4.607891        1.724215       -1.477105
F          4.559652        1.221368        0.619351
H         -1.071936       -0.801433       -0.112616
H          0.136892        0.994228       -2.763867
H         -3.183650       -2.045329       -2.273847
H         -4.078882       -2.825717       -0.977150
H         -5.640052       -1.956478       -2.662902
H         -4.928575       -0.354945       -2.543605
H         -6.714762       -1.786612       -0.539186
H         -6.875226       -0.172694       -1.208586
H         -5.286969       -1.121853        1.149731
H         -6.018831        0.450148        0.876972
H         -2.968385       -1.561548        0.503024
H         -4.126805        0.900643       -0.816085
H         -3.670022        2.834229        0.107871
H         -4.879361        2.520233        1.381903
H         -3.217405        2.969810        1.819413
H         -4.535845        0.513474        2.838262
H         -2.847589        0.982199        3.123441
H         -3.211593       -0.609061        2.443327
H          0.150478       -2.301328       -1.214737
H          4.285089       -1.959988       -0.088567
H          2.184527        1.473269       -1.606944
N         -0.526438       -0.760423        2.716110
O         -0.755358       -1.553247        1.810159
O         -1.001331       -0.806469        3.823617
C          0.457511        0.342845        2.393779
C         -0.170577        1.498370        1.722331
H         -1.247123        1.414857        1.546386
O          0.210946        1.488986        3.115364
C          0.539030        2.413336        0.793632
C          1.776170        4.081210       -1.070829
C         -0.142873        2.804332       -0.361044
C          1.831430        2.889826        1.031266
C          2.449999        3.712914        0.094624
C          0.474381        3.634216       -1.293351
H         -1.160559        2.452875       -0.527056
H          2.341745        2.635642        1.955369
H          3.459828        4.067457        0.275316
H         -0.066155        3.931366       -2.187365
H          2.261212        4.726596       -1.796643
C          1.845421       -0.215245        2.292016
H          1.815584       -1.191189        1.805864
H          2.254216       -0.329313        3.300141
H          2.487191        0.451653        1.716763
```

RS epoxide:Catalyst, binary complex 17; Energy = -2449.844553; 6-31G(d) basis set.

N	-0.785184	0.073623	-0.885692
H	-0.410349	-0.834382	-1.148715
C	-2.160262	0.236920	-1.002160
S	-2.868648	1.720164	-1.332894
N	-2.804298	-0.927505	-0.824776
H	-2.238741	-1.690776	-0.463445
C	0.173153	1.077529	-0.685233
C	2.237577	2.887658	-0.095623
C	-0.047170	2.129233	0.211661
C	1.421133	0.950536	-1.299350
C	2.443873	1.837122	-0.980028
C	0.978067	3.025631	0.481318
H	-1.006378	2.229698	0.704756
H	1.596491	0.146261	-2.004990
H	3.038400	3.579186	0.145171
C	3.823652	1.618622	-1.530107
C	0.730245	4.185013	1.406339
F	3.823404	0.800346	-2.592580
F	4.409345	2.764774	-1.891969
F	4.624207	1.048684	-0.605388
F	-0.311814	3.966182	2.217289
F	1.801385	4.429233	2.177637
F	0.476741	5.311501	0.725372
C	-4.248071	-1.188897	-0.840052
C	-6.478559	-0.931072	0.269577
C	-6.349636	-1.390499	-2.203228
C	-7.123203	-0.676549	-1.094078
C	-4.887573	-0.942101	-2.211083
C	-5.010983	-0.479436	0.306505
H	-6.541869	-2.004990	0.497037
H	-6.402194	-2.476368	-2.039257
H	-7.128895	0.402865	-1.297217
H	-4.829629	0.123355	-2.452228
H	-4.989286	0.596608	0.102549
H	-4.313965	-2.268077	-0.645526
H	-7.013869	-0.405334	1.065878
H	-6.803774	-1.194096	-3.180039
H	-8.168056	-1.004984	-1.082409
H	-4.313831	-1.482754	-2.972206
N	-4.452092	-0.661934	1.645088
C	-4.106469	-2.021227	2.012282
H	-4.903057	-2.714241	1.726927
H	-3.988490	-2.079025	3.100042
H	-3.156941	-2.371449	1.568155
C	-3.406030	0.263751	2.038132
H	-2.408858	0.012034	1.631240
H	-3.317859	0.258490	3.131031
H	-3.663660	1.275901	1.715310
O	1.388247	-1.865803	-0.528848
C	1.984066	-2.951213	0.180917
C	1.310682	-1.812196	0.858214
H	1.413063	-3.876858	0.119908
N	-0.089689	-2.139916	1.319605
O	-0.409480	-1.779192	2.427992
O	-0.794979	-2.772262	0.546479
C	3.467145	-3.050209	0.130387
C	6.246371	-3.226962	0.083795
C	4.217491	-2.081519	-0.535800
C	4.107474	-4.117973	0.761058
C	5.496133	-4.202745	0.738192
C	5.605456	-2.167357	-0.554812
H	3.710129	-1.269423	-1.045564
H	3.521622	-4.879633	1.269022
H	5.993163	-5.032144	1.230915
H	6.179110	-1.402608	-1.068708
H	7.329465	-3.295804	0.068761
C	1.967580	-0.717706	1.642270
H	2.139351	-1.046691	2.668502
H	1.340137	0.176938	1.656225
H	2.923415	-0.478753	1.172809

RS epoxide:Catalyst, binary complex 18; Energy = -2449.842890; 6-31G(d) basis set.

N	0.571906	0.702712	-0.356902

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H          0.557644       -0.312923       -0.424912
C          1.796582        1.299650       -0.552136
S          2.027993        2.943071       -0.833876
N          2.802118        0.412204       -0.506801
H          2.578223       -0.541614       -0.239767
C         -0.696234        1.297544       -0.288115
C         -3.307234        2.319509       -0.101538
C         -1.776690        0.589888       -0.825751
C         -0.930473        2.513397        0.360517
C         -2.225680        3.013617        0.427734
C         -3.065346        1.097147       -0.716919
H         -1.605019       -0.348857       -1.345002
H         -0.108850        3.056707        0.808427
H         -4.312843        2.718016       -0.031305
C         -2.442167        4.357498        1.066612
C         -4.225040        0.285302       -1.217736
F         -2.165887        5.356700        0.216864
F         -3.712665        4.518910        1.465506
F         -1.656167        4.527091        2.139091
F         -3.874700       -0.516560       -2.234880
F         -4.722874       -0.499191       -0.248895
F         -5.229474        1.063941       -1.644275
C          4.220238        0.699596       -0.683724
C          6.533495       -0.088107       -0.101654
C          6.074679        0.696766       -2.431791
C          6.869773       -0.288781       -1.577438
C          4.581610        0.526429       -2.165697
C          5.036149       -0.238762        0.214782
H          6.828179        0.921925        0.211397
H          6.378587        1.722701       -2.184040
H          6.621137       -1.315796       -1.880206
H          4.270712       -0.481329       -2.476203
H          4.725086       -1.268635       -0.061242
H          4.391844        1.741024       -0.391164
H          7.097865       -0.785431        0.526988
H          6.282262        0.550526       -3.496970
H          7.945906       -0.162321       -1.736599
H          3.985074        1.241592       -2.742028
N          4.856245       -0.037881        1.660522
C          3.734677        0.740375        2.163806
H          3.638265        1.688278        1.628744
H          3.940698        0.976502        3.213728
H          2.765093        0.216004        2.123495
C          4.971580       -1.292503        2.383132
H          4.101677       -1.955032        2.222831
H          5.057489       -1.091385        3.456004
H          5.873576       -1.828183        2.071400
O         -0.257971       -2.252534       -0.641381
C         -1.048259       -2.380417        0.548014
C          0.062715       -3.306005        0.209032
H         -0.822311       -1.621296        1.298570
N          1.338571       -3.017895        0.963567
O          1.907307       -3.954248        1.473254
O          1.692726       -1.851422        1.033811
C         -2.474504       -2.767051        0.385641
C         -5.138271       -3.542028        0.145586
C         -2.993726       -3.099204       -0.866344
C         -3.295377       -2.802407        1.514638
C         -4.623477       -3.195301        1.393408
C         -4.325710       -3.484704       -0.983324
H         -2.358607       -3.040096       -1.745830
H         -2.893759       -2.524350        2.485752
H         -5.258564       -3.223930        2.272864
H         -4.729678       -3.730976       -1.960117
H         -6.176923       -3.842983        0.052524
C         -0.051820       -4.724523       -0.251655
H          0.007479       -5.400909        0.601216
H          0.753645       -4.960186       -0.951180
H         -1.013202       -4.854084       -0.748740

RS epoxide:Catalyst, binary complex 19; Energy = -2449.844469; 6-31G(d) basis set.
N         -0.800838        0.067424       -0.942941
H         -0.430994       -0.848073       -1.185935
C         -2.175563        0.235791       -1.040407
S         -2.878796        1.720794       -1.375882
```

N	-2.823932	-0.923173	-0.841971
H	-2.259223	-1.682890	-0.471857
C	0.162804	1.065173	-0.737123
C	2.236458	2.863355	-0.141747
C	1.406143	0.942695	-1.363375
C	-0.047074	2.105594	0.173106
C	0.984327	2.994255	0.449589
C	2.432268	1.823469	-1.042766
H	1.572485	0.147887	-2.081675
H	-1.006091	2.207345	0.667787
H	3.037996	3.555881	0.092462
C	0.772197	4.048738	1.499950
C	3.805658	1.617433	-1.613471
F	1.557981	5.115095	1.299545
F	-0.495589	4.473412	1.534767
F	1.062116	3.572889	2.723010
F	3.799935	0.788326	-2.667133
F	4.370591	2.767349	-1.995753
F	4.627623	1.068262	-0.694788
C	-4.269397	-1.175692	-0.838269
C	-6.486322	-0.891032	0.291959
C	-6.386918	-1.375530	-2.177245
C	-7.143098	-0.644381	-1.067337
C	-4.921690	-0.938448	-2.204887
C	-5.015082	-0.449852	0.309310
H	-6.555276	-1.962355	0.529895
H	-6.446164	-2.459226	-2.001568
H	-7.142250	0.433026	-1.280948
H	-4.858486	0.123968	-2.457806
H	-4.987768	0.624067	0.094823
H	-4.340081	-2.252435	-0.632230
H	-7.009572	-0.354122	1.088833
H	-6.849754	-1.185473	-3.151217
H	-8.190376	-0.964229	-1.041590
H	-4.359822	-1.491115	-2.966242
N	-4.442724	-0.623389	1.643614
C	-4.105352	-1.982048	2.021017
H	-4.911980	-2.670314	1.753074
H	-3.974257	-2.029215	3.107768
H	-3.164635	-2.345739	1.569106
C	-3.381802	0.295438	2.012623
H	-2.393060	0.029087	1.594472
H	-3.277967	0.299897	3.104147
H	-3.633830	1.306894	1.683106
O	1.394665	-1.835767	-0.524509
C	1.987391	-2.909772	0.204381
C	1.315944	-1.757487	0.861205
H	1.414765	-3.835271	0.159049
N	-0.085850	-2.074025	1.326440
O	-0.406493	-1.692796	2.427741
O	-0.791251	-2.719106	0.564023
C	3.470369	-3.012233	0.155495
C	6.249162	-3.194804	0.108405
C	4.221452	-2.057647	-0.529979
C	4.109685	-4.068937	0.805538
C	5.498181	-4.156611	0.782307
C	5.609216	-2.146347	-0.549358
H	3.714454	-1.254397	-1.053997
H	3.523096	-4.819810	1.328486
H	5.994603	-4.977566	1.289576
H	6.183624	-1.392593	-1.078461
H	7.332109	-3.265932	0.093053
C	1.977088	-0.653518	1.628575
H	2.155180	-0.971030	2.657426
H	1.351387	0.242393	1.638064
H	2.930457	-0.421486	1.150676

RS epoxide:Catalyst, binary complex 20; Energy = -2449.842716; 6-31G(d) basis set.

N	-0.588039	-0.690538	-0.404170
H	-0.575271	0.325503	-0.466361
C	-1.812503	-1.289440	-0.592082
S	-2.040309	-2.930942	-0.888333
N	-2.820450	-0.405820	-0.528088
H	-2.597196	0.544796	-0.249390
C	0.680207	-1.284598	-0.329431

C	3.286700	-2.306956	-0.124016
C	1.760704	-0.585556	-0.872466
C	0.909162	-2.496160	0.334473
C	2.201075	-2.994096	0.413555
C	3.050435	-1.094515	-0.755105
H	1.591525	0.346492	-1.404296
H	0.084118	-3.036142	0.778299
H	4.291410	-2.710539	-0.050768
C	2.472184	-4.292566	1.121007
C	4.213249	-0.294384	-1.267650
F	3.282495	-4.108013	2.177200
F	1.354781	-4.873348	1.568972
F	3.091231	-5.167488	0.314284
F	3.860712	0.513712	-2.278864
F	4.730524	0.481699	-0.302500
F	5.204215	-1.083442	-1.706443
C	-4.239033	-0.695788	-0.696206
C	-6.549590	0.076553	-0.081843
C	-6.109781	-0.675384	-2.426380
C	-6.899850	0.296158	-1.551555
C	-4.614865	-0.503494	-2.172137
C	-5.049729	0.227223	0.222874
H	-6.838785	-0.938384	0.220246
H	-6.407981	-1.705500	-2.189237
H	-6.656950	1.327903	-1.842641
H	-4.310439	0.509572	-2.471603
H	-4.744446	1.261749	-0.041744
H	-4.404155	-1.741734	-0.416426
H	-7.109885	0.763819	0.561405
H	-6.328003	-0.515752	-3.487493
H	-7.977041	0.168675	-1.702617
H	-4.021407	-1.208352	-2.764155
N	-4.855426	0.007238	1.663946
C	-3.729846	-0.778432	2.146074
H	-3.638532	-1.718436	1.596307
H	-3.926764	-1.029669	3.194260
H	-2.760482	-0.253673	2.104849
C	-4.963591	1.251791	2.404757
H	-4.094050	1.915475	2.247084
H	-5.041254	1.035944	3.475418
H	-5.867340	1.792721	2.107534
O	0.251729	2.260740	-0.639206
C	1.052829	2.346213	0.546641
C	-0.052836	3.290887	0.245293
H	0.827153	1.566632	1.276111
N	-1.325316	2.992579	1.000977
O	-1.880317	3.918975	1.543079
O	-1.691498	1.828360	1.038322
C	2.480132	2.729268	0.383835
C	5.143256	3.506664	0.144752
C	3.307629	2.739493	1.508462
C	2.992510	3.086955	-0.863971
C	4.324145	3.473704	-0.980478
C	4.635431	3.133779	1.387890
H	2.911299	2.441281	2.475725
H	2.351828	3.047753	-1.740478
H	4.722529	3.741022	-1.954017
H	5.275484	3.143800	2.264122
H	6.181487	3.809193	0.052100
C	0.071727	4.722093	-0.171780
H	0.043212	5.370420	0.704220
H	-0.746781	4.992849	-0.842716
H	1.022819	4.854275	-0.687542

RS epoxide:Catalyst, binary complex 21; Energy = -2449.850250; 6-31G(d) basis set.

N	-0.686873	-0.655019	-1.004055
H	-0.800416	0.285196	-1.377972
C	-1.824405	-1.348311	-0.669098
S	-1.826382	-2.968248	-0.210416
N	-2.932842	-0.598511	-0.759952
H	-2.820316	0.389657	-0.962253
C	0.651164	-1.029319	-0.767277
C	3.374964	-1.440039	-0.238307
C	1.054218	-1.581706	0.451158
C	1.611844	-0.688186	-1.717957

C	2.960754	-0.890537	-1.443321
C	2.405988	-1.783810	0.697518
H	0.313768	-1.812979	1.209360
H	1.303767	-0.234265	-2.655464
H	4.428286	-1.563912	-0.018373
C	3.972958	-0.481881	-2.474829
C	2.813073	-2.325597	2.039043
F	3.708485	0.743238	-2.963138
F	5.215770	-0.452818	-1.975123
F	3.981657	-1.316803	-3.523970
F	2.165285	-1.694083	3.035711
F	2.529478	-3.628232	2.161781
F	4.126327	-2.177076	2.262895
C	-4.293846	-1.018987	-0.447752
C	-6.508563	-0.228599	0.436351
C	-6.474322	-1.762985	-1.537202
C	-7.195280	-0.588318	-0.879073
C	-5.003814	-1.415402	-1.750383
C	-5.020259	0.123569	0.276025
H	-6.565397	-1.079150	1.128177
H	-6.553950	-2.648011	-0.891708
H	-7.177994	0.276320	-1.557265
H	-4.928670	-0.572019	-2.451650
H	-4.941192	1.007255	-0.390565
H	-4.228922	-1.894174	0.206812
H	-7.018273	0.607078	0.927779
H	-6.937825	-2.022778	-2.494694
H	-8.247949	-0.829427	-0.697553
H	-4.451915	-2.252546	-2.191362
N	-4.491316	0.458440	1.607913
C	-3.175251	0.000564	2.015645
H	-3.044165	-1.065806	1.816130
H	-3.091657	0.147229	3.098252
H	-2.339331	0.547860	1.539707
C	-4.653523	1.871269	1.902214
H	-3.949977	2.505593	1.333368
H	-4.487765	2.045607	2.970518
H	-5.672228	2.192729	1.666394
O	0.509000	2.100867	-1.067010
C	0.761758	1.857708	0.321337
C	0.153086	3.112144	-0.185910
H	0.062387	1.148190	0.767665
N	-1.348892	3.154841	-0.006384
O	-1.816841	4.131961	0.531696
O	-1.985445	2.188017	-0.390304
C	2.183403	1.724172	0.735172
C	4.833485	1.312872	1.491703
C	2.477281	1.201221	1.995082
C	3.218486	2.036586	-0.148329
C	4.541354	1.831246	0.231385
C	3.800835	0.996548	2.372652
H	1.670073	0.920755	2.666866
H	2.981220	2.384959	-1.148988
H	5.341347	2.051996	-0.468314
H	4.021490	0.566759	3.344543
H	5.865196	1.140264	1.781991
C	0.782838	4.466676	-0.266607
H	0.530136	5.050590	0.618308
H	0.430550	4.994002	-1.156653
H	1.865196	4.346565	-0.322959

RS epoxide:Catalyst, binary complex 22; Energy = -2449.852711; 6-31G(d) basis set.

N	-0.254300	-1.521941	0.100128
H	-0.801150	-0.948608	0.793133
C	-0.989356	-1.936020	-0.954511
S	-0.398549	-2.550097	-2.409190
N	-2.335129	-1.753801	-0.786791
H	-2.829377	-2.051304	-1.621804
C	1.130056	-1.346838	0.193410
C	3.863730	-0.808513	0.556473
C	1.548114	-0.233904	0.934012
C	2.088068	-2.208018	-0.346091
C	3.438264	-1.922304	-0.157182
C	2.897658	0.030760	1.103765
H	0.798169	0.433465	1.347786

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H          1.783263       -3.083118       -0.904374
H          4.920732       -0.602101        0.688090
C          4.467590       -2.819930       -0.787352
C          3.335856        1.233765        1.888650
F          4.031536       -4.081671       -0.893543
F          4.790662       -2.408335       -2.022484
F          5.603875       -2.841066       -0.073652
F          3.933730        0.890502        3.037598
F          4.220636        1.972935        1.197884
F          2.304720        2.036605        2.197760
C         -3.136202       -1.950226        0.443609
C         -4.270519       -0.965129        2.488707
C         -5.603664       -2.440665        0.998496
C         -5.652710       -1.204224        1.889343
C         -4.549676       -2.257942       -0.086615
C         -3.185015       -0.749278        1.419889
H         -4.005746       -1.837093        3.102072
H         -5.362741       -3.321499        1.608468
H         -5.957463       -0.333488        1.293795
H         -4.838204       -1.417344       -0.733775
H         -3.439469        0.125803        0.810568
H         -2.751811       -2.833994        0.975944
H         -4.284054       -0.098418        3.159065
H         -6.575373       -2.630035        0.531546
H         -6.392975       -1.326713        2.686490
H         -4.492378       -3.152026       -0.717879
N         -1.869340       -0.443580        2.027432
C         -1.793271        0.923241        2.536366
H         -2.127000        1.620668        1.766914
H         -0.754926        1.159618        2.794032
H         -2.401517        1.069407        3.442052
C         -1.431168       -1.384126        3.059607
H         -1.991460       -1.278306        3.999395
H         -0.372787       -1.198553        3.272673
H         -1.525525       -2.414058        2.706312
O         -1.259068        1.240512       -0.415524
C         -1.583790        2.560788       -0.859001
C         -1.487668        1.402375       -1.778848
H         -2.593031        2.870293       -0.591026
N         -2.826719        0.801424       -2.157049
O         -3.750339        0.947563       -1.377196
O         -2.888085        0.207789       -3.211658
C         -0.516338        3.593828       -0.760626
C          1.451765        5.559314       -0.555322
C          0.763707        3.260780       -0.317400
C         -0.812695        4.917495       -1.091044
C          0.172315        5.895460       -0.995055
C          1.745222        4.241700       -0.212042
H          0.983417        2.231959       -0.051754
H         -1.814195        5.181504       -1.421388
H         -0.061137        6.922654       -1.256922
H          2.734164        3.970924        0.144279
H          2.216257        6.325500       -0.473331
C         -0.402614        1.151774       -2.775897
H         -0.208475        0.080861       -2.871179
H          0.501368        1.659880       -2.436976
H         -0.693812        1.548334       -3.750275

RS epoxide:Catalyst, binary complex 23; Energy = -2449.842321; 6-31G(d) basis set.
N          0.647892        0.682924        0.402043
H          0.528991       -0.314468        0.567116
C          1.940393        1.095354        0.151176
S          2.306975        2.477544       -0.731356
N          2.835785        0.229726        0.660713
H          2.455712       -0.512935        1.238621
C         -0.539806        1.390602        0.159578
C         -3.012092        2.680354       -0.175596
C         -0.684875        2.735915        0.517790
C         -1.631046        0.703548       -0.369517
C         -2.857847        1.345652       -0.516563
C         -1.908110        3.363322        0.332812
H          0.152056        3.274459        0.944887
H         -1.519388       -0.329138       -0.685408
H         -3.967097        3.178838       -0.294478
C         -4.024733        0.538937       -1.011258
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C	-2.046587	4.821742	0.669087
F	-5.061346	1.312036	-1.360039
F	-3.694436	-0.201588	-2.081956
F	-4.461399	-0.314710	-0.070594
F	-1.189697	5.196474	1.628196
F	-1.812923	5.600844	-0.396782
F	-3.285640	5.110377	1.097161
C	4.282310	0.155108	0.434913
C	6.166954	-0.325682	-1.149504
C	6.557538	1.134787	0.863932
C	6.931254	0.878273	-0.596240
C	5.050976	1.357624	0.996643
C	4.645897	-0.148811	-1.036688
H	6.473792	-1.224806	-0.595893
H	6.861433	0.271261	1.472765
H	6.687149	1.768522	-1.191437
H	4.760469	2.258712	0.449628
H	4.362916	0.724455	-1.634664
H	4.587235	-0.720412	1.024280
H	6.410666	-0.501754	-2.201677
H	7.096879	2.004500	1.253567
H	8.009784	0.714193	-0.694785
H	4.762960	1.502149	2.044091
N	3.957398	-1.300433	-1.624777
C	3.916218	-2.493826	-0.808901
H	4.898498	-2.714442	-0.382308
H	3.623057	-3.347284	-1.430489
H	3.188337	-2.427074	0.024937
C	2.659379	-1.039423	-2.220967
H	1.830466	-1.025941	-1.490418
H	2.436357	-1.824180	-2.954349
H	2.670509	-0.076733	-2.737981
O	-0.274151	-2.158583	-0.050982
C	-1.235403	-2.508607	0.954271
C	-0.047623	-3.342902	0.639469
H	-1.155567	-1.900268	1.855969
N	1.084313	-3.165543	1.623862
O	1.678539	-4.156708	1.975095
O	1.310026	-2.029061	2.013207
C	-2.609348	-2.840338	0.495492
C	-5.214040	-3.407913	-0.307885
C	-2.914837	-2.933466	-0.862743
C	-3.611404	-3.018847	1.451493
C	-4.909787	-3.308540	1.048715
C	-4.218267	-3.215188	-1.261139
H	-2.139242	-2.759213	-1.603426
H	-3.374996	-2.924122	2.508154
H	-5.686711	-3.446452	1.793632
H	-4.456263	-3.268361	-2.318562
H	-6.230828	-3.623672	-0.620354
C	-0.016445	-4.650152	-0.084675
H	0.894402	-4.721346	-0.684694
H	-0.887709	-4.706264	-0.737994
H	-0.041538	-5.476858	0.625500

RS epoxide:Catalyst, binary complex 24; Energy = -2449.844426; 6-31G(d) basis set.

N	-0.777632	0.150379	-0.850478
H	-0.470614	-0.730455	-1.256175
C	-2.138511	0.423194	-0.923122
S	-2.747393	1.985440	-0.963077
N	-2.862733	-0.707518	-0.957390
H	-2.349130	-1.565500	-0.775178
C	0.251441	1.078110	-0.612479
C	2.427250	2.751187	-0.021875
C	0.158405	2.016948	0.417550
C	1.436501	0.980088	-1.346313
C	2.512379	1.802971	-1.035810
C	1.238770	2.848084	0.691276
H	-0.746904	2.081184	1.010307
H	1.519785	0.253367	-2.146944
H	3.269546	3.393451	0.211983
C	3.813522	1.662328	-1.772480
C	1.098633	3.881910	1.774034
F	3.715212	0.839862	-2.824223
F	4.267665	2.841980	-2.211541

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F          4.771864        1.157383       -0.968308
F          0.386676        3.414316        2.809652
F          2.293563        4.268929        2.243842
F          0.471928        4.979919        1.331757
C         -4.323474       -0.859198       -0.951625
C         -6.484077       -0.641667        0.303435
C         -6.486574       -0.620626       -2.212429
C         -7.147997       -0.068478       -0.949492
C         -4.990326       -0.303887       -2.215507
C         -4.979847       -0.336022        0.349748
H         -6.642898       -1.729221        0.320928
H         -6.635414       -1.709114       -2.252780
H         -7.054146        1.025951       -0.943092
H         -4.843293        0.778966       -2.257530
H         -4.861979        0.752625        0.365018
H         -4.467531       -1.948137       -0.965708
H         -6.937432       -0.239041        1.214269
H         -6.954570       -0.201940       -3.109512
H         -8.219003       -0.297862       -0.945134
H         -4.497923       -0.736649       -3.093680
N         -4.395106       -0.837321        1.592912
C         -4.176305       -2.269019        1.655926
H         -5.064366       -2.811092        1.318867
H         -3.982881       -2.555720        2.695303
H         -3.308573       -2.611683        1.063837
C         -3.247135       -0.110323        2.102972
H         -3.411782        0.965432        1.996693
H         -2.293734       -0.365190        1.602904
H         -3.122218       -0.341279        3.167499
O          1.282052       -1.863321       -0.658465
C          1.877429       -3.016072       -0.063897
C          1.056836       -2.041268        0.699634
H          1.382730       -3.948383       -0.335895
N         -0.348876       -2.523003        0.955418
O         -0.742818       -2.484968        2.098245
O         -0.980573       -2.945689       -0.001903
C          3.360390       -3.031646        0.045404
C          6.133944       -3.076335        0.288770
C          3.994940       -4.155875        0.575376
C          4.115385       -1.935867       -0.373904
C          5.500727       -1.958909       -0.251235
C          5.380458       -4.174402        0.700338
H          3.406267       -5.014185        0.888759
H          3.614435       -1.076022       -0.807393
H          6.079804       -1.102644       -0.580969
H          5.871972       -5.048160        1.116048
H          7.214910       -3.094524        0.384977
C          1.540039       -1.049521        1.713630
H          1.698455       -1.540979        2.674733
H          0.806340       -0.249784        1.840745
H          2.480590       -0.622108        1.361940

RS epoxide:Catalyst, binary complex 25; Energy = -2449.842172; 6-31G(d) basis set.
N         -0.637358        0.699411       -0.389543
H         -0.519984       -0.295560       -0.569411
C         -1.929793        1.108285       -0.131716
S         -2.297573        2.477840        0.769645
N         -2.825065        0.248440       -0.651203
H         -2.445455       -0.486945       -1.238676
C          0.553165        1.401030       -0.144816
C          3.028207        2.683365        0.210315
C          1.650893        0.699371        0.351135
C          0.694441        2.757271       -0.461036
C          1.919033        3.379519       -0.267850
C          2.878173        1.337849        0.507986
H          1.543200       -0.341622        0.639703
H         -0.150101        3.312543       -0.849949
H          3.979720        3.182451        0.352199
C          2.078139        4.821100       -0.662397
C          4.043575        0.518361        0.984950
F          2.495124        4.937729       -1.934641
F          0.927708        5.497469       -0.564563
F          2.986635        5.445281        0.101615
F          3.724530       -0.210185        2.067439
F          4.448201       -0.348527        0.042344
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F          5.097920        1.278736        1.307136
C         -4.273512        0.178450       -0.435965
C         -6.172971       -0.303046        1.130142
C         -6.540308        1.173947       -0.875414
C         -6.925895        0.909576        0.580202
C         -5.031576        1.388703       -0.995761
C         -4.650040       -0.134516        1.030394
H         -6.481037       -1.196125        0.567534
H         -6.844862        0.316381       -1.492295
H         -6.680477        1.794125        1.183311
H         -4.739801        2.284911       -0.441423
H         -4.366544        0.732136        1.637523
H         -4.577922       -0.691559       -1.033750
H         -6.425707       -0.485479        2.179097
H         -7.071690        2.049463       -1.262968
H         -8.006087        0.751517        0.669997
H         -4.735174        1.537690       -2.040256
N         -3.973047       -1.294981        1.614576
C         -3.933809       -2.482257        0.789676
H         -4.914139       -2.692494        0.353533
H         -3.651673       -3.342626        1.406770
H         -3.199067       -2.413884       -0.037858
C         -2.677052       -1.046349        2.220418
H         -1.844273       -1.028100        1.494381
H         -2.461501       -1.840362        2.946045
H         -2.686843       -0.089726        2.748542
O          0.256872       -2.149819        0.042408
C          1.215320       -2.521466       -0.957854
C          0.016063       -3.337073       -0.637729
H          1.145153       -1.920312       -1.865128
N         -1.111325       -3.153354       -1.626144
O         -1.715613       -4.140224       -1.972388
O         -1.323313       -2.017027       -2.023499
C          2.583964       -2.865064       -0.491896
C          5.180275       -3.449380        0.325902
C          2.884836       -2.943597        0.868320
C          3.586403       -3.066591       -1.442833
C          4.880609       -3.364657       -1.032757
C          4.184220       -3.233770        1.273889
H          2.108971       -2.751425        1.604376
H          3.353553       -2.982889       -2.501206
H          5.658064       -3.519819       -1.773729
H          4.419030       -3.275435        2.332528
H          6.193958       -3.671489        0.643942
C         -0.033510       -4.636869        0.098710
H         -0.945468       -4.689494        0.698911
H          0.836579       -4.698330        0.753217
H         -0.019407       -5.470715       -0.603313

RS epoxide:Catalyst, binary complex 26; Energy = -2449.838153; 6-31G(d) basis set.
N         -0.038793       -1.105281        1.033800
H         -0.198604       -0.176784        1.411534
C         -1.172146       -1.689645        0.496635
S         -1.126716       -3.046370       -0.493857
N         -2.276151       -1.006130        0.836440
H         -2.134007       -0.146024        1.355611
C          1.296615       -1.305670        0.638748
C          4.007809       -1.547153       -0.043595
C          2.069532       -0.172174        0.388095
C          1.886522       -2.570229        0.562704
C          3.228125       -2.671905        0.213890
C          3.412429       -0.296875        0.053742
H          1.619853        0.815011        0.448290
H          1.304370       -3.453970        0.787317
H          5.057562       -1.645412       -0.296886
C          3.853660       -4.033244        0.085568
C          4.190720        0.947745       -0.267228
F          5.148990       -4.012182        0.435482
F          3.240070       -4.940597        0.855912
F          3.799356       -4.484225       -1.176505
F          5.507094        0.774144       -0.088195
F          4.014408        1.322686       -1.545352
F          3.806550        1.981085        0.497079
C         -3.677040       -1.261989        0.495913
C         -5.554472       -1.166931       -1.127861
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C         -5.666332       -2.775726        0.803900
C         -6.024785       -2.545024       -0.661400
C         -4.158860       -2.628161        0.998581
C         -4.033136       -0.996027       -0.985868
H         -6.063100       -0.396785       -0.530011
H         -6.197635       -2.042519        1.426874
H         -5.549944       -3.319706       -1.278248
H         -3.638512       -3.420425        0.453982
H         -3.551798       -1.771065       -1.604348
H         -4.213706       -0.490063        1.064394
H         -5.852877       -1.016902       -2.169003
H         -5.990241       -3.768881        1.131879
H         -7.105837       -2.632279       -0.814168
H         -3.884356       -2.723387        2.054912
N         -3.544703        0.345104       -1.406398
C         -2.243249        0.238036       -2.065502
H         -1.514886       -0.263339       -1.431081
H         -1.865519        1.243227       -2.285495
H         -2.309660       -0.320256       -3.016117
C         -4.435612        1.049649       -2.326391
H         -4.598422        0.508229       -3.274636
H         -3.979104        2.011044       -2.581972
H         -5.404346        1.253152       -1.867713
O         -0.837548        1.637848        0.380311
C         -0.236591        2.752935        1.054224
C         -1.649957        2.740174        0.603489
H         -0.077365        2.579658        2.119233
N         -2.628252        2.472453        1.721738
O         -3.557659        3.237672        1.831233
O         -2.396103        1.529700        2.463036
C          0.837029        3.479486        0.325286
C          2.889507        4.830615       -0.985180
C          1.173372        3.134859       -0.985728
C          1.537324        4.492096        0.983497
C          2.556556        5.171028        0.324507
C          2.201620        3.810245       -1.636632
H          0.645041        2.323579       -1.480065
H          1.286132        4.745860        2.010179
H          3.097307        5.960026        0.837035
H          2.473521        3.527991       -2.648350
H          3.692808        5.353880       -1.493839
C         -2.246940        3.509927       -0.529327
H         -3.103997        2.956807       -0.919761
H         -1.493427        3.630696       -1.308689
H         -2.574430        4.491328       -0.185035

RS epoxide:Catalyst, binary complex 27; Energy = -2449.841685; 6-31G(d) basis set.
N          0.178836       -0.896162       -0.527532
H          0.217914        0.118066       -0.555962
C          1.408955       -1.501793       -0.375896
S          1.617541       -3.106378        0.077438
N          2.401985       -0.623238       -0.602057
H          2.131212        0.307419       -0.908562
C         -1.112431       -1.380509       -0.287679
C         -3.790703       -2.119869        0.161088
C         -1.525004       -2.696952       -0.522503
C         -2.051968       -0.443035        0.147648
C         -3.372556       -0.811992        0.363774
C         -2.849340       -3.044532       -0.282865
H         -0.822479       -3.431819       -0.889794
H         -1.742750        0.584692        0.320202
H         -4.820146       -2.410536        0.335449
C         -4.336131        0.254674        0.797654
C         -3.267648       -4.477015       -0.467673
F         -3.838212        0.979009        1.817912
F         -4.589825        1.123242       -0.193654
F         -5.507558       -0.252076        1.197576
F         -4.554225       -4.571987       -0.835944
F         -2.532334       -5.096735       -1.399985
F         -3.135798       -5.177460        0.668868
C          3.850835       -0.805993       -0.482684
C          5.863220       -1.095441        0.975573
C          5.950417       -1.804068       -1.441106
C          6.446151       -2.095837       -0.024534
C          4.421897       -1.813418       -1.488817
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C	4.327843	-1.092735	0.961024
H	6.235045	-0.089158	0.732960
H	6.322932	-0.820229	-1.760154
H	6.141402	-3.111746	0.261348
H	4.047826	-2.813825	-1.250807
H	3.987564	-2.098142	1.231939
H	4.246560	0.181262	-0.759687
H	6.191486	-1.318399	1.995329
H	6.348681	-2.539102	-2.148283
H	7.540522	-2.068615	0.012779
H	4.058603	-1.556160	-2.490104
N	3.813096	-0.187646	1.990483
C	3.836076	1.218352	1.660232
H	4.779330	1.504811	1.186167
H	3.726185	1.810869	2.576147
H	3.006826	1.500041	0.981646
C	2.537790	-0.549599	2.583141
H	1.667429	-0.261975	1.965383
H	2.437036	-0.044922	3.551632
H	2.493907	-1.628244	2.748660
O	0.486419	2.067683	-0.076732
C	0.016635	3.089544	-0.968611
C	1.185506	3.271774	-0.073469
H	0.253164	2.884543	-2.012103
N	2.509220	3.138036	-0.791106
O	3.345548	3.979976	-0.558183
O	2.635518	2.213141	-1.576820
C	-1.313874	3.691740	-0.692559
C	-3.818846	4.834099	-0.262402
C	-1.843134	4.587911	-1.623783
C	-2.044421	3.362873	0.450892
C	-3.299462	3.928504	0.659011
C	-3.088716	5.164971	-1.402731
H	-1.280583	4.830935	-2.521341
H	-1.637686	2.658665	1.171636
H	-3.873398	3.648371	1.535613
H	-3.494317	5.864726	-2.126152
H	-4.796808	5.275030	-0.098367
C	1.254142	4.105232	1.166216
H	1.615560	5.105380	0.926479
H	1.931436	3.644905	1.889988
H	0.255230	4.174594	1.597701

RS epoxide:Catalyst, binary complex 28; Energy = -2449.844529; 6-31G(d) basis set.

N	-0.779860	0.074812	-0.885965
H	-0.404604	-0.831805	-1.153026
C	-2.155168	0.237925	-1.000956
S	-2.864659	1.722494	-1.322616
N	-2.798307	-0.927970	-0.830060
H	-2.232026	-1.693097	-0.473889
C	0.177732	1.079095	-0.683884
C	2.240379	2.896016	-0.100794
C	-0.038767	2.125573	0.216552
C	1.425364	0.956252	-1.303393
C	2.445583	1.844282	-0.987324
C	0.986051	3.026874	0.483070
H	-0.995497	2.220727	0.717251
H	1.599556	0.153684	-2.011300
H	3.038736	3.591313	0.133570
C	3.823698	1.631409	-1.543468
C	0.705702	4.165336	1.424824
F	3.823216	0.809123	-2.602775
F	4.401494	2.779399	-1.912333
F	4.631682	1.069573	-0.620141
F	-0.021231	5.123851	0.835727
F	0.012258	3.752622	2.496340
F	1.834773	4.735513	1.867821
C	-4.241829	-1.190602	-0.847899
C	-6.473878	-0.941032	0.260568
C	-6.341727	-1.387371	-2.214461
C	-7.117422	-0.680273	-1.102423
C	-4.880200	-0.937227	-2.218280
C	-5.006869	-0.487951	0.301462
H	-6.536234	-2.016147	0.482535
H	-6.393150	-2.474168	-2.056382

H	-7.124301	0.400177	-1.299940
H	-4.823198	0.129599	-2.453590
H	-4.986253	0.589142	0.103137
H	-4.306863	-2.270847	-0.659093
H	-7.010575	-0.419881	1.058944
H	-6.794996	-1.186301	-3.190735
H	-8.161860	-1.010110	-1.093595
H	-4.305049	-1.473116	-2.981704
N	-4.449522	-0.676753	1.639785
C	-4.102515	-2.037499	2.000278
H	-4.897591	-2.730158	1.709857
H	-3.986263	-2.100964	3.087914
H	-3.151729	-2.383880	1.555860
C	-3.405337	0.248290	2.039215
H	-2.407397	0.000343	1.631989
H	-3.318272	0.236924	3.132148
H	-3.664155	1.261863	1.721911
O	1.396786	-1.857393	-0.529346
C	1.994059	-2.943097	0.178740
C	1.315007	-1.808431	0.857635
H	1.426254	-3.870417	0.113115
N	-0.085336	-2.142402	1.314247
O	-0.408530	-1.787699	2.423572
O	-0.786939	-2.773530	0.536782
C	3.477595	-3.037059	0.132309
C	6.257513	-3.204304	0.093402
C	4.119648	-4.104438	0.761855
C	4.226626	-2.063921	-0.528901
C	5.614911	-2.145070	-0.544154
C	5.508652	-4.184427	0.742880
H	3.534883	-4.869497	1.265963
H	3.717927	-1.252107	-1.037810
H	6.187418	-1.376974	-1.054321
H	6.007007	-5.013498	1.234822
H	7.340870	-3.269472	0.081392
C	1.966401	-0.714546	1.647204
H	2.138436	-1.047385	2.672153
H	1.335381	0.177499	1.664696
H	2.921757	-0.469737	1.179766

RS epoxide:Catalyst, binary complex 29; Energy = -2449.841675; 6-31G(d) basis set.

N	0.175573	-0.887186	-0.542047
H	0.222540	0.126943	-0.559899
C	1.400372	-1.503415	-0.386727
S	1.590808	-3.111693	0.061255
N	2.401665	-0.632722	-0.605495
H	2.140028	0.301576	-0.908967
C	-1.117187	-1.364544	-0.293204
C	-3.792445	-2.093939	0.180290
C	-1.544263	-2.670135	-0.557996
C	-2.039983	-0.431644	0.185585
C	-3.359686	-0.795746	0.414445
C	-2.867617	-3.013699	-0.306385
H	-0.852892	-3.400237	-0.955009
H	-1.716060	0.585873	0.386668
H	-4.820783	-2.381279	0.366963
C	-4.312210	0.260396	0.896348
C	-3.301932	-4.436905	-0.523000
F	-3.750489	1.027827	1.850030
F	-4.676529	1.091126	-0.092348
F	-5.430472	-0.265217	1.409484
F	-4.593107	-4.510277	-0.879993
F	-2.582210	-5.039332	-1.478578
F	-3.165359	-5.167221	0.593680
C	3.847908	-0.826335	-0.473464
C	5.844024	-1.132723	1.003833
C	5.948483	-1.839887	-1.412820
C	6.428385	-2.136776	0.008221
C	4.420535	-1.837208	-1.475117
C	4.309012	-1.117946	0.974583
H	6.225936	-0.129105	0.765866
H	6.331782	-0.858746	-1.727379
H	6.112937	-3.150457	0.290369
H	4.036538	-2.834858	-1.241531
H	3.958474	-2.120925	1.241260

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H           4.253646        0.158185       -0.745667
H           6.160746       -1.359297        2.026464
H           6.347761       -2.577462       -2.116770
H           7.522538       -2.118301        0.055924
H           4.068626       -1.576332       -2.479511
N           3.791253       -0.209902        1.999856
C           3.828096        1.196436        1.672241
H           4.777712        1.476050        1.206852
H           3.715090        1.788147        2.588277
H           3.006988        1.486173        0.987117
C           2.508542       -0.563119        2.581517
H           1.645250       -0.267223        1.957741
H           2.403894       -0.059925        3.550377
H           2.454683       -1.641770        2.744077
O           0.505114        2.072021       -0.086964
C           0.044457        3.088644       -0.989601
C           1.205686        3.275176       -0.085296
H           0.290326        2.876927       -2.029572
N           2.535755        3.133790       -0.790044
O           3.373267        3.973142       -0.552116
O           2.665777        2.205483       -1.571069
C          -1.289606        3.690308       -0.729955
C          -3.805219        4.821180       -0.332646
C          -2.026795        3.370712        0.411892
C          -1.817332        4.571818       -1.675802
C          -3.068368        5.143475       -1.471006
C          -3.287156        3.930079        0.603644
H          -1.621014        2.678211        1.144249
H          -1.249898        4.807342       -2.572319
H          -3.472800        5.832169       -2.205617
H          -3.865540        3.657111        1.479510
H          -4.787215        5.257644       -0.181324
C           1.265588        4.116161        1.149700
H           1.631428        5.113927        0.906772
H           1.935840        3.658781        1.881884
H           0.263259        4.190600        1.572265

RS epoxide:Catalyst, binary complex 30; Energy = -2449.852369; 6-31G(d) basis set.
N           0.498621       -0.794396       -0.250231
H          -0.002702        0.049838        0.012211
C          -0.288711       -1.919582       -0.310768
S           0.297949       -3.493967       -0.225930
N          -1.597168       -1.619596       -0.418454
H          -1.870821       -0.645084       -0.330050
C           1.886747       -0.723605       -0.059567
C           4.648436       -0.387987        0.300034
C           2.372329        0.218701        0.846612
C           2.787953       -1.500573       -0.796286
C           4.150214       -1.329453       -0.599054
C           3.744252        0.385130        1.012276
H           1.675193        0.803100        1.441730
H           2.420274       -2.221242       -1.514549
H           5.717042       -0.261821        0.436118
C           5.131478       -2.180369       -1.355410
C           4.238476        1.454710        1.943118
F           5.651423       -3.143422       -0.580035
F           4.571444       -2.778449       -2.413873
F           6.163634       -1.447049       -1.803616
F           5.481463        1.208463        2.374867
F           4.261315        2.656991        1.342049
F           3.448305        1.578754        3.019633
C          -2.671511       -2.592758       -0.307337
C          -5.022117       -2.986336        0.408553
C          -4.000446       -4.405835       -1.420964
C          -5.287007       -3.793578       -0.866633
C          -2.930999       -3.332790       -1.624450
C          -3.959268       -1.899805        0.163874
H          -4.681380       -3.659060        1.207307
H          -3.619729       -5.157680       -0.716648
H          -5.722261       -3.126447       -1.623776
H          -3.258623       -2.606019       -2.380343
H          -4.319260       -1.268656       -0.666612
H          -2.365393       -3.336761        0.440602
H          -5.956346       -2.529217        0.749112
H          -4.198746       -4.925806       -2.363848
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H	-6.030717	-4.572189	-0.666965
H	-1.993269	-3.775085	-1.970821
N	-3.715905	-0.966708	1.281054
C	-4.962095	-0.371166	1.753796
H	-5.564545	-0.039887	0.900674
H	-4.734042	0.495146	2.381318
H	-5.573007	-1.069602	2.347144
C	-3.001932	-1.558978	2.410568
H	-3.554008	-2.389643	2.879314
H	-2.851234	-0.782792	3.167315
H	-2.016310	-1.915657	2.101422
O	-1.598075	1.468543	-0.593622
C	-1.064619	2.724108	-0.153663
C	-2.267497	2.097106	0.450374
H	-0.141059	2.625134	0.417502
N	-1.974870	1.423505	1.767423
O	-2.698885	1.694249	2.700198
O	-0.992816	0.704264	1.821046
C	-1.144491	3.876071	-1.088787
C	-1.263148	6.071963	-2.797404
C	-1.781559	3.762250	-2.325126
C	-0.556820	5.085438	-0.713223
C	-0.621496	6.182659	-1.565043
C	-1.838305	4.861518	-3.177170
H	-2.211554	2.809350	-2.619348
H	-0.047373	5.166560	0.243543
H	-0.165046	7.121825	-1.269439
H	-2.326421	4.768999	-4.142096
H	-1.306935	6.927211	-3.464173
C	-3.686195	2.530473	0.273985
H	-4.012778	3.121902	1.129090
H	-4.322081	1.647971	0.178073
H	-3.758847	3.131546	-0.633494

RS epoxide:Catalyst, binary complex 31; Energy = -2449.844962; 6-31G(d) basis set.

N	-0.935293	-0.443489	-0.003893
H	-0.601349	-0.456217	-0.962602
C	-0.093272	-1.016755	0.925955
S	-0.558511	-1.441322	2.485225
N	1.144786	-1.215461	0.440644
H	1.352739	-0.915515	-0.509983
C	-2.308201	-0.164902	0.114814
C	-5.048059	0.443152	0.174762
C	-2.869662	0.424960	1.249440
C	-3.117252	-0.426653	-0.994143
C	-4.470835	-0.118605	-0.957991
C	-4.230730	0.709204	1.266989
H	-2.250617	0.659766	2.105086
H	-2.688107	-0.885103	-1.880310
H	-6.107587	0.671682	0.202983
C	-5.321844	-0.359036	-2.172439
C	-4.829812	1.286126	2.519450
F	-6.564804	-0.730759	-1.835583
F	-5.436510	0.748902	-2.922016
F	-4.809696	-1.314386	-2.960671
F	-5.953665	1.971640	2.261158
F	-5.147626	0.328468	3.401753
F	-3.979203	2.119383	3.135423
C	2.240748	-1.853787	1.160267
C	4.249165	-3.342663	0.937385
C	4.256993	-1.478910	2.630724
C	5.105434	-2.301278	1.660288
C	3.095870	-0.814504	1.892293
C	3.078633	-2.699729	0.181378
H	3.861027	-4.058843	1.674481
H	3.859189	-2.137829	3.414563
H	5.558148	-1.626510	0.919288
H	3.492030	-0.100235	1.156839
H	3.510873	-2.014897	-0.562697
H	1.785670	-2.515499	1.905344
H	4.842651	-3.915600	0.218354
H	4.866153	-0.719002	3.131527
H	5.929296	-2.793262	2.188106
H	2.452959	-0.254793	2.580725
N	2.334995	-3.713036	-0.568738

C	1.428429	-4.521496	0.228434
H	1.934278	-4.902765	1.119591
H	1.104255	-5.382528	-0.365294
H	0.525377	-3.972177	0.551534
C	1.681008	-3.257878	-1.782231
H	0.700404	-2.779628	-1.609570
H	1.510690	-4.114676	-2.444702
H	2.321342	-2.542409	-2.308317
O	3.024644	0.325358	-1.369041
C	2.436974	1.543781	-0.904261
C	2.619805	1.227280	-2.343487
H	1.428324	1.414636	-0.506368
N	1.353195	0.762998	-3.020999
O	1.055894	1.296698	-4.062516
O	0.698898	-0.104489	-2.460617
C	3.317717	2.505050	-0.189190
C	4.927034	4.334998	1.158291
C	4.681812	2.251140	-0.033673
C	2.758054	3.668812	0.340301
C	3.564291	4.584645	1.007953
C	5.483183	3.166896	0.641592
H	5.102177	1.329326	-0.426703
H	1.692713	3.854852	0.232934
H	3.127488	5.489648	1.417397
H	6.541871	2.964965	0.768936
H	5.553682	5.047199	1.685587
C	3.609137	1.837966	-3.285481
H	3.165050	2.691851	-3.797072
H	3.926660	1.101402	-4.027730
H	4.475341	2.169550	-2.712316

RS epoxide:Catalyst, binary complex 32; Energy = -2449.844464; 6-31G(d) basis set.

N	-1.023004	-0.650878	-0.442167
H	-0.631424	0.017262	-1.097087
C	-0.118014	-1.548795	0.070600
S	-0.476557	-2.774656	1.166556
N	1.125845	-1.341851	-0.407397
H	1.297742	-0.535421	-1.004751
C	-2.367392	-0.385200	-0.150183
C	-5.052469	0.358419	0.268886
C	-3.241923	-1.251569	0.515237
C	-2.855304	0.843217	-0.617261
C	-4.179020	1.201091	-0.407882
C	-4.561228	-0.860956	0.718037
H	-2.898088	-2.216093	0.859413
H	-2.192776	1.517107	-1.156549
H	-6.087705	0.637192	0.426543
C	-4.642710	2.549752	-0.880790
C	-5.471563	-1.775048	1.491301
F	-4.232891	3.526788	-0.054866
F	-4.155759	2.843303	-2.095410
F	-5.977589	2.623701	-0.948527
F	-6.751573	-1.630495	1.116649
F	-5.143314	-3.062871	1.329486
F	-5.419322	-1.518080	2.808039
C	2.278839	-2.193110	-0.138769
C	4.397412	-3.141458	-1.079715
C	4.243304	-2.623966	1.383344
C	5.162842	-2.680363	0.162671
C	3.041848	-1.723061	1.103377
C	3.192865	-2.238384	-1.379860
H	4.052483	-4.172504	-0.922193
H	3.890096	-3.636498	1.621785
H	5.579215	-1.678976	-0.019058
H	3.392572	-0.695980	0.933506
H	3.581984	-1.223033	-1.544314
H	1.887347	-3.198710	0.052886
H	5.043508	-3.151340	-1.962754
H	4.787753	-2.260787	2.261495
H	6.010986	-3.347753	0.349409
H	2.352043	-1.700869	1.953794
N	2.543798	-2.638975	-2.628717
C	1.700077	-3.817242	-2.531573
H	2.229171	-4.630187	-2.027458
H	1.448181	-4.158408	-3.541150

H	0.753729	-3.631597	-1.991584
C	1.870356	-1.585308	-3.367190
H	0.847793	-1.370711	-3.008609
H	1.787651	-1.877518	-4.420582
H	2.453540	-0.660107	-3.316014
O	2.909877	1.099974	-0.897834
C	2.363314	1.719818	0.269809
C	2.453957	2.402271	-1.045902
H	1.380570	1.331752	0.544935
N	1.140210	2.440403	-1.786990
O	0.763042	3.513083	-2.191563
O	0.527340	1.388649	-1.904524
C	3.291693	2.030004	1.389163
C	4.987129	2.610213	3.520636
C	2.768887	2.547889	2.574975
C	4.662515	1.791102	1.274120
C	5.507232	2.080417	2.341670
C	3.618131	2.842777	3.636584
H	1.699015	2.714667	2.668611
H	5.055014	1.361452	0.356384
H	6.571447	1.886658	2.253873
H	3.209649	3.245684	4.557593
H	5.647079	2.834278	4.352656
C	3.387239	3.506549	-1.431925
H	2.920050	4.475421	-1.255734
H	3.651369	3.423351	-2.489115
H	4.290829	3.426185	-0.827062

RS epoxide:Catalyst, binary complex 33; Energy = -2449.852268; 6-31G(d) basis set.

N	-0.511495	-0.797984	0.258279
H	-0.007656	0.050299	0.014166
C	0.274562	-1.924683	0.305756
S	-0.312377	-3.497951	0.201464
N	1.583407	-1.628184	0.419015
H	1.859905	-0.653683	0.340900
C	-1.898373	-0.721086	0.060727
C	-4.658050	-0.389788	-0.329489
C	-2.805982	-1.518588	0.764622
C	-2.377087	0.243060	-0.827412
C	-3.746554	0.407574	-1.007087
C	-4.167465	-1.349670	0.552006
H	-2.444871	-2.264081	1.461140
H	-1.675066	0.840950	-1.403154
H	-5.724171	-0.275740	-0.489598
C	-4.231623	1.491581	-1.926021
C	-5.139679	-2.172555	1.350324
F	-4.253526	2.685578	-1.308660
F	-3.434718	1.628081	-2.996187
F	-5.472808	1.255798	-2.368482
F	-6.277805	-2.386671	0.674132
F	-4.632337	-3.364847	1.683835
F	-5.477846	-1.555679	2.495362
C	2.655002	-2.604378	0.306934
C	5.003691	-3.007807	-0.408579
C	3.976098	-4.423242	1.420748
C	5.265085	-3.815532	0.866996
C	2.910730	-3.346123	1.623764
C	3.945093	-1.916861	-0.165064
H	4.660588	-3.679613	-1.207110
H	3.592898	-5.173549	0.716149
H	5.702187	-3.149722	1.624253
H	3.240467	-2.621143	2.380476
H	4.308121	-1.285895	0.664328
H	2.345929	-3.346611	-0.441298
H	5.939760	-2.554501	-0.749122
H	4.172070	-4.944004	2.363683
H	6.006245	-4.596729	0.667956
H	1.970769	-3.784814	1.968916
N	3.704501	-0.985150	-1.283904
C	4.952833	-0.398309	-1.761850
H	5.560148	-0.068638	-0.911558
H	4.727851	0.468025	-2.390450
H	5.557521	-1.101876	-2.355500
C	2.983547	-1.575454	-2.410088
H	3.528299	-2.411563	-2.877770

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H          2.837162       -0.800234       -3.168648
H          1.995828       -1.923688       -2.097996
O          1.592561        1.464231        0.598703
C          1.076838        2.725734        0.154222
C          2.271571        2.080666       -0.446638
H          0.152447        2.637480       -0.417251
N          1.971389        1.408125       -1.762317
O          2.695055        1.674064       -2.696860
O          0.984304        0.695862       -1.813072
C          1.172835        3.880076        1.084902
C          1.325456        6.082130        2.782877
C          1.803634        3.761026        2.323938
C          0.608462        5.097958        0.701251
C          0.690174        6.198156        1.547692
C          1.877235        4.863385        3.170699
H          2.215899        2.802201        2.624144
H          0.104323        5.183600       -0.257906
H          0.252269        7.144018        1.245456
H          2.360419        4.766954        4.137716
H          1.382437        6.939772        3.445579
C          3.695639        2.495440       -0.268816
H          4.032891        3.076580       -1.126847
H          4.318508        1.604592       -0.165200
H          3.774223        3.101334        0.634969

RS epoxide:Catalyst, binary complex 34; Energy = -2449.848601; 6-31G(d) basis set.
N         -0.695177        0.602244       -0.730691
H         -0.346434       -0.053386       -1.425375
C          0.121372        1.692176       -0.473059
S         -0.446020        3.171573        0.085077
N          1.415254        1.435368       -0.725009
H          1.700738        0.466534       -0.853489
C         -2.066184        0.479320       -0.435597
C         -4.769731        0.032633        0.152560
C         -2.584923        0.858068        0.807547
C         -2.896945       -0.133497       -1.369992
C         -4.236793       -0.358597       -1.065620
C         -3.927130        0.643787        1.078897
H         -1.941210        1.309220        1.551554
H         -2.501542       -0.437368       -2.334464
H         -5.816303       -0.137616        0.381324
C         -5.095379       -1.078529       -2.065850
C         -4.508679        1.089042        2.390792
F         -4.756700       -0.759098       -3.324281
F         -4.974213       -2.409930       -1.956901
F         -6.393956       -0.786949       -1.908736
F         -5.309344        0.147109        2.914249
F         -3.561922        1.363965        3.296725
F         -5.256866        2.193578        2.247506
C          2.485200        2.419919       -0.648949
C          4.904073        2.785769       -0.139259
C          3.748315        4.232977       -1.854562
C          5.066311        3.577170       -1.440277
C          2.634083        3.191710       -1.964266
C          3.798273        1.724069       -0.268767
H          4.652919        3.475212        0.677796
H          3.464415        4.984987       -1.105972
H          5.396031        2.895090       -2.236476
H          2.860857        2.479490       -2.769628
H          4.075300        1.057876       -1.103893
H          2.214134        3.137542        0.133376
H          5.849830        2.301393        0.127125
H          3.864071        4.760674       -2.806797
H          5.851361        4.331683       -1.324653
H          1.675102        3.664363       -2.200620
N          3.616606        0.846163        0.891203
C          4.811069        0.078093        1.205980
H          5.241096       -0.324188        0.284736
H          4.541848       -0.771434        1.845997
H          5.586429        0.665849        1.725584
C          3.097016        1.510242        2.078658
H          3.757514        2.305526        2.462040
H          2.985070        0.764894        2.873190
H          2.107464        1.935978        1.882414
O          1.271795       -1.533636       -0.940924
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C	1.612379	-2.840674	-0.458071
C	0.722180	-1.925048	0.281594
H	1.124109	-3.628624	-1.030822
N	-0.745712	-2.245648	0.123299
O	-1.428860	-2.189829	1.123023
O	-1.135011	-2.540872	-0.990722
C	3.030377	-3.056523	-0.049704
C	5.685879	-3.552590	0.629575
C	3.336611	-3.657296	1.171388
C	4.053095	-2.702347	-0.930007
C	5.378927	-2.955852	-0.591746
C	4.665057	-3.900783	1.511546
H	2.536736	-3.936022	1.852854
H	3.806027	-2.229899	-1.876940
H	6.173584	-2.684100	-1.279800
H	4.900986	-4.365142	2.463758
H	6.720562	-3.747990	0.893153
C	1.054947	-1.172614	1.530202
H	0.911234	-1.802570	2.409862
H	0.411194	-0.292303	1.617010
H	2.093631	-0.844849	1.448177

RS epoxide:Catalyst, binary complex 35; Energy = -2449.846132; 6-31G(d) basis set.

N	-1.180067	-0.321682	-0.117064
H	-0.681758	0.531365	-0.355712
C	-0.395220	-1.335026	0.381950
S	-0.977409	-2.675987	1.216356
N	0.911027	-1.127635	0.133197
H	1.168072	-0.298084	-0.396849
C	-2.570660	-0.150904	-0.014321
C	-5.330492	0.352121	0.075521
C	-3.479534	-1.201267	-0.177713
C	-3.047260	1.148184	0.171707
C	-4.416533	1.387983	0.210241
C	-4.841531	-0.936538	-0.117843
H	-3.122163	-2.206081	-0.357885
H	-2.344516	1.970502	0.281787
H	-6.396938	0.544351	0.101510
C	-4.893882	2.791012	0.455537
C	-5.815770	-2.075071	-0.237361
F	-4.804806	3.122534	1.753026
F	-4.159885	3.686189	-0.223109
F	-6.172542	2.955814	0.091580
F	-6.958551	-1.686412	-0.824192
F	-5.315947	-3.087832	-0.957556
F	-6.145733	-2.569851	0.964896
C	2.008489	-2.007435	0.516794
C	4.273786	-2.866768	-0.193544
C	3.812892	-2.434387	2.239650
C	4.865943	-2.389600	1.133065
C	2.614823	-1.569679	1.855588
C	3.050361	-2.044002	-0.620063
H	3.986217	-3.922951	-0.098949
H	3.482833	-3.470962	2.392743
H	5.228042	-1.356587	1.021757
H	2.948383	-0.525592	1.773724
H	3.399395	-1.012718	-0.781191
H	1.580984	-3.006888	0.644864
H	5.011597	-2.808701	-0.999920
H	4.232574	-2.088770	3.190342
H	5.733044	-3.004012	1.398233
H	1.828659	-1.604583	2.617847
N	2.548932	-2.519023	-1.912089
C	1.715185	-3.707492	-1.845421
H	2.192312	-4.479242	-1.234801
H	1.591971	-4.111483	-2.855574
H	0.709332	-3.513129	-1.431825
C	1.943443	-1.515525	-2.768912
H	0.915611	-1.234808	-2.476508
H	1.895219	-1.904368	-3.792545
H	2.559370	-0.611378	-2.777217
O	2.262469	1.326986	-1.085671
C	2.887485	1.721594	0.143323
C	2.285797	2.689382	-0.806250
H	2.281298	1.494700	1.021176

N	0.919460	3.171474	-0.373164
O	0.693208	4.353832	-0.472088
O	0.150079	2.338451	0.079339
C	4.350724	1.491843	0.269841
C	7.077001	1.001133	0.581245
C	4.949712	1.641108	1.522740
C	5.116918	1.083989	-0.824493
C	6.477533	0.838598	-0.666361
C	6.311844	1.401762	1.675244
H	4.347725	1.936345	2.378498
H	4.640649	0.935385	-1.789917
H	7.067737	0.514282	-1.517277
H	6.773253	1.519583	2.650270
H	8.137691	0.806724	0.703610
C	3.000407	3.642125	-1.710610
H	3.100777	4.614587	-1.228575
H	2.446253	3.762279	-2.644591
H	3.991819	3.243095	-1.926633

RS epoxide:Catalyst, binary complex 36; Energy = -2449.846234; 6-31G(d) basis set.

N	1.180587	-0.331110	0.107791
H	0.683684	0.524856	0.338662
C	0.391655	-1.351691	-0.369401
S	0.965927	-2.707577	-1.184884
N	-0.912867	-1.138351	-0.116168
H	-1.166595	-0.299083	0.399981
C	2.570367	-0.160753	-0.002226
C	5.329126	0.345732	-0.118900
C	3.044026	1.137779	-0.200468
C	3.482316	-1.209270	0.157631
C	4.843197	-0.942890	0.082960
C	4.412558	1.379446	-0.249855
H	2.339669	1.956851	-0.323176
H	3.128443	-2.214511	0.341425
H	6.394890	0.537844	-0.164881
C	5.820863	-2.079832	0.188127
C	4.885369	2.796993	-0.401097
F	5.325281	-3.102740	0.896439
F	6.151953	-2.558501	-1.020486
F	6.962984	-1.694211	0.778508
F	6.162050	2.861574	-0.800165
F	4.145030	3.471909	-1.293088
F	4.799550	3.468939	0.759114
C	-2.014046	-2.019909	-0.484534
C	-4.283049	-2.856983	0.239668
C	-3.819652	-2.468894	-2.200621
C	-4.872916	-2.400802	-1.095372
C	-2.618304	-1.602612	-1.830774
C	-3.056511	-2.031973	0.652285
H	-3.999899	-3.915882	0.164041
H	-3.493654	-3.509223	-2.335852
H	-5.230729	-1.364483	-1.002274
H	-2.947294	-0.555816	-1.766781
H	-3.401204	-0.996528	0.794857
H	-1.590990	-3.023291	-0.595596
H	-5.021000	-2.781666	1.044492
H	-4.237667	-2.137763	-3.157196
H	-5.742413	-3.016217	-1.350179
H	-1.832024	-1.653948	-2.591949
N	-2.557930	-2.485976	1.952977
C	-1.728244	-3.678204	1.908119
H	-2.208236	-4.459324	1.311849
H	-1.606591	-4.064170	2.925510
H	-0.721615	-3.495285	1.491267
C	-1.950797	-1.469311	2.792864
H	-1.901378	-1.841991	3.822403
H	-2.566562	-0.565014	2.787860
H	-0.923333	-1.193244	2.494737
O	-2.255095	1.342729	1.062592
C	-2.878978	1.720537	-0.172240
C	-2.274773	2.700821	0.762870
H	-2.273294	1.479055	-1.046515
N	-0.907037	3.172655	0.323019
O	-0.677164	4.355587	0.405007
O	-0.140101	2.330927	-0.117319

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C         -4.342836        1.492893       -0.295490
C         -7.070456        1.004733       -0.599757
C         -5.110573        1.105108        0.805115
C         -4.941035        1.623198       -1.550837
C         -6.303767        1.385088       -1.699936
C         -6.471833        0.861061        0.650555
H         -4.635082        0.970346        1.772928
H         -4.338107        1.903232       -2.411017
H         -6.764526        1.488533       -2.676905
H         -7.063122        0.552078        1.506385
H         -8.131653        0.811323       -0.719286
C         -2.986792        3.668952        1.652809
H         -3.083166        4.634781        1.156810
H         -2.433081        3.800582        2.585503
H         -3.979830        3.276692        1.873621

RS epoxide:Catalyst, binary complex 37; Energy = -2449.839256; 6-31G(d) basis set.
N          1.159637        0.467922       -0.058085
H          0.586032       -0.201054       -0.561715
C          0.546163        1.669919        0.218304
S          1.359492        3.082462        0.636645
N         -0.784577        1.594584        0.068689
H         -1.199161        0.678429       -0.086680
C          2.515766        0.122578        0.022311
C          5.183124       -0.753935        0.134924
C          3.364573        0.585736        1.030895
C          3.003374       -0.792967       -0.915315
C          4.320659       -1.226844       -0.847445
C          4.684891        0.151742        1.063970
H          2.996033        1.274140        1.779798
H          2.351579       -1.155108       -1.705524
H          6.214237       -1.085660        0.177296
C          4.805693       -2.262761       -1.820940
C          5.593836        0.713767        2.121508
F          4.626433       -3.506676       -1.345659
F          4.150346       -2.195724       -2.988733
F          6.113531       -2.129173       -2.078608
F          6.661072       -0.070785        2.329127
F          6.054622        1.926287        1.782734
F          4.958464        0.851716        3.294418
C         -1.734796        2.684427        0.247720
C         -3.953390        3.616320       -0.468344
C         -3.391221        3.606793        1.964248
C         -4.513983        3.451693        0.941749
C         -2.296038        2.586480        1.675995
C         -2.842676        2.609560       -0.817594
H         -3.519263        4.618287       -0.577617
H         -2.978319        4.622192        1.900125
H         -4.969636        2.456635        1.048849
H         -2.701422        1.573339        1.810156
H         -3.265759        1.582869       -0.753583
H         -1.185091        3.624306        0.134801
H         -4.754999        3.542863       -1.209838
H         -3.764815        3.475734        2.985209
H         -5.306750        4.186918        1.115046
H         -1.453794        2.692841        2.368194
N         -2.400896        2.891858       -2.191552
C         -1.015532        2.634318       -2.558706
H         -0.324193        3.161043       -1.896836
H         -0.865378        3.024586       -3.570510
H         -0.750090        1.561395       -2.568961
C         -3.278842        2.262422       -3.160461
H         -3.138864        1.163926       -3.208100
H         -3.076807        2.662672       -4.158641
H         -4.327875        2.461576       -2.926397
O         -2.781922       -0.688148        0.213160
C         -2.707588       -2.116485        0.228812
C         -3.186997       -1.342888       -0.944365
H         -1.688649       -2.496211        0.162476
N         -2.150099       -1.210783       -2.034212
O         -2.515576       -1.403122       -3.170093
O         -1.006490       -0.945267       -1.697384
C         -3.642505       -2.844328        1.126738
C         -5.372944       -4.255032        2.790922
C         -4.581689       -2.157512        1.896959
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C	-3.561830	-4.236144	1.198267
C	-4.430438	-4.939568	2.025906
C	-5.444660	-2.865298	2.728578
H	-4.620238	-1.072825	1.852559
H	-2.818266	-4.767107	0.609449
H	-4.367101	-6.021642	2.078469
H	-6.170457	-2.329411	3.331773
H	-6.046352	-4.805420	3.440230
C	-4.595362	-1.226855	-1.435292
H	-4.802282	-1.997916	-2.177789
H	-4.757744	-0.244441	-1.887066
H	-5.268726	-1.350774	-0.586435

RS epoxide:Catalyst, binary complex 38; Energy = -2449.838915; 6-31G(d) basis set.

N	-0.819747	-0.656088	0.168690
H	-0.495447	-0.954695	-0.746478
C	0.064067	-0.876514	1.207472
S	-0.365646	-0.896952	2.832027
N	1.312330	-1.103230	0.770570
H	1.497117	-1.073569	-0.230681
C	-2.194650	-0.376092	0.223077
C	-4.946016	0.192612	0.143250
C	-3.003197	-0.914757	-0.782104
C	-2.765349	0.466581	1.179534
C	-4.130479	0.727280	1.132617
C	-4.360430	-0.623223	-0.818120
H	-2.571336	-1.575982	-1.528441
H	-2.150685	0.904654	1.955305
H	-6.009136	0.401344	0.124521
C	-4.702586	1.657689	2.165872
C	-5.193595	-1.167487	-1.943712
F	-4.304603	1.327225	3.400928
F	-4.303141	2.923398	1.956718
F	-6.042293	1.657870	2.155482
F	-5.148411	-0.364730	-3.019672
F	-4.764272	-2.374024	-2.341558
F	-6.481334	-1.286953	-1.596478
C	2.456947	-1.451377	1.607119
C	4.679932	-2.616918	1.632437
C	4.459045	-0.421132	2.804829
C	5.392460	-1.315186	1.991512
C	3.179979	-0.158265	2.016143
C	3.380420	-2.406005	0.837891
H	4.414095	-3.158344	2.549507
H	4.212921	-0.917648	3.752971
H	5.691693	-0.788764	1.073854
H	3.427765	0.398788	1.101640
H	3.628956	-1.891482	-0.111790
H	2.074838	-1.949530	2.505096
H	5.341489	-3.277293	1.061812
H	4.942187	0.528909	3.056512
H	6.309722	-1.532418	2.549045
H	2.473579	0.452974	2.587998
N	2.809679	-3.734251	0.552069
C	1.368955	-3.924941	0.583261
H	0.937360	-3.551956	1.515010
H	1.174850	-5.001813	0.537825
H	0.833915	-3.457084	-0.264088
C	3.350843	-4.269495	-0.683732
H	2.966321	-3.737360	-1.575170
H	3.084804	-5.326982	-0.777450
H	4.441892	-4.195474	-0.689222
O	2.942383	0.262653	-1.385341
C	2.047099	1.369003	-1.257181
C	2.379623	0.738979	-2.560676
H	1.080458	1.100651	-0.825365
N	1.307445	-0.196860	-3.065689
O	0.953328	-0.066266	-4.212186
O	0.848417	-1.011766	-2.276166
C	2.619123	2.674907	-0.836772
C	3.640298	5.141496	-0.044566
C	3.991682	2.827414	-0.633271
C	1.757271	3.753446	-0.631332
C	2.269275	4.986212	-0.241352
C	4.498759	4.061435	-0.236407

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H          4.651907        1.975333       -0.770917
H          0.687123        3.625509       -0.772743
H          1.596685        5.822969       -0.082935
H          5.565161        4.177291       -0.071305
H          4.037674        6.102121        0.267308
C          3.233745        1.308959       -3.648844
H          2.619703        1.858896       -4.362246
H          3.761127        0.508448       -4.173163
H          3.959777        1.986987       -3.199253

RS epoxide:Catalyst, binary complex 39; Energy = -2449.839841; 6-31G(d) basis set.
N         -0.057373       -0.696671       -1.097552
H         -0.002543        0.077690       -1.756424
C          1.118314       -1.381549       -0.879444
S          1.196738       -2.877594       -0.117911
N          2.168010       -0.715651       -1.400881
H          1.989426        0.264479       -1.591435
C         -1.360462       -0.976456       -0.665686
C         -4.037663       -1.350887        0.108938
C         -1.659978       -1.568344        0.563973
C         -2.408327       -0.546660       -1.490880
C         -3.726108       -0.731476       -1.097060
C         -2.990330       -1.757985        0.924607
H         -0.863111       -1.883145        1.225220
H         -2.186992       -0.078340       -2.445842
H         -5.068528       -1.513431        0.401776
C         -4.838946       -0.214565       -1.963935
C         -3.270548       -2.375486        2.266662
F         -5.229324        1.012937       -1.579829
F         -4.473443       -0.123641       -3.249274
F         -5.920540       -1.003075       -1.900427
F         -2.535928       -3.477002        2.466950
F         -2.974676       -1.526059        3.264066
F         -4.559456       -2.715357        2.403918
C          3.586206       -1.062455       -1.334059
C          5.683033       -1.242334        0.003911
C          5.469957       -2.498525       -2.170829
C          6.074835       -2.506200       -0.766232
C          3.949211       -2.334675       -2.109860
C          4.152877       -1.104509        0.098796
H          6.100642       -0.364221       -0.509755
H          5.906398       -1.669624       -2.746264
H          5.710677       -3.387418       -0.221155
H          3.499839       -3.202053       -1.618185
H          3.754669       -2.009152        0.572995
H          4.077214       -0.233427       -1.860971
H          6.120083       -1.262207        1.008666
H          5.722280       -3.421425       -2.703244
H          7.165419       -2.592781       -0.820269
H          3.521804       -2.268254       -3.116084
N          3.667594        0.014114        0.911381
C          3.921664       -0.194171        2.326847
H          3.482754       -1.145776        2.642447
H          3.450558        0.613380        2.896565
H          4.993962       -0.195671        2.588418
C          4.137032        1.326138        0.498213
H          5.213527        1.488093        0.679585
H          3.579636        2.089034        1.053875
H          3.937582        1.489663       -0.564974
O          1.124650        1.955560       -0.691789
C         -0.078867        2.241989        0.031489
C          0.488474        3.156389       -0.979786
H         -0.928554        1.641260       -0.295247
N         -0.219887        3.070799       -2.311263
O         -0.478884        4.114424       -2.865352
O         -0.504411        1.958691       -2.726283
C          0.062176        2.471009        1.495041
C          0.244892        2.777059        4.249901
C         -0.688996        3.457223        2.133776
C          0.906571        1.633497        2.225902
C          0.989818        1.789936        3.607592
C         -0.592297        3.612700        3.513538
H         -1.346021        4.099443        1.552622
H          1.487292        0.870079        1.705767
H          1.630000        1.133354        4.188854
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H         -1.170419        4.383577        4.012870
H          0.314788        2.893535        5.326897
C          1.182589        4.457162       -0.729533
H          0.467375        5.280459       -0.733369
H          1.937286        4.638533       -1.498402
H          1.665430        4.397111        0.247283

RS epoxide:Catalyst, binary complex 40; Energy = -2449.846682; 6-31G(d) basis set.
N         -0.729357        0.068491       -0.142049
H         -0.220238       -0.065947       -1.011646
C         -0.067584        0.713356        0.861148
S         -0.353519        0.480554        2.499239
N          0.969288        1.482931        0.422395
H          1.475121        1.891803        1.202696
C         -1.974845       -0.563580       -0.037620
C         -4.521143       -1.727930       -0.006438
C         -2.201253       -1.759816       -0.712263
C         -3.016802        0.051166        0.660369
C         -4.273197       -0.532663        0.665615
C         -3.473100       -2.328388       -0.690829
H         -1.385299       -2.242628       -1.243039
H         -2.831388        0.993723        1.164452
H         -5.510580       -2.169448       -0.008445
C         -5.373566        0.169453        1.408870
C         -3.679778       -3.632938       -1.406330
F         -6.586469       -0.245046        1.018147
F         -5.292240       -0.027395        2.731299
F         -5.318142        1.499296        1.210559
F         -3.082215       -4.648623       -0.765005
F         -4.977330       -3.943872       -1.523114
F         -3.158217       -3.600118       -2.643150
C          0.860083        2.395298       -0.726350
C         -0.096320        4.615844       -1.499611
C          2.237203        3.991153       -2.145165
C          1.314834        5.144153       -1.752553
C          2.260452        2.915600       -1.059577
C         -0.112526        3.549230       -0.392154
H         -0.475939        4.179213       -2.432737
H          1.883846        3.552304       -3.088259
H          1.699244        5.627009       -0.843621
H          2.696061        3.343582       -0.143637
H          0.284563        4.012101        0.524149
H          0.486485        1.833955       -1.591606
H         -0.779589        5.429620       -1.228461
H          3.255442        4.350935       -2.325521
H          1.296443        5.908020       -2.537030
H          2.886961        2.067313       -1.344630
N         -1.444023        3.042086       -0.045873
C         -2.286509        2.746695       -1.194372
H         -2.586338        3.643822       -1.760690
H         -3.198698        2.250070       -0.849480
H         -1.771559        2.062323       -1.877599
C         -2.142007        3.888436        0.908905
H         -3.093116        3.416071        1.177502
H         -2.366640        4.897598        0.520595
H         -1.543873        3.985884        1.819535
O          3.872689        0.264583       -0.181249
C          4.498886       -0.950294       -0.592538
C          3.244140       -0.906991        0.199179
H          4.385508       -1.157270       -1.656858
N          2.010822       -1.176955       -0.624581
O          1.854035       -0.552920       -1.661379
O          1.254754       -2.029173       -0.206808
C          5.807329       -1.293949        0.027318
C          8.255970       -1.964638        1.178180
C          6.376176       -0.463134        0.993463
C          6.472054       -2.455280       -0.370598
C          7.691637       -2.791306        0.208296
C          7.598803       -0.799427        1.566354
H          5.860356        0.448468        1.279483
H          6.034106       -3.095367       -1.132292
H          8.203891       -3.697034       -0.100493
H          8.039924       -0.147880        2.314061
H          9.209309       -2.226250        1.626522
C          3.075168       -1.253219        1.645836
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H          2.852826       -2.314374        1.760396
H          2.253326       -0.672148        2.076425
H          4.004092       -1.019288        2.167224

RS epoxide:Catalyst, binary complex 41; Energy = -2449.841730; 6-31G(d) basis set.
N          1.202394       -0.361291        0.064895
H          0.700302        0.496895        0.275401
C          0.421086       -1.394828       -0.393296
S          1.002453       -2.781520       -1.148782
N         -0.887437       -1.173534       -0.171349
H         -1.147877       -0.345430        0.359628
C          2.593578       -0.190361       -0.022499
C          5.352887        0.324546       -0.095157
C          3.066964        1.108464       -0.223191
C          3.506068       -1.234019        0.162338
C          4.867551       -0.963390        0.109404
C          4.434977        1.354139       -0.250867
H          2.362560        1.924630       -0.363123
H          3.152804       -2.238805        0.349231
H          6.418613        0.519924       -0.123972
C          5.844558       -2.098096        0.242517
C          4.907102        2.771857       -0.403058
F          6.988219       -1.699040        0.820519
F          5.348160       -3.100982        0.978774
F          6.171819       -2.610080       -0.953208
F          4.166064        3.446341       -1.294707
F          4.822747        3.444112        0.757042
F          6.183556        2.836239       -0.803139
C         -1.974835       -2.099006       -0.480050
C         -4.301824       -2.792638        0.187174
C         -3.754802       -2.597265       -2.241648
C         -4.841343       -2.402232       -1.186309
C         -2.530586       -1.765709       -1.873297
C         -3.056297       -1.993839        0.603653
H         -4.025331       -3.854944        0.192140
H         -3.479489       -3.659137       -2.294189
H         -5.156166       -1.348142       -1.175994
H         -2.814325       -0.702937       -1.883688
H         -3.338445       -0.925013        0.644174
H         -1.555881       -3.111210       -0.494667
H         -5.073697       -2.667061        0.954403
H         -4.113477       -2.309100       -3.235445
H         -5.728548       -2.998839       -1.423998
H         -1.718096       -1.893421       -2.596188
N         -2.652000       -2.448396        1.944548
C         -1.240602       -2.558010        2.277299
H         -0.698563       -3.132605        1.522526
H         -1.163299       -3.100953        3.225341
H         -0.731158       -1.585793        2.409156
C         -3.347506       -1.694336        2.970891
H         -2.985777       -0.650053        3.041361
H         -3.203341       -2.171836        3.945129
H         -4.422041       -1.667871        2.764666
O         -2.220775        1.312739        1.034980
C         -2.827910        1.682990       -0.210452
C         -2.238046        2.669172        0.728042
H         -2.210701        1.435364       -1.075106
N         -0.867132        3.144939        0.303954
O         -0.638958        4.327449        0.395369
O         -0.095061        2.307400       -0.135665
C         -4.291178        1.463173       -0.355879
C         -7.016570        0.990910       -0.701316
C         -5.075624        1.069882        0.731114
C         -4.871527        1.609097       -1.617478
C         -6.233936        1.379946       -1.786722
C         -6.435082        0.832078        0.555732
H         -4.611096        0.922914        1.702597
H         -4.256123        1.894800       -2.466843
H         -6.681529        1.495811       -2.768414
H         -7.039506        0.517640        1.400567
H         -8.076806        0.803014       -0.837090
C         -2.966086        3.639263        1.602823
H         -3.061540        4.601611        1.099860
H         -2.424853        3.779657        2.541499
H         -3.959475        3.242429        1.813622
```

RS epoxide:Catalyst, binary complex 42; Energy = -2449.841635; 6-31G(d) basis set.

N	1.200503	-0.355809	0.079314
H	0.696596	0.501059	0.291044
C	0.424139	-1.386514	-0.394412
S	1.015384	-2.763504	-1.160015
N	-0.886027	-1.170625	-0.178616
H	-1.151549	-0.348212	0.358679
C	2.591600	-0.183021	-0.011915
C	5.348971	0.328481	-0.112526
C	3.063281	1.114613	-0.237757
C	3.502977	-1.220879	0.190270
C	4.866562	-0.952185	0.123910
C	4.428924	1.358068	-0.280385
H	2.357237	1.926946	-0.386159
H	3.150543	-2.221542	0.402301
H	6.414728	0.522346	-0.156348
C	5.830037	-2.094250	0.288937
C	4.929880	2.762304	-0.463275
F	5.415284	-2.955733	1.229099
F	5.970311	-2.793155	-0.846614
F	7.051861	-1.667358	0.641888
F	5.222729	3.338306	0.714121
F	6.050540	2.793452	-1.198779
F	4.024289	3.543440	-1.067732
C	-1.971092	-2.090244	-0.511876
C	-4.304780	-2.791309	0.125653
C	-3.738767	-2.553727	-2.295221
C	-4.832865	-2.375530	-1.244776
C	-2.516024	-1.730910	-1.902934
C	-3.060238	-2.003314	0.565521
H	-4.031135	-3.854274	0.114124
H	-3.464624	-3.614949	-2.364590
H	-5.146335	-1.321312	-1.218453
H	-2.797960	-0.667564	-1.896052
H	-3.340457	-0.934678	0.623204
H	-1.551993	-3.101973	-0.541790
H	-5.082162	-2.676964	0.889086
H	-4.089600	-2.247307	-3.286341
H	-5.719117	-2.966422	-1.499606
H	-1.698453	-1.846689	-2.622136
N	-2.666414	-2.482974	1.900622
C	-1.257497	-2.600743	2.241404
H	-0.711392	-3.164526	1.481446
H	-1.188087	-3.159114	3.181038
H	-0.747017	-1.631871	2.392018
C	-3.368262	-1.746736	2.935528
H	-3.006503	-0.704063	3.026796
H	-3.230511	-2.241293	3.902155
H	-4.441477	-1.716122	2.723021
O	-2.229055	1.291705	1.059535
C	-2.831297	1.692199	-0.178915
C	-2.246688	2.655361	0.786400
H	-2.210134	1.467020	-1.046895
N	-0.874600	3.143217	0.380130
O	-0.648327	4.323316	0.502730
O	-0.099640	2.318116	-0.077583
C	-4.293614	1.474368	-0.336342
C	-7.016527	1.007510	-0.706319
C	-4.868309	1.651982	-1.596465
C	-5.082394	1.052545	0.736659
C	-6.440654	0.817303	0.548944
C	-6.229640	1.425548	-1.777724
H	-4.249256	1.959563	-2.435507
H	-4.621804	0.882366	1.706283
H	-7.048614	0.480674	1.382661
H	-6.673081	1.565249	-2.758202
H	-8.075803	0.821505	-0.851818
C	-2.979604	3.602424	1.682093
H	-3.077087	4.576029	1.201692
H	-2.440825	3.722209	2.625030
H	-3.972173	3.197601	1.881255

RS epoxide:Catalyst, binary complex 43; Energy = -2449.851281; 6-31G(d) basis set.

N	0.816648	2.818784	-0.711911

```
H          0.775955        3.825888       -0.808564
C          2.069186        2.289993       -0.970416
S          3.240695        3.244422       -1.709281
N          2.239654        1.034054       -0.552770
H          1.486235        0.609579       -0.012142
C         -0.408604        2.132594       -0.770034
C         -2.923285        0.880778       -0.935079
C         -1.498353        2.635585       -0.052180
C         -0.584126        0.994099       -1.563732
C         -1.827316        0.376159       -1.624225
C         -2.738317        2.014279       -0.149617
H         -1.366173        3.501896        0.588559
H          0.247432        0.590083       -2.132252
H         -3.887426        0.387036       -0.985991
C         -1.975948       -0.849346       -2.483515
C         -3.868541        2.484232        0.720826
F         -0.894038       -1.639963       -2.387678
F         -3.044458       -1.575118       -2.134809
F         -2.111499       -0.532342       -3.779206
F         -3.872580        1.816511        1.892951
F         -3.775371        3.785356        1.013690
F         -5.059879        2.271076        0.150202
C          3.337894        0.141535       -0.914552
C          4.739680       -1.809331       -0.188646
C          3.806612       -1.823224       -2.500699
C          4.162371       -2.687395       -1.294851
C          2.827681       -0.735043       -2.073769
C          3.785635       -0.701335        0.293687
H          5.648207       -1.310977       -0.550636
H          4.719697       -1.364798       -2.902504
H          3.259381       -3.200360       -0.934001
H          1.886489       -1.205462       -1.751640
H          2.865285       -1.179197        0.696376
H          4.171935        0.763869       -1.254639
H          5.042312       -2.422175        0.665401
H          3.366557       -2.422648       -3.304412
H          4.883533       -3.464203       -1.569821
H          2.586421       -0.067623       -2.910151
N          4.480462        0.048254        1.349373
C          4.162391        1.457412        1.534742
H          4.302428        2.018372        0.608595
H          4.863738        1.858567        2.273597
H          3.138953        1.636895        1.907723
C          4.387041       -0.637637        2.625936
H          3.376659       -0.566256        3.072832
H          5.091819       -0.192782        3.335000
H          4.639729       -1.695953        2.523938
O          0.329709       -1.001469        0.654781
C         -0.985874       -0.863530        1.202205
C          0.214280       -1.101567        2.039504
H         -1.346897        0.165320        1.204000
N          0.704233        0.162140        2.709770
O          1.029805        0.079394        3.874634
O          0.709703        1.180229        2.041605
C         -1.983462       -1.913072        0.874459
C         -3.921088       -3.808285        0.236741
C         -3.322249       -1.679545        1.197594
C         -1.617032       -3.089631        0.220387
C         -2.588073       -4.034899       -0.096323
C         -4.288021       -2.628584        0.882530
H         -3.605207       -0.746065        1.678843
H         -0.580954       -3.243464       -0.066448
H         -2.303783       -4.945067       -0.614681
H         -5.327728       -2.444160        1.133473
H         -4.676658       -4.545829       -0.015177
C          0.601588       -2.357830        2.751646
H          0.240875       -2.333438        3.780037
H          1.689732       -2.467106        2.759472
H          0.155607       -3.206691        2.232241

RS epoxide:Catalyst, binary complex 44; Energy = -2449.835964; 6-31G(d) basis set.
N         -1.129840       -0.545153        0.027445
H         -0.502375        0.100354       -0.442802
C         -0.587723       -1.782668        0.303982
S         -1.484049       -3.178327        0.578454
```

N	0.753600	-1.749982	0.288565
H	1.203532	-0.843120	0.195053
C	-2.478245	-0.162481	0.013157
C	-5.124473	0.778973	-0.038791
C	-2.887225	0.750064	-0.960370
C	-3.397778	-0.599194	0.972329
C	-4.704201	-0.131496	0.926309
C	-4.197096	1.217014	-0.974075
H	-2.183709	1.082457	-1.719424
H	-3.092176	-1.300015	1.738646
H	-6.149184	1.130179	-0.063426
C	-5.661539	-0.567425	2.000291
C	-4.582963	2.233400	-2.010341
F	-6.937517	-0.454647	1.605250
F	-5.457404	-1.838833	2.365057
F	-5.526870	0.182625	3.106988
F	-4.117630	3.454449	-1.696239
F	-4.075150	1.927875	-3.213683
F	-5.910469	2.338018	-2.142396
C	1.643115	-2.899536	0.423264
C	4.162328	-3.031875	0.214300
C	3.060687	-2.065309	2.330752
C	4.339515	-2.157008	1.466250
C	2.033210	-3.105138	1.892565
C	2.863327	-2.688471	-0.517026
H	4.152229	-4.097053	0.473944
H	3.301144	-2.193196	3.390290
H	4.639221	-1.149487	1.149137
H	1.120694	-3.052567	2.494629
H	2.919304	-1.600755	-0.754425
H	1.089604	-3.778234	0.085909
H	5.025543	-2.875499	-0.437871
H	2.614228	-1.068202	2.233643
H	5.173027	-2.555722	2.052986
H	2.438711	-4.115683	2.016381
N	2.681273	-3.433612	-1.762644
C	1.455223	-3.029763	-2.447365
H	0.570691	-3.251495	-1.845925
H	1.371321	-3.592477	-3.380599
H	1.447286	-1.950877	-2.693592
C	3.802151	-3.246445	-2.673317
H	3.999978	-2.175109	-2.878136
H	3.570583	-3.730299	-3.625410
H	4.712046	-3.704869	-2.283002
O	2.636136	0.683395	0.340137
C	2.582216	2.075797	0.015786
C	3.188602	1.060346	-0.880581
H	1.585266	2.416481	-0.261139
N	2.288860	0.650299	-2.023399
O	2.805665	0.495368	-3.105520
O	1.100114	0.511009	-1.783685
C	3.411354	3.003263	0.829858
C	4.945896	4.786291	2.319232
C	4.234799	2.527440	1.850992
C	3.346866	4.371838	0.562556
C	4.117896	5.260899	1.303634
C	5.000113	3.421658	2.593928
H	4.258398	1.463263	2.069157
H	2.691976	4.739902	-0.223016
H	4.068015	6.324098	1.092169
H	5.635896	3.052098	3.392062
H	5.543696	5.480495	2.901157
C	4.644382	0.852709	-1.154558
H	4.950664	1.427461	-2.029247
H	4.848081	-0.206702	-1.336772
H	5.211270	1.186083	-0.284216

RS epoxide:Catalyst, binary complex 45; Energy = -2449.832283; 6-31G(d) basis set.

N	0.562600	1.040275	0.266272
H	0.199849	1.163845	1.206398
C	-0.381676	1.036162	-0.734427
S	-0.221283	0.222654	-2.195841
N	-1.482578	1.753061	-0.440787
H	-2.214718	1.675153	-1.137679
C	1.847959	0.463764	0.207765

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C          4.437527       -0.598651        0.216196
C          2.710331        0.720428       -0.862051
C          2.281727       -0.313404        1.278836
C          3.574131       -0.832446        1.275776
C          3.986973        0.179623       -0.848735
H          2.382320        1.342170       -1.685933
H          1.611003       -0.516081        2.109197
H          5.445350       -0.999255        0.223042
C          4.003884       -1.709357        2.417832
C          4.909195        0.412291       -2.013139
F          5.336934       -1.748723        2.540308
F          3.498153       -1.283164        3.584386
F          3.584773       -2.973767        2.251700
F          4.932343       -0.643955       -2.839148
F          4.543798        1.476968       -2.738291
F          6.171333        0.611492       -1.604045
C         -1.602337        2.857993        0.521470
C         -2.689089        5.094166        0.926249
C         -2.632779        3.450151        2.794560
C         -3.454561        4.546916        2.126598
C         -2.317239        2.351736        1.784631
C         -2.353230        4.030716       -0.134073
H         -1.736544        5.525234        1.260837
H         -1.698654        3.880434        3.180589
H         -4.420339        4.136180        1.801868
H         -3.248466        1.863624        1.468002
H         -3.303612        3.603266       -0.516739
H         -0.589139        3.196451        0.776002
H         -3.245257        5.906617        0.448608
H         -3.162733        3.016503        3.648479
H         -3.671659        5.355711        2.831893
H         -1.707895        1.570698        2.254725
N         -1.625719        4.708617       -1.219096
C         -0.569043        4.005872       -1.932764
H          0.180510        3.608595       -1.242733
H         -0.063590        4.736102       -2.573040
H         -0.920952        3.182026       -2.576693
C         -2.552923        5.289098       -2.176365
H         -3.061965        4.521128       -2.788057
H         -2.011213        5.957882       -2.851965
H         -3.319292        5.877568       -1.665530
O         -2.822689       -1.165203       -0.273952
C         -3.327731       -2.358088        0.328756
C         -1.989786       -1.805747        0.638179
H         -4.105590       -2.180580        1.068275
N         -1.928550       -0.987681        1.914049
O         -2.971564       -0.607128        2.397224
O         -0.820537       -0.727016        2.356754
C         -3.491775       -3.547943       -0.551304
C         -3.822261       -5.795997       -2.163751
C         -3.110809       -3.504702       -1.893234
C         -4.048375       -4.712909       -0.020855
C         -4.208419       -5.836451       -0.825388
C         -3.277236       -4.629556       -2.695996
H         -2.695055       -2.586575       -2.299022
H         -4.357090       -4.738478        1.021292
H         -4.638105       -6.742031       -0.408960
H         -2.983283       -4.593122       -3.740242
H         -3.950578       -6.671829       -2.792236
C         -0.671097       -2.390428        0.244095
H         -0.305517       -3.043137        1.040658
H          0.065270       -1.610726        0.048542
H         -0.808638       -2.974054       -0.666745

RS epoxide:Catalyst, binary complex 46; Energy = -2449.834742; 6-31G(d) basis set.
N          1.040415       -0.475445       -0.376766
H          0.532681        0.405337       -0.432996
C          0.317351       -1.609377       -0.660295
S          0.982412       -3.126380       -0.951401
N         -1.008146       -1.367597       -0.695009
H         -1.310727       -0.464993       -0.344229
C          2.428600       -0.326032       -0.225508
C          5.177771        0.145701        0.114895
C          3.004284        0.865791       -0.669993
C          3.231677       -1.278637        0.412499
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C	4.589562	-1.034207	0.562700
C	4.365469	1.092270	-0.491690
H	2.388413	1.615693	-1.158736
H	2.797379	-2.199093	0.777946
H	6.241441	0.317684	0.234111
C	5.440682	-2.031380	1.297581
C	4.934917	2.405354	-0.947773
F	6.685168	-2.078301	0.798738
F	5.557670	-1.709998	2.597481
F	4.931878	-3.267509	1.243496
F	6.273169	2.382790	-0.996208
F	4.489690	2.740510	-2.167939
F	4.583691	3.404564	-0.121764
C	-2.048058	-2.382564	-0.876850
C	-4.391811	-1.403217	-1.146800
C	-2.810896	-1.465791	-3.126603
C	-3.712093	-0.583993	-2.244059
C	-2.306135	-2.690185	-2.352397
C	-3.342937	-1.916054	-0.147791
H	-4.922468	-2.252260	-1.596938
H	-3.364937	-1.802991	-4.008965
H	-3.105968	0.195796	-1.765112
H	-1.393228	-3.093008	-2.799413
H	-3.077740	-1.050836	0.498472
H	-1.683667	-3.300206	-0.410511
H	-5.133619	-0.790434	-0.621080
H	-1.962889	-0.879172	-3.494483
H	-4.459724	-0.056915	-2.845246
H	-3.054113	-3.492019	-2.374809
N	-3.840004	-3.005240	0.696036
C	-2.967296	-3.189076	1.849784
H	-1.933363	-3.363754	1.542332
H	-3.297811	-4.058462	2.424713
H	-2.978710	-2.305459	2.516413
C	-5.195289	-2.777553	1.179081
H	-5.287493	-1.832779	1.747170
H	-5.473230	-3.601514	1.842074
H	-5.909321	-2.755819	0.354419
O	-1.592214	1.219175	0.823679
C	-2.515731	2.011622	0.062732
C	-1.505688	2.597947	0.976501
H	-2.260494	2.068474	-0.995653
N	-0.301440	3.142328	0.237679
O	0.088145	4.241610	0.552914
O	0.168799	2.450078	-0.651377
C	-3.960137	1.870656	0.381121
C	-6.687481	1.564468	0.870217
C	-4.895235	2.352504	-0.537847
C	-4.392776	1.219604	1.538343
C	-5.755428	1.072161	1.781727
C	-6.256006	2.202954	-0.291115
H	-4.555539	2.833907	-1.451582
H	-3.663428	0.802730	2.227494
H	-6.088625	0.562320	2.680335
H	-6.978368	2.578354	-1.008517
H	-7.749047	1.442924	1.060440
C	-1.732013	3.240016	2.307938
H	-1.829994	4.319141	2.190796
H	-0.892412	3.027588	2.974080
H	-2.648412	2.840217	2.741982

RS epoxide:Catalyst, binary complex 47; Energy = -2449.832952; 6-31G(d) basis set.

N	0.963177	-0.508225	-0.307072
H	0.346348	0.285975	-0.145640
C	0.369075	-1.693044	-0.669228
S	1.196180	-3.061165	-1.197645
N	-0.969032	-1.647332	-0.556712
H	-1.387884	-0.782123	-0.234582
C	2.330447	-0.181480	-0.292909
C	5.017354	0.629940	-0.208276
C	3.313654	-1.059079	0.171324
C	2.695520	1.104451	-0.695853
C	4.026216	1.500673	-0.643166
C	4.640716	-0.646530	0.195245
H	3.039936	-2.048747	0.512203

```
H          1.937636        1.793880       -1.054751
H          6.055738        0.939727       -0.178101
C          4.378938        2.910675       -1.020762
C          5.691987       -1.622267        0.644892
F          5.651932        3.016535       -1.424375
F          3.597962        3.367243       -2.012080
F          4.224030        3.753353        0.012716
F          6.778139       -0.995815        1.121560
F          5.235309       -2.431110        1.611876
F          6.103225       -2.407958       -0.361204
C         -1.900060       -2.726127       -0.870054
C         -4.381452       -3.048088       -0.633670
C         -3.426723       -1.615844       -2.522999
C         -4.699876       -2.105696       -1.808502
C         -2.314775       -2.646772       -2.350118
C         -3.106620       -2.622333        0.101621
H         -4.236965       -4.076087       -0.986088
H         -3.628339       -1.422089       -3.580310
H         -5.280114       -1.246639       -1.450404
H         -1.426100       -2.402274       -2.939191
H         -3.223549       -1.547137        0.382813
H         -1.383006       -3.672284       -0.691897
H         -5.237727       -3.069715        0.042687
H         -3.093131       -0.659321       -2.094181
H         -5.344482       -2.636601       -2.516898
H         -2.661892       -3.629529       -2.689674
N         -2.879166       -3.406953        1.317173
C         -1.598846       -3.106107        1.947572
H         -0.761032       -3.379646        1.302825
H         -1.516082       -3.689795        2.867945
H         -1.499134       -2.033763        2.208886
C         -3.937492       -3.195550        2.294919
H         -4.059259       -2.124649        2.553496
H         -3.690859       -3.738348        3.210691
H         -4.894879       -3.575568        1.936873
O         -1.863020        1.007144        0.346624
C         -2.341818        2.352135        0.243452
C         -1.911162        1.741160        1.527058
H         -1.624018        3.025936       -0.222937
N         -0.527163        2.169247        1.951432
O         -0.406809        2.566443        3.088359
O          0.357280        2.120279        1.115471
C         -3.774876        2.542465       -0.102939
C         -6.455064        2.949659       -0.742916
C         -4.256969        3.838217       -0.295418
C         -4.632537        1.450439       -0.242363
C         -5.970910        1.655870       -0.563117
C         -5.597142        4.039609       -0.609460
H         -3.583936        4.686397       -0.200739
H         -4.244883        0.443466       -0.110144
H         -6.635928        0.804821       -0.673856
H         -5.970991        5.047850       -0.755048
H         -7.499264        3.109317       -0.991868
C         -2.784375        1.301210        2.659375
H         -2.900561        2.109634        3.381319
H         -2.341517        0.436860        3.161197
H         -3.761957        1.025265        2.261624

RS epoxide:Catalyst, binary complex 48; Energy = -2449.838645; 6-31G(d) basis set.
N          0.294371       -0.647871        0.195510
H          0.517711        0.342661        0.155136
C          1.350126       -1.503754       -0.021558
S          1.351490       -3.101771        0.488450
N          2.352495       -0.887006       -0.686339
H          2.178774        0.091623       -0.892278
C         -1.055652       -0.920027        0.427398
C         -3.846118       -1.141127        0.684724
C         -1.796444        0.080918        1.066651
C         -1.715439       -2.047290       -0.061789
C         -3.097449       -2.140940        0.079552
C         -3.171984       -0.025426        1.174410
H         -1.284478        0.950161        1.465585
H         -1.161073       -2.829684       -0.565853
H         -4.924925       -1.220327        0.761889
C         -3.787910       -3.307151       -0.568469
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C         -3.961609        1.076864        1.819193
F         -3.843015       -3.145650       -1.904467
F         -3.142844       -4.457992       -0.344850
F         -5.048206       -3.452339       -0.138976
F         -3.242082        2.202314        1.952331
F         -5.052497        1.381639        1.095341
F         -4.393641        0.735751        3.041514
C          3.780645       -1.204908       -0.626295
C          5.853224       -1.290055        0.767990
C          5.708843       -2.618521       -1.373123
C          6.282907       -2.570190        0.044754
C          4.183359       -2.493895       -1.348744
C          4.320514       -1.174458        0.816330
H          6.270394       -0.421898        0.238118
H          6.137643       -1.796599       -1.964055
H          5.922750       -3.441231        0.608682
H          3.746574       -3.352748       -0.832545
H          3.926502       -2.066059        1.321320
H          4.252384       -0.381358       -1.178663
H          6.260953       -1.270756        1.785349
H          5.996816       -3.550402       -1.870707
H          7.375719       -2.638384        0.016873
H          3.772543       -2.476834       -2.364041
N          3.781376       -0.030014        1.555993
C          3.953970       -0.169744        2.991314
H          3.553453       -1.135097        3.314425
H          3.393319        0.620771        3.500888
H          5.005630       -0.098129        3.320453
C          4.247855        1.269107        1.101268
H          5.325710        1.439108        1.265773
H          3.706651        2.049138        1.648674
H          4.037234        1.411772        0.035898
O          1.250318        2.001118       -0.736709
C          0.361558        2.731571       -1.612555
C          0.964130        3.320646       -0.398907
H          0.851026        2.980341       -2.553112
N          2.155828        4.212350       -0.687247
O          2.945398        3.829858       -1.524183
O          2.216349        5.254942       -0.069059
C         -1.051315        2.255501       -1.668707
C         -3.660538        1.285275       -1.792262
C         -2.111932        3.044986       -1.221911
C         -1.303220        0.986603       -2.198404
C         -2.605751        0.500352       -2.255194
C         -3.414802        2.557591       -1.281469
H         -1.921036        4.039019       -0.826303
H         -0.474295        0.370844       -2.541004
H         -2.796221       -0.497625       -2.638725
H         -4.235599        3.165407       -0.915332
H         -4.675210        0.899849       -1.818801
C          0.296025        3.624735        0.906963
H         -0.012410        4.669756        0.943574
H          0.990594        3.433523        1.729093
H         -0.583355        2.988455        1.013659

RS epoxide:Catalyst, binary complex 49; Energy = -2449.839625; 6-31G(d) basis set.
N         -1.719114       -1.289551       -0.866584
C         -0.467246       -1.791442       -0.944162
S         -0.122774       -3.432929       -0.965397
C         -2.924825       -2.080376       -0.672651
C         -3.864229       -1.356367        0.302859
C         -4.989021       -2.330060        0.723966
C         -5.347787       -3.324169       -0.398372
C         -5.146882       -2.679420       -1.771819
C         -3.659939       -2.341577       -2.000225
N         -3.122984       -0.721145        1.394712
C         -2.338108       -1.633669        2.215388
N          0.465254       -0.785587       -1.047493
C          1.823832       -0.739972       -0.718115
C          2.494180        0.450551       -1.041251
C          3.817214        0.630219       -0.670507
C          4.518034       -0.363575        0.006211
C          3.846644       -1.538649        0.313134
C          2.512480       -1.741714       -0.027982
C          4.495867        1.943691       -0.945903
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F          5.792337        1.769022       -1.247963
C          4.577608       -2.655334        1.007055
F          3.798730       -3.270804        1.908363
C         -3.971120        0.122523        2.221456
F          3.927969        2.598238       -1.966131
F          4.450422        2.747864        0.124794
F          4.983874       -3.593186        0.138777
F          5.667511       -2.212382        1.648995
H         -1.804855       -0.324373       -0.555188
H          0.083374        0.116820       -1.314145
H         -3.565519       -1.447914       -2.628441
H         -3.147706       -3.156182       -2.522328
H         -5.509400       -3.336704       -2.567480
H         -5.752108       -1.764949       -1.823177
H         -4.711972       -4.215127       -0.329099
H         -6.379020       -3.668880       -0.276641
H         -4.680927       -2.882111        1.619290
H         -5.873597       -1.745865        1.001800
H         -2.612974       -3.036072       -0.238178
H         -4.321429       -0.521649       -0.248971
H         -4.662837       -0.453698        2.859147
H         -3.342763        0.737055        2.876288
H         -4.555376        0.791320        1.582802
H         -2.953060       -2.310191        2.830560
H         -1.717272       -1.042428        2.897623
H         -1.671156       -2.238510        1.593529
H          1.974181        1.239965       -1.578191
H          5.555318       -0.220616        0.286637
H          2.016163       -2.663992        0.241995
N          1.287194        2.893661        0.639378
O          1.854523        2.744280        1.700512
O          1.702439        3.520848       -0.313811
C         -0.078729        2.255820        0.504819
C         -1.045041        3.087474       -0.246208
H         -0.666804        4.044841       -0.602402
O         -0.362683        1.979156       -0.835734
C         -2.521633        2.959369       -0.086034
C         -5.305603        2.904230        0.054185
C         -3.189105        3.745498        0.854893
C         -3.247115        2.132055       -0.943632
C         -4.638827        2.112017       -0.877397
C         -4.578303        3.712403        0.927526
H         -2.621105        4.390879        1.519976
H         -2.723873        1.533457       -1.685483
H         -5.201743        1.483454       -1.561637
H         -5.094278        4.324826        1.660005
H         -6.389908        2.891805        0.101798
C         -0.401003        1.253839        1.565662
H          0.355861        0.463289        1.583351
H         -1.382777        0.816539        1.351489
H         -0.420386        1.737010        2.544685

RS epoxide:Catalyst, binary complex 50; Energy = -2449.855802; 6-31G(d) basis set.
N          2.737849       -2.635476       -1.259977
O          3.006816       -1.529481       -1.690285
O          3.514955       -3.561893       -1.170536
N          2.107144        1.244661       -0.692770
C          0.905350        1.809955       -0.477280
S          0.727271        3.314237        0.258685
C          3.384921        1.828712       -0.314357
C          4.364808        0.708287        0.060886
C          5.686507        1.339300        0.528430
C          6.282632        2.230842       -0.565722
C          5.295181        3.319057       -0.990142
C          3.963830        2.706764       -1.427862
N          3.745992       -0.248687        0.985965
C          3.328162        0.324968        2.257681
N         -0.121161        1.021013       -0.939591
C         -1.507204        1.054990       -0.752570
C         -2.215793       -0.012985       -1.324349
C         -3.587796       -0.120388       -1.163448
C         -4.308702        0.835719       -0.456293
C         -3.603218        1.902466        0.081829
C         -2.222759        2.029684       -0.048918
C         -4.274093       -1.332195       -1.723075
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F	-3.836124	-1.630651	-2.954369
C	-4.322865	2.958254	0.875620
F	-4.058616	2.850025	2.186787
C	4.562285	-1.435861	1.186409
F	-4.037354	-2.422773	-0.962548
F	-5.600719	-1.181239	-1.785380
F	-3.950267	4.191191	0.505579
F	-5.652947	2.876335	0.730638
H	2.154527	0.293366	-1.054214
H	0.183472	0.176438	-1.415405
H	4.108639	2.089850	-2.325514
H	3.233807	3.484683	-1.674044
H	5.116290	3.997509	-0.144925
H	5.715299	3.924473	-1.799895
H	7.219036	2.677499	-0.215311
H	6.532859	1.610148	-1.437110
H	5.509665	1.940827	1.430363
H	6.397426	0.550935	0.800224
H	3.202638	2.466258	0.557419
H	4.575362	0.134207	-0.854247
H	5.438141	-1.263690	1.833776
H	3.953940	-2.220521	1.654587
H	4.913061	-1.808715	0.218882
H	2.823009	-0.450224	2.843665
H	2.612024	1.136297	2.095899
H	4.166618	0.704340	2.864803
H	-1.680679	-0.772992	-1.888649
H	-5.382585	0.755521	-0.339767
H	-1.711036	2.876867	0.385858
C	1.338345	-2.880423	-0.755628
C	0.936893	-1.953016	0.331416
H	1.695983	-1.217582	0.624213
O	0.504005	-1.807886	-1.033774
C	0.865153	-4.284780	-0.966229
H	-0.131500	-4.385550	-0.534767
H	1.543964	-4.985731	-0.480561
H	0.820800	-4.510301	-2.034702
C	-0.099720	-2.320345	1.332735
C	-2.019240	-2.969992	3.247731
C	-1.427903	-2.516694	0.953914
C	0.266345	-2.451924	2.673420
C	-0.690838	-2.782889	3.626618
C	-2.386429	-2.833991	1.911343
H	-1.714462	-2.409620	-0.086418
H	1.300953	-2.298282	2.970284
H	-0.401217	-2.885637	4.667472
H	-3.419366	-2.966303	1.605748
H	-2.766854	-3.215421	3.995436

RS epoxide:Catalyst, binary complex 51; Energy = -2449.842776; 6-31G(d) basis set.

N	-0.069567	-0.541900	-0.515085
H	0.076786	0.392874	-0.887805
C	1.055628	-1.281395	-0.220974
S	0.984519	-2.669436	0.731351
N	2.173391	-0.753654	-0.754666
H	2.049669	0.038549	-1.376121
C	-1.403943	-0.876650	-0.211150
C	-4.101607	-1.445868	0.304006
C	-2.233059	0.093509	0.354846
C	-1.930818	-2.129114	-0.530874
C	-3.266313	-2.402798	-0.261128
C	-3.572238	-0.195296	0.597935
H	-1.836085	1.070963	0.613030
H	-1.296132	-2.878869	-0.988583
H	-5.142146	-1.670293	0.510090
C	-3.795722	-3.773681	-0.576969
C	-4.478229	0.861984	1.160695
F	-3.405917	-4.678368	0.331004
F	-5.136046	-3.794407	-0.608376
F	-3.356293	-4.203473	-1.769572
F	-5.165952	1.496107	0.190745
F	-5.390143	0.338898	1.991537
F	-3.800198	1.799441	1.835706
C	3.562519	-1.212031	-0.628832
C	5.540279	-1.710996	0.838700

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C          5.275077       -2.940871       -1.330064
C          5.754446       -3.042326        0.118080
C          3.804123       -2.525095       -1.387757
C          4.058836       -1.300666        0.827540
H          6.145047       -0.940108        0.341417
H          5.888944       -2.199448       -1.860803
H          5.192813       -3.833152        0.633091
H          3.180258       -3.305507       -0.938921
H          3.489343       -2.101573        1.306072
H          4.140079       -0.420342       -1.126036
H          5.890173       -1.771020        1.876672
H          5.409131       -3.895355       -1.849738
H          6.812115       -3.324923        0.152710
H          3.475624       -2.399194       -2.425392
N          3.753654       -0.074001        1.571471
C          3.518003       -0.329351        2.983955
H          2.732606       -1.082198        3.092635
H          3.179717        0.595302        3.465026
H          4.420486       -0.674591        3.519366
C          4.726905        0.994505        1.403501
H          5.685597        0.795053        1.911253
H          4.317557        1.920732        1.821232
H          4.935093        1.166297        0.342088
O          1.173310        1.929489       -1.526335
C          0.792700        3.313896       -1.396986
C          1.695821        2.638618       -0.447804
H          1.250617        3.942776       -2.160421
N          3.156721        2.939694       -0.654471
O          3.641274        3.751358        0.106774
O          3.737538        2.353350       -1.544350
C         -0.637046        3.550276       -1.045749
C         -3.312241        3.912232       -0.368252
C         -0.986501        4.487655       -0.073177
C         -1.625576        2.803191       -1.687433
C         -2.963156        2.984639       -1.347131
C         -2.325205        4.667085        0.263101
H         -0.211173        5.061158        0.428555
H         -1.344282        2.071473       -2.441330
H         -3.730655        2.390077       -1.831648
H         -2.596547        5.386200        1.029334
H         -4.353129        4.034298       -0.087436
C          1.395873        2.212429        0.958383
H          0.320911        2.055421        1.063541
H          1.710522        2.994314        1.652658
H          1.937993        1.280446        1.176225

RS epoxide:Catalyst, binary complex 52; Energy = -2449.838637; 6-31G(d) basis set.
N         -0.295764       -0.646260       -0.164496
H         -0.520187        0.343691       -0.116796
C         -1.351465       -1.505953        0.034013
S         -1.344395       -3.098817       -0.493154
N         -2.360571       -0.898626        0.696774
H         -2.188883        0.076738        0.919443
C          1.052909       -0.918470       -0.406872
C          3.837589       -1.147869       -0.688012
C          1.786311        0.069752       -1.070143
C          1.715720       -2.038224        0.099410
C          3.094329       -2.136588       -0.054011
C          3.161994       -0.040535       -1.189653
H          1.271197        0.931659       -1.480825
H          1.163181       -2.808841        0.622585
H          4.915860       -1.231390       -0.775461
C          3.817214       -3.269482        0.617379
C          3.946323        1.049383       -1.861643
F          4.168017       -2.930863        1.873713
F          3.064895       -4.370849        0.705651
F          4.947807       -3.592805       -0.025285
F          4.362898        0.688039       -3.083537
F          3.227672        2.174063       -2.003608
F          5.046552        1.362983       -1.155712
C         -3.786928       -1.220355        0.622160
C         -5.847629       -1.307236       -0.789604
C         -5.716310       -2.643608        1.347684
C         -6.279321       -2.591369       -0.074604
C         -4.191238       -2.513204        1.336815
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C         -4.314888       -1.188106       -0.825080
H         -6.271501       -0.442064       -0.260146
H         -6.153006       -1.825774        1.938477
H         -5.912026       -3.459045       -0.639143
H         -3.746356       -3.368409        0.821381
H         -3.915403       -2.077926       -1.328676
H         -4.266539       -0.400128        1.172664
H         -6.246913       -1.285434       -1.810254
H         -6.005158       -3.578612        1.838880
H         -7.372100       -2.663006       -0.055692
H         -3.789437       -2.498067        2.355718
N         -3.771561       -0.041503       -1.557942
C         -3.929066       -0.179348       -2.995124
H         -3.522247       -1.142996       -3.315480
H         -3.365404        0.613579       -3.497647
H         -4.977454       -0.110211       -3.335012
C         -4.244843        1.255658       -1.105426
H         -5.321220        1.424450       -1.280569
H         -3.699160        2.037768       -1.645378
H         -4.045752        1.395571       -0.037435
O         -1.266893        1.995238        0.781054
C         -0.359608        2.740663        1.624725
C         -0.994646        3.311318        0.418840
H         -0.826856        2.999739        2.573842
N         -2.181295        4.203346        0.725051
O         -2.257986        5.239432        0.097661
O         -2.950990        3.828046        1.583443
C          1.056904        2.272819        1.653347
C          3.675360        1.321889        1.735734
C          1.329997        1.016562        2.202336
C          2.101710        3.059654        1.166424
C          3.408978        2.581846        1.205234
C          2.636898        0.540016        2.238509
H          0.514138        0.403468        2.579304
H          1.895316        4.044774        0.756631
H          4.216613        3.187129        0.806989
H          2.843988       -0.448173        2.638187
H          4.692781        0.942947        1.745401
C         -0.361280        3.600291       -0.907626
H         -1.078179        3.402140       -1.708741
H          0.513585        2.960729       -1.030942
H         -0.051923        4.644205       -0.963681

RS epoxide:Catalyst, binary complex 53; Energy = -2449.842827; 6-31G(d) basis set.
N         -0.070544       -0.538985       -0.534570
H          0.075219        0.397791       -0.902633
C          1.056071       -1.274982       -0.235611
S          0.986746       -2.663851        0.715491
N          2.174645       -0.742861       -0.763204
H          2.051341        0.049970       -1.383970
C         -1.404677       -0.875244       -0.231565
C         -4.100118       -1.450755        0.284223
C         -2.238638        0.096864        0.321735
C         -1.925228       -2.134875       -0.539292
C         -3.258678       -2.411355       -0.268788
C         -3.577944       -0.195598        0.565719
H         -1.846763        1.079028        0.569956
H         -1.286504       -2.886202       -0.987194
H         -5.140359       -1.677608        0.490896
C         -3.794308       -3.788937       -0.541835
C         -4.488710        0.863791        1.117016
F         -3.176765       -4.364160       -1.582940
F         -3.631076       -4.600952        0.511620
F         -5.108195       -3.760590       -0.814199
F         -3.816909        1.797462        1.803583
F         -5.160096        1.502480        0.138774
F         -5.414114        0.342636        1.933986
C          3.563624       -1.202812       -0.640180
C          5.541489       -1.718040        0.820998
C          5.276715       -2.922509       -1.362005
C          5.756992       -3.040498        0.084469
C          3.805434       -2.506931       -1.414502
C          4.059399       -1.309971        0.815055
H          6.145252       -0.940407        0.333067
H          5.889662       -2.174367       -1.884295
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H          5.196653       -3.838009        0.590506
H          3.181660       -3.292612       -0.974445
H          3.491682       -2.118329        1.282720
H          4.141966       -0.405357       -1.127070
H          5.891456       -1.790206        1.858166
H          5.411331       -3.870683       -1.892984
H          6.815012       -3.322231        0.115082
H          3.476797       -2.369176       -2.450601
N          3.751604       -0.094157        1.575477
C          3.513329       -0.369888        2.983688
H          2.727676       -1.124203        3.079886
H          3.174188        0.547733        3.477410
H          4.414969       -0.722804        3.515600
C          4.724601        0.977111        1.424732
H          5.681760        0.771484        1.932970
H          4.313286        1.897624        1.853041
H          4.936340        1.162679        0.366361
O          1.177931        1.943966       -1.513463
C          0.802011        3.328230       -1.368643
C          1.698433        2.637831       -0.424129
H          1.265901        3.964700       -2.122169
N          3.161017        2.937102       -0.621776
O          3.644688        3.739221        0.150027
O          3.743814        2.358912       -1.515737
C         -0.628594        3.566027       -1.022365
C         -3.306729        3.932503       -0.359508
C         -0.979803        4.486059       -0.034023
C         -1.616741        2.838511       -1.686890
C         -2.955791        3.022356       -1.354057
C         -2.320043        4.667758        0.295051
H         -0.204849        5.044471        0.484961
H         -1.333985        2.120169       -2.452967
H         -3.723446        2.443408       -1.856826
H         -2.592945        5.372908        1.073572
H         -4.349081        4.055904       -0.084726
C          1.392557        2.195593        0.975912
H          0.317261        2.036899        1.075135
H          1.704246        2.969733        1.680200
H          1.934301        1.261518        1.185753

RS epoxide:Catalyst, binary complex 54; Energy = -2449.852596; 6-31G(d) basis set.
N          0.329490        0.746961        1.620921
H          0.458267       -0.063321        2.220850
C          1.468530        1.165478        0.961685
S          1.473556        2.424681       -0.157036
N          2.549409        0.448005        1.317440
H          2.407916       -0.292782        1.997043
C         -1.017503        0.921749        1.252518
C         -3.724496        1.021124        0.500951
C         -1.850588       -0.187603        1.428376
C         -1.560092        2.108186        0.753611
C         -2.898556        2.130461        0.370322
C         -3.183745       -0.134158        1.053605
H         -1.438662       -1.100746        1.848298
H         -0.948139        2.993850        0.658004
H         -4.764508        1.060352        0.197327
C         -3.440296        3.385228       -0.255012
C         -4.015823       -1.378928        1.155835
F         -4.772140        3.467949       -0.134683
F         -2.910857        4.485647        0.294429
F         -3.162732        3.434802       -1.570401
F         -5.316143       -1.102766        1.306496
F         -3.900285       -2.137405        0.050129
F         -3.635232       -2.148556        2.188592
C          3.944884        0.601150        0.886675
C          5.664731        0.588419       -0.936935
C          6.079026        1.926490        1.150669
C          6.302653        1.854353       -0.360653
C          4.589079        1.857586        1.487417
C          4.156412        0.543965       -0.641364
H          6.160156       -0.290863       -0.502415
H          6.601317        1.087844        1.632209
H          5.854334        2.736944       -0.836295
H          4.073556        2.738336        1.087487
H          3.716488        1.453833       -1.055315
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H          4.441383       -0.277855        1.320049
H          5.818999        0.537363       -2.021710
H          6.508963        2.846071        1.561043
H          7.373322        1.876070       -0.590238
H          4.436047        1.852904        2.572084
N          3.430978       -0.577362       -1.244168
C          2.995928       -0.291793       -2.602774
H          2.404014        0.628369       -2.613051
H          2.361489       -1.113087       -2.957348
H          3.834054       -0.186977       -3.314687
C          4.135176       -1.851796       -1.194809
H          4.968161       -1.906949       -1.916487
H          3.429345       -2.659016       -1.414212
H          4.533613       -2.029023       -0.192868
C          0.367360       -2.864619        0.406113
N          1.393729       -2.524908        1.457883
O          0.963224       -2.022777        2.495258
O          2.563676       -2.667788        1.204820
C         -0.861744       -3.542207        0.944472
H         -1.014576       -3.301371        1.996432
H         -0.738147       -4.623671        0.841534
H         -1.740448       -3.229857        0.376189
C          0.499918       -1.948332       -0.764465
C         -0.674178       -1.585154       -1.594757
C         -2.947043       -0.806462       -3.003517
C         -0.935626       -0.228986       -1.806001
C         -1.527572       -2.552325       -2.129281
C         -2.659882       -2.159624       -2.836706
C         -2.080837        0.159912       -2.493767
H         -0.243389        0.520097       -1.425096
H         -1.295025       -3.605377       -1.997013
H         -3.324043       -2.911672       -3.250945
H         -2.294412        1.216186       -2.625723
H         -3.839367       -0.505064       -3.543590
H          1.333368       -1.235263       -0.724665
O          0.941352       -3.315539       -0.760472

RS epoxide:Catalyst, binary complex 55; Energy = -2449.845442; 6-31G(d) basis set.
N          0.462196       -1.656186       -0.330810
H          0.505864       -1.912288       -1.313645
C          1.679945       -1.635779        0.330337
S          1.837467       -1.765044        1.994843
N          2.702970       -1.560141       -0.543509
H          2.435167       -1.295834       -1.486926
C         -0.845549       -1.503498        0.141178
C         -3.556341       -1.125899        0.837973
C         -1.873604       -1.849002       -0.748096
C         -1.189199       -0.952194        1.382961
C         -2.530362       -0.786825        1.711893
C         -3.202721       -1.648327       -0.400754
H         -1.632359       -2.269923       -1.719908
H         -0.421168       -0.637862        2.074585
H         -4.595540       -0.975063        1.104995
C         -2.867669       -0.210771        3.060403
C         -4.257352       -1.935120       -1.431347
F         -2.882867       -1.151368        4.014117
F         -1.981650        0.719829        3.435872
F         -4.081968        0.366401        3.058606
F         -4.332887       -0.936754       -2.332791
F         -3.991953       -3.053715       -2.118134
F         -5.471737       -2.065097       -0.886853
C          4.093488       -1.204434       -0.244264
C          5.705354        0.508449        0.614225
C          6.363131       -1.923341        0.554889
C          6.514615       -0.595543        1.300668
C          4.890125       -2.323415        0.435331
C          4.219058        0.124674        0.530691
H          6.105735        0.670332       -0.396296
H          6.798389       -1.823165       -0.449418
H          6.158319       -0.717644        2.332208
H          4.472641       -2.512233        1.428710
H          3.866582       -0.068381        1.548768
H          4.537585       -1.056576       -1.238021
H          5.811202        1.456249        1.155443
H          6.921462       -2.715139        1.064746
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H	7.570074	-0.309195	1.358794
H	4.780689	-3.243448	-0.148333
N	3.324794	1.150136	-0.017728
C	2.987177	2.162505	0.970005
H	2.557133	1.682621	1.854090
H	2.235541	2.841827	0.551294
H	3.850265	2.776484	1.282026
C	3.804152	1.769857	-1.245699
H	4.659387	2.446775	-1.080416
H	2.990822	2.343099	-1.702186
H	4.103572	1.004492	-1.967363
C	-0.255148	1.268026	-2.562872
N	0.517396	0.025841	-2.918119
O	-0.131358	-0.967563	-3.199265
O	1.728276	0.060398	-2.828179
C	0.163957	1.815025	-1.255393
C	-0.789727	2.599713	-0.421079
C	-2.505446	4.016075	1.254463
C	-1.966473	2.008102	0.036069
C	-0.482684	3.912085	-0.059113
C	-1.343151	4.619061	0.775627
C	-2.819395	2.710915	0.882217
H	-2.214425	0.997289	-0.276523
H	0.424255	4.376025	-0.437749
H	-1.104746	5.639944	1.056309
H	-3.723676	2.236639	1.251460
H	-3.169035	4.566179	1.913976
C	-1.615685	1.332804	-3.187903
H	-2.244718	0.509606	-2.844528
H	-1.532107	1.287525	-4.276606
H	-2.071366	2.281197	-2.901220
H	0.990878	1.298985	-0.752908
O	0.558982	2.383680	-2.515494

RS epoxide:Catalyst, binary complex 56; Energy = -2449.860508; 6-31G(d) basis set.

N	-1.759692	-1.519765	-0.827775
C	-1.191177	-2.665144	-1.202128
S	-2.032153	-4.041281	-1.698185
C	-3.172386	-1.332796	-0.532963
C	-3.316502	-0.510806	0.756320
C	-4.809988	-0.391668	1.100881
C	-5.569463	0.285516	-0.045022
C	-5.390296	-0.480671	-1.356932
C	-3.907914	-0.654006	-1.691801
N	-2.436758	-1.011956	1.818303
C	-2.662970	-2.397295	2.204913
N	0.186236	-2.688347	-1.203563
C	1.100952	-1.923717	-0.462093
C	2.432490	-1.932190	-0.898700
C	3.408437	-1.256641	-0.183220
C	3.094309	-0.538636	0.965361
C	1.771680	-0.530028	1.382144
C	0.768389	-1.217796	0.701501
C	4.828137	-1.314544	-0.672310
F	5.582216	-0.342009	-0.143177
C	1.386755	0.215721	2.628157
F	2.381608	0.980987	3.092169
C	-2.442403	-0.143540	2.986279
F	5.410868	-2.481889	-0.363605
F	4.892487	-1.192487	-2.009442
F	0.331869	1.025182	2.413331
F	1.024709	-0.619363	3.614206
H	-1.178031	-0.697864	-0.695356
H	0.562957	-3.506138	-1.666372
H	-3.446049	0.327340	-1.873490
H	-3.773194	-1.257367	-2.595776
H	-5.852418	-1.472931	-1.264520
H	-5.902985	0.033376	-2.176526
H	-6.632371	0.370905	0.204537
H	-5.185133	1.307739	-0.165373
H	-5.233048	-1.388899	1.285877
H	-4.932542	0.188952	2.021554
H	-3.598043	-2.332012	-0.394925
H	-2.951031	0.501012	0.534814
H	-3.365534	-0.226194	3.584056

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H         -1.596305       -0.399876        3.630667
H         -2.330165        0.897327        2.666714
H         -3.654280       -2.568773        2.657604
H         -1.905087       -2.678332        2.943665
H         -2.551223       -3.064667        1.344484
H          2.695653       -2.466444       -1.807365
H          3.854609        0.015338        1.502180
H         -0.251154       -1.203073        1.094200
N         -2.450851        3.300120       -0.659566
O         -2.884771        2.801788        0.360921
O         -2.950332        4.230670       -1.256247
C         -1.160642        2.738221       -1.223887
C         -0.193719        2.323429       -0.177238
H         -0.522905        2.478720        0.847286
O         -1.011986        1.394033       -0.894151
C          1.274319        2.273259       -0.405359
C          4.036682        2.264258       -0.797356
C          2.112807        2.931831        0.496471
C          1.826265        1.574619       -1.481356
C          3.203278        1.581054       -1.681247
C          3.490321        2.930271        0.297741
H          1.685360        3.439513        1.357372
H          1.178535        1.008179       -2.145066
H          3.629636        1.029709       -2.513646
H          4.136375        3.445496        1.001557
H          5.110878        2.257407       -0.950496
C         -0.867817        3.221031       -2.609480
H         -0.840091        4.310510       -2.630043
H         -1.643285        2.875074       -3.297381
H          0.098402        2.831959       -2.928649

RS epoxide:Catalyst, binary complex 57; Energy = -2449.857114; 6-31G(d) basis set.
N          2.227781       -0.975257       -0.543683
C          1.726530       -1.674086       -1.574884
S          2.624053       -2.509034       -2.723918
C          3.645964       -0.956451       -0.198869
C          3.846676        0.125204        0.874474
C          5.328334        0.194293        1.272936
C          5.817314       -1.153011        1.808322
C          5.580251       -2.255303        0.775773
C          4.110520       -2.308665        0.357480
N          3.237620        1.399667        0.477070
C          4.025735        2.154662       -0.487084
N          0.349190       -1.668623       -1.703581
C         -0.673814       -1.544162       -0.756710
C         -1.986531       -1.663959       -1.237088
C         -3.070870       -1.533568       -0.381005
C         -2.896427       -1.267360        0.971192
C         -1.593703       -1.146726        1.437228
C         -0.487711       -1.298936        0.609140
C         -4.452062       -1.680159       -0.956068
F         -5.397889       -1.243885       -0.115914
C         -1.334872       -0.814865        2.880484
F         -2.425775       -0.332573        3.489553
C          2.889356        2.210737        1.632826
F         -4.583136       -0.992872       -2.104199
F         -4.731226       -2.960324       -1.244184
F         -0.926423       -1.884548        3.577180
F         -0.366293        0.113481        2.999296
H          1.736059       -0.108029       -0.300864
H          0.062811       -2.089510       -2.579651
H          3.483846       -2.550715        1.227394
H          3.950607       -3.087636       -0.390815
H          6.201289       -2.063919       -0.109914
H          5.887873       -3.227895        1.173412
H          6.878699       -1.091309        2.071031
H          5.273118       -1.396951        2.731007
H          5.928246        0.467037        0.394806
H          5.474348        0.983503        2.019633
H          4.232839       -0.717183       -1.098322
H          3.276789       -0.210956        1.754853
H          2.186836        1.661236        2.267289
H          3.760358        2.508879        2.241421
H          2.394263        3.127037        1.298483
H          4.981179        2.520502       -0.077587
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H	3.453383	3.028369	-0.815340
H	4.230158	1.542115	-1.370314
H	-2.157132	-1.841435	-2.296183
H	-3.744411	-1.112169	1.626895
H	0.504212	-1.196040	1.027781
N	1.247331	2.411975	-2.043509
O	1.614782	3.434636	-2.589466
O	1.567759	1.284892	-2.357095
C	0.281724	2.570385	-0.894446
C	-0.829709	1.589991	-0.931357
H	-0.809310	0.902722	-1.777188
O	0.298771	1.454225	-0.067487
C	-2.152917	1.805959	-0.290838
C	-4.667441	2.010947	0.893989
C	-3.305106	1.670914	-1.066281
C	-2.261107	2.042024	1.081046
C	-3.517821	2.144454	1.670298
C	-4.560160	1.773994	-0.475121
H	-3.219619	1.449165	-2.127178
H	-1.361708	2.084043	1.688893
H	-3.597738	2.306535	2.740556
H	-5.452528	1.645533	-1.079559
H	-5.646876	2.079370	1.357062
C	0.220825	3.962361	-0.346395
H	1.218116	4.324871	-0.088860
H	-0.409216	3.961947	0.543529
H	-0.206463	4.635526	-1.091131

RS epoxide:Catalyst, binary complex 58; Energy = -2449.854922; 6-31G(d) basis set.

N	2.976178	-0.568398	1.549413
C	1.639263	-0.544709	1.780925
S	0.959646	-1.655845	2.861387
C	3.647840	-0.069401	0.338373
C	3.872512	1.470886	0.388389
C	5.251033	1.853210	-0.160496
C	6.366820	1.235576	0.697070
C	6.036238	-0.214470	1.119753
C	4.976980	-0.822927	0.199020
N	2.735365	2.164009	-0.253880
C	2.779875	2.158072	-1.713272
N	0.979462	0.416702	1.092551
C	-0.381526	0.712437	0.961408
C	-0.685788	1.583376	-0.097302
C	-1.990397	1.963390	-0.349329
C	-3.042584	1.469638	0.418512
C	-2.733984	0.605988	1.458214
C	-1.423334	0.234523	1.758959
C	-2.274488	2.837780	-1.534788
F	-3.341092	3.621322	-1.333939
C	-3.835426	0.064673	2.327057
F	-3.611800	-1.211460	2.676800
C	2.530930	3.516375	0.254276
F	-1.231957	3.632752	-1.827504
F	-2.527654	2.115149	-2.643155
F	-3.953741	0.763388	3.467338
F	-5.027315	0.110629	1.713392
H	3.421537	-1.355186	2.006666
H	1.564978	1.036437	0.493761
H	4.809473	-1.884396	0.408608
H	5.309768	-0.766616	-0.843111
H	6.940412	-0.829329	1.118207
H	5.657318	-0.226173	2.149250
H	7.302551	1.260317	0.129869
H	6.525205	1.851874	1.588460
H	5.342194	1.503934	-1.195748
H	5.355818	2.943542	-0.187878
H	3.001627	-0.315117	-0.514520
H	3.840355	1.758747	1.447343
H	2.408915	3.483444	1.340528
H	3.362162	4.195765	0.009310
H	1.615298	3.928141	-0.182677
H	3.578611	2.799879	-2.114626
H	1.825309	2.527086	-2.102595
H	2.926128	1.140627	-2.086319
H	0.117737	1.944368	-0.731508

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H         -4.069791        1.738799        0.200259
H         -1.220260       -0.440172        2.579617
N          1.765776       -3.147002       -1.360964
O          2.078368       -4.187306       -1.904483
O          2.348308       -2.634898       -0.425771
C          0.526380       -2.451576       -1.876764
C         -0.333592       -1.903988       -0.800450
H          0.019270       -2.065439        0.220662
O          0.546263       -1.092516       -1.585327
C         -1.799623       -1.719768       -0.973804
C         -4.558191       -1.391056       -1.216753
C         -2.319474       -0.888973       -1.965695
C         -2.663807       -2.370697       -0.089767
C         -4.039068       -2.209154       -0.214207
C         -3.697735       -0.727958       -2.087542
H         -1.641876       -0.337031       -2.610776
H         -2.254700       -2.980056        0.712725
H         -4.704463       -2.701469        0.487892
H         -4.094012       -0.063699       -2.848990
H         -5.631933       -1.256083       -1.304238
C          0.092729       -2.935839       -3.225231
H          0.872540       -2.741998       -3.965759
H         -0.816750       -2.407363       -3.511014
H         -0.106208       -4.007199       -3.196504

RS epoxide:Catalyst, binary complex 59; Energy = -2449.856123; 6-31G(d) basis set.
N         -3.177109        0.215713        2.219536
C         -1.910185       -0.252556        2.364093
S         -1.233116       -0.415962        3.897049
C         -3.750289        0.815930        1.009592
C         -4.517641       -0.177606        0.105599
C         -5.013871        0.587829       -1.127438
C         -5.924472        1.749720       -0.722477
C         -5.202258        2.718091        0.212644
C         -4.648891        1.981029        1.431135
N         -3.658066       -1.346242       -0.205760
C         -3.925510       -2.459108        0.708260
N         -1.338114       -0.594032        1.176096
C         -0.054555       -1.044614        0.873008
C          0.081195       -1.692424       -0.366098
C          1.320474       -2.136356       -0.794176
C          2.453756       -1.979734       -0.000103
C          2.312650       -1.320884        1.214499
C          1.084399       -0.837233        1.658142
C          1.475814       -2.746978       -2.158260
F          2.117209       -1.906572       -2.990836
C          3.517547       -1.130567        2.095644
F          4.657036       -1.126735        1.377039
C         -3.688887       -1.835724       -1.582799
F          2.207288       -3.869983       -2.111983
F          0.300569       -3.047285       -2.719232
F          3.466395        0.028540        2.763533
F          3.633097       -2.107954        3.003081
H         -3.616835        0.453391        3.100585
H         -2.038508       -0.774507        0.424746
H         -5.480544        1.586811        2.033155
H         -4.076203        2.660735        2.071069
H         -4.372065        3.193167       -0.327238
H         -5.874374        3.519734        0.534283
H         -6.273571        2.273051       -1.618209
H         -6.815470        1.352854       -0.217534
H         -4.149545        0.975689       -1.682967
H         -5.554453       -0.088138       -1.795788
H         -2.916395        1.209921        0.412271
H         -5.406366       -0.527878        0.659776
H         -3.378551       -1.055638       -2.277212
H         -2.971853       -2.659015       -1.664067
H         -4.676781       -2.224514       -1.876069
H         -3.900327       -2.112659        1.742649
H         -3.155407       -3.226164        0.580260
H         -4.909930       -2.914842        0.513281
H         -0.790605       -1.822007       -1.002061
H          3.420996       -2.342242       -0.332526
H          1.010818       -0.312718        2.600993
N         -0.525216        0.669869       -2.116471
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O         -0.135368       -0.044359       -3.012589
O         -1.599849        0.557933       -1.547939
C          0.385194        1.782058       -1.644529
C          1.831255        1.518599       -1.850984
H          2.080747        0.543160       -2.268224
O          1.055916        2.339285       -2.725175
C          2.876365        2.197560       -1.036521
C          4.832331        3.416760        0.535262
C          3.767837        1.421198       -0.296412
C          2.986445        3.589462       -1.012581
C          3.963615        4.194762       -0.227972
C          4.736060        2.027586        0.497292
H          3.708695        0.339402       -0.350275
H          2.317168        4.188512       -1.622853
H          4.048906        5.276744       -0.215519
H          5.411293        1.411523        1.081912
H          5.589023        3.892586        1.150886
C         -0.232987        2.635338       -0.581649
H         -1.138100        3.118572       -0.957190
H          0.486340        3.395540       -0.277425
H         -0.490987        2.021388        0.284893

RS epoxide:Catalyst, binary complex 60; Energy = -2449.850301; 6-31G(d) basis set.
N          3.401439        0.655739       -0.770819
C          2.199743        1.215744       -0.986559
S          1.773168        1.774866       -2.518463
C          3.907753        0.051551        0.454443
C          5.205813       -0.699490        0.102277
C          5.701080       -1.452804        1.345661
C          5.975242       -0.473281        2.491627
C          4.736518        0.366682        2.809276
C          4.209727        1.075378        1.559215
N          5.044410       -1.477916       -1.123626
C          4.099135       -2.580823       -1.019191
N          1.388468        1.262982        0.123746
C          0.081914        1.766108        0.233981
C         -0.788815        1.118615        1.117716
C         -2.088244        1.584878        1.277259
C         -2.543967        2.697016        0.579794
C         -1.659330        3.348296       -0.271363
C         -0.352786        2.908523       -0.445758
C         -3.050289        0.869628        2.183049
F         -3.769559        1.739196        2.909895
C         -2.139442        4.543138       -1.048607
F         -3.060215        5.236872       -0.361759
C          6.312101       -1.923066       -1.677695
F         -3.938370        0.146188        1.474670
F         -2.437741        0.041266        3.032021
F         -1.138777        5.381000       -1.346092
F         -2.709865        4.179077       -2.206536
H          3.904798        0.385668       -1.612417
H          1.647398        0.635945        0.878354
H          4.958662        1.779762        1.175599
H          3.321336        1.667253        1.801498
H          3.950379       -0.286668        3.212397
H          4.962852        1.104071        3.585981
H          6.304916       -1.017234        3.382827
H          6.798743        0.193613        2.202658
H          4.943744       -2.183193        1.660638
H          6.609372       -2.014490        1.100936
H          3.177869       -0.683649        0.832656
H          5.953006        0.072829       -0.139542
H          6.997737       -1.074283       -1.758842
H          6.800771       -2.709771       -1.077911
H          6.142268       -2.324829       -2.681050
H          4.443598       -3.382474       -0.344103
H          3.958605       -3.014018       -2.013828
H          3.126047       -2.218602       -0.676701
H         -0.461864        0.240795        1.668654
H         -3.556324        3.062549        0.715098
H          0.323110        3.444939       -1.097053
N          0.288504       -1.556574       -0.394698
O          0.825625       -1.360063       -1.461913
O          0.866366       -1.693428        0.673328
C         -1.213653       -1.680028       -0.410157
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C	-1.692640	-2.936606	0.216843
H	-0.920970	-3.594827	0.616585
O	-1.746314	-1.668762	0.868096
C	-2.975624	-3.569918	-0.189829
C	-5.353116	-4.784975	-0.983494
C	-4.196121	-2.946970	0.072041
C	-2.945801	-4.805812	-0.838462
C	-4.133337	-5.409266	-1.238726
C	-5.382152	-3.557663	-0.325422
H	-4.206982	-1.997093	0.597061
H	-1.993206	-5.293700	-1.029495
H	-4.106596	-6.367868	-1.747152
H	-6.331617	-3.074461	-0.117465
H	-6.279748	-5.257838	-1.293521
C	-1.862679	-0.924439	-1.530719
H	-1.492797	0.104602	-1.562046
H	-2.939790	-0.920553	-1.357720
H	-1.646601	-1.400841	-2.487988

RS epoxide:Catalyst, binary complex 61; Energy = -2449.847183; 6-31G(d) basis set.

N	0.243899	-1.847722	-0.877134
C	0.130095	-1.062802	-1.954167
S	1.294712	-0.933939	-3.169699
C	1.423542	-2.639903	-0.529811
C	2.486265	-1.735992	0.140749
C	1.965663	-1.286300	1.512834
C	1.621048	-2.461230	2.428711
C	0.549254	-3.330510	1.768753
C	1.010598	-3.796506	0.383636
N	3.763473	-2.462301	0.224498
C	4.728290	-1.795394	1.092711
N	-1.037427	-0.347371	-2.074910
C	-2.097283	-0.239935	-1.155711
C	-1.854824	-0.090739	0.214935
C	-2.921168	-0.010302	1.098077
C	-4.237334	-0.021455	0.646015
C	-4.465216	-0.118074	-0.721119
C	-3.412732	-0.246178	-1.622250
C	-2.659229	0.107978	2.575774
F	-1.396194	-0.215948	2.886661
C	-5.870001	-0.067695	-1.256384
F	-6.771523	-0.383386	-0.319501
C	4.369035	-2.595092	-1.098806
F	-2.886900	1.344847	3.027723
F	-3.467144	-0.713880	3.266400
F	-6.175343	1.157785	-1.707384
F	-6.034430	-0.913124	-2.284340
H	-0.568351	-1.961739	-0.282750
H	-1.166262	0.059809	-2.992500
H	0.236689	-4.393981	-0.111875
H	1.893914	-4.432761	0.501988
H	0.313774	-4.201625	2.388684
H	-0.383271	-2.747426	1.699614
H	2.516147	-3.068435	2.614755
H	1.265817	-2.090914	3.396234
H	2.681025	-0.604299	1.984339
H	1.056252	-0.693735	1.347369
H	1.808088	-3.038563	-1.469636
H	2.603503	-0.840508	-0.492669
H	4.597382	-1.612074	-1.547527
H	5.300856	-3.161204	-1.010538
H	3.716763	-3.134365	-1.787292
H	4.902754	-0.741114	0.805553
H	5.682008	-2.326460	1.025272
H	4.407460	-1.827006	2.136337
H	-0.838443	0.003405	0.579577
H	-5.065752	0.037399	1.343588
H	-3.612173	-0.366915	-2.682918
N	-0.221939	3.006112	0.701547
O	-0.545643	2.247445	1.594839
O	-0.721882	4.089400	0.478951
C	0.924425	2.583119	-0.193030
C	2.004315	1.883295	0.546626
H	1.835244	1.773049	1.617571
O	1.032515	1.199795	-0.245702

C	3.421022	1.847461	0.097870
C	6.104732	1.750309	-0.653489
C	3.773623	1.383537	-1.171677
C	4.414428	2.249242	0.993077
C	5.753461	2.204507	0.616297
C	5.114403	1.338705	-1.543324
H	3.001875	1.019942	-1.847646
H	4.138799	2.589806	1.988129
H	6.521681	2.517847	1.316175
H	5.384327	0.968448	-2.527622
H	7.149475	1.709840	-0.945512
C	1.042957	3.399612	-1.440702
H	0.142570	3.280936	-2.048728
H	1.905825	3.052462	-2.009041
H	1.168259	4.454491	-1.196066

RS epoxide:Catalyst, binary complex 62; Energy = -2449.851995; 6-31G(d) basis set.

N	2.083999	-1.156644	0.097452
C	1.717489	-2.110681	-0.768371
S	2.745110	-3.252633	-1.449994
C	3.417101	-1.054436	0.687978
C	4.293365	-0.058241	-0.108335
C	3.732893	1.355860	0.102439
C	3.693171	1.758338	1.578233
C	2.824361	0.773603	2.365635
C	3.320768	-0.660338	2.165658
N	5.690770	-0.172087	0.328853
C	6.525837	0.894244	-0.209952
N	0.381018	-2.124605	-1.125020
C	-0.760411	-1.733449	-0.415084
C	-0.766748	-1.323179	0.923844
C	-1.964622	-0.951915	1.525329
C	-3.179342	-1.005981	0.856023
C	-3.166497	-1.436461	-0.465127
C	-1.983225	-1.786431	-1.100464
C	-1.905905	-0.479227	2.951417
F	-1.642516	-1.484421	3.797792
C	-4.447045	-1.540382	-1.245957
F	-4.325551	-0.986842	-2.465412
C	6.263321	-1.458601	-0.059276
F	-0.928939	0.431442	3.120658
F	-3.053878	0.086781	3.342796
F	-4.797747	-2.820214	-1.439367
F	-5.468550	-0.935589	-0.628744
H	1.469690	-0.348262	0.168500
H	0.208609	-2.738115	-1.912274
H	2.677800	-1.377522	2.688755
H	4.328567	-0.750651	2.585771
H	2.828214	1.020673	3.432396
H	1.778230	0.865606	2.034267
H	4.708977	1.757555	1.993060
H	3.300709	2.776727	1.679473
H	4.272311	2.086088	-0.507985
H	2.706832	1.347798	-0.276697
H	3.831521	-2.058217	0.609198
H	4.201804	-0.316106	-1.182083
H	5.762428	-2.287497	0.443860
H	6.200633	-1.633321	-1.148110
H	7.315393	-1.483459	0.236888
H	6.465634	0.968059	-1.311301
H	7.566433	0.696563	0.060163
H	6.253403	1.861477	0.218441
H	0.147283	-1.294163	1.504599
H	-4.098016	-0.691439	1.335471
H	-2.000700	-2.094740	-2.142908
N	1.420863	1.875818	-2.308447
O	1.920753	2.770207	-2.958742
O	1.613576	0.686202	-2.462018
C	0.448883	2.286097	-1.222313
C	-0.753659	1.419916	-1.169636
H	-0.782119	0.626945	-1.916887
O	0.338284	1.289529	-0.255545
C	-2.061109	1.836447	-0.601640
C	-4.566501	2.423450	0.465019
C	-3.202356	1.723460	-1.396508

C	-2.173928	2.241683	0.729168
C	-3.427001	2.535079	1.259636
C	-4.453274	2.017628	-0.863762
H	-3.114435	1.375405	-2.422244
H	-1.289099	2.271585	1.357978
H	-3.513521	2.830568	2.300395
H	-5.340084	1.911302	-1.480506
H	-5.544038	2.641230	0.883818
C	0.560208	3.720039	-0.815142
H	1.553246	3.915117	-0.400962
H	-0.196694	3.927726	-0.057768
H	0.401766	4.370774	-1.675214

RS epoxide:Catalyst, binary complex 63; Energy = -2449.846403; 6-31G(d) basis set.

N	-1.978113	0.537260	0.000606
C	-1.543748	0.275642	-1.251598
S	-2.456925	-0.599439	-2.358436
C	-1.763578	1.805864	0.706206
C	-2.669410	2.897065	0.100725
C	-2.548278	4.198262	0.908656
C	-2.867640	3.967062	2.386566
C	-1.936917	2.906167	2.976044
C	-2.036950	1.594564	2.195992
N	-2.418889	3.012276	-1.331875
C	-1.241395	3.782102	-1.691710
N	-0.273849	0.692916	-1.589622
C	0.897385	0.701794	-0.818170
C	0.947444	0.287584	0.517562
C	2.163366	0.244186	1.181648
C	3.354075	0.592319	0.554160
C	3.293847	0.995357	-0.774107
C	2.086625	1.067025	-1.456907
C	2.190635	-0.155569	2.631133
F	2.367799	0.911653	3.425512
C	4.574742	1.260612	-1.512426
F	5.110208	0.115983	-1.969357
C	-3.580416	3.443086	-2.089537
F	1.047541	-0.745173	3.013630
F	3.194560	-1.004026	2.894280
F	4.389197	2.059029	-2.572071
F	5.493353	1.834242	-0.724414
H	-2.887857	0.114624	0.181276
H	-0.115792	0.626295	-2.588108
H	-3.047147	1.175550	2.311116
H	-1.337545	0.850801	2.596471
H	-0.901316	3.270965	2.938373
H	-2.171860	2.726170	4.029652
H	-2.776485	4.905532	2.943011
H	-3.909531	3.634616	2.489463
H	-1.524736	4.587566	0.822622
H	-3.214737	4.954467	0.477091
H	-0.718322	2.106520	0.577040
H	-3.701921	2.530772	0.204541
H	-3.886054	4.481657	-1.869697
H	-3.354387	3.378237	-3.158312
H	-4.423104	2.777534	-1.882696
H	-1.367428	4.869038	-1.549317
H	-1.014474	3.603805	-2.748129
H	-0.373441	3.457348	-1.108736
H	0.050372	-0.038247	1.026194
H	4.301113	0.539904	1.080758
H	2.070624	1.383852	-2.495759
N	-3.667059	-2.743475	-0.122167
O	-4.475742	-3.067822	-0.961527
O	-3.851360	-1.912199	0.750568
C	-2.321351	-3.440264	-0.152479
C	-1.245740	-2.702036	0.519778
H	-1.529444	-1.754676	0.976347
O	-1.916347	-3.812270	1.129234
C	0.189318	-2.840779	0.138357
C	2.910230	-2.769877	-0.466296
C	1.131548	-3.167097	1.116098
C	0.609331	-2.508563	-1.150301
C	1.970354	-2.466698	-1.447771
C	2.488853	-3.137107	0.812065

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H          0.797268       -3.425720        2.116978
H         -0.131300       -2.249091       -1.905300
H          2.297369       -2.185866       -2.444729
H          3.218910       -3.376181        1.578555
H          3.970234       -2.715942       -0.696505
C         -2.173157       -4.401749       -1.288559
H         -2.935076       -5.181149       -1.226093
H         -1.182316       -4.853721       -1.223875
H         -2.276812       -3.877245       -2.241048

RS epoxide:Catalyst, binary complex 64; Energy = -2449.840519; 6-31G(d) basis set.
N         -1.824209        0.708240       -0.192424
C         -1.354996        0.331014       -1.399647
S         -2.321805       -0.439608       -2.538308
C         -1.446044        1.950906        0.498378
C         -1.907208        3.177192       -0.329269
C         -3.441419        3.211193       -0.341830
C         -4.026903        3.272685        1.070949
C         -3.574185        2.064258        1.894878
C         -2.045920        1.955158        1.905543
N         -1.305037        4.390485        0.236109
C         -1.901155        5.611769       -0.292260
N         -0.037147        0.615439       -1.686750
C          1.092980        0.523717       -0.851206
C          1.038066        0.039562        0.461675
C          2.206513       -0.103924        1.191385
C          3.448659        0.226593        0.655659
C          3.489820        0.716190       -0.641631
C          2.330069        0.869182       -1.395378
C          2.141620       -0.586241        2.614372
F          0.914873       -1.008108        2.951550
C          4.796750        1.149429       -1.245373
F          4.881948        0.797942       -2.536876
C          0.133503        4.426714       -0.007103
F          2.995808       -1.596500        2.833841
F          2.475638        0.392400        3.469400
F          4.938369        2.482692       -1.196125
F          5.843791        0.614034       -0.606783
H         -2.776641        0.387315       -0.032145
H          0.166543        0.494433       -2.672170
H         -1.716626        1.057679        2.443777
H         -1.628063        2.825490        2.422003
H         -3.937629        2.142605        2.924444
H         -4.026376        1.149573        1.485537
H         -3.692772        4.192259        1.568296
H         -5.119937        3.307945        1.020409
H         -3.800318        4.037589       -0.960817
H         -3.789052        2.297792       -0.842719
H         -0.361708        1.960217        0.588808
H         -1.555340        3.035561       -1.371920
H          0.377334        4.363244       -1.083997
H          0.539369        5.364263        0.380892
H          0.652154        3.614585        0.507771
H         -1.865968        5.660631       -1.396058
H         -1.351775        6.469847        0.103396
H         -2.940343        5.709291        0.027476
H          0.091212       -0.243347        0.902960
H          4.357144        0.105406        1.235525
H          2.391424        1.244913       -2.413087
N         -3.921069       -2.284177       -0.240476
O         -4.772247       -2.504004       -1.070462
O         -3.973148       -1.406925        0.606808
C         -2.696850       -3.178158       -0.248499
C         -1.523482       -2.596737        0.414159
H         -1.664082       -1.609230        0.851669
O         -2.355511       -3.579380        1.042457
C         -0.125172       -2.958521        0.040777
C          2.567142       -3.344827       -0.567166
C          0.755358       -3.409024        1.026376
C          0.338643       -2.723299       -1.254592
C          1.686034       -2.911788       -1.554857
C          2.098785       -3.604795        0.720297
H          0.387140       -3.589476        2.032425
H         -0.353716       -2.371943       -2.017046
H          2.047298       -2.719725       -2.560828
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H          2.782658       -3.948531        1.489262
H          3.618119       -3.486632       -0.799912
C         -2.691286       -4.173614       -1.364707
H         -3.563082       -4.827053       -1.295105
H         -1.780761       -4.769141       -1.283920
H         -2.707619       -3.659216       -2.328273

RS epoxide:Catalyst, binary complex 65; Energy = -2449.850942; 6-31G(d) basis set.
N         -2.733711        0.883275        0.208598
C         -2.857376        2.198981       -0.011961
S         -4.314123        3.041622       -0.028596
C         -3.809114       -0.001856        0.645642
C         -4.511079       -0.649937       -0.571020
C         -3.497993       -1.554728       -1.285226
C         -2.948939       -2.642262       -0.356593
C         -2.290964       -2.031234        0.886055
C         -3.249617       -1.067537        1.594344
N         -5.699875       -1.386255       -0.118206
C         -6.280548       -2.200499       -1.178044
N         -1.679404        2.871068       -0.249548
C         -0.375778        2.471002        0.093199
C         -0.120155        1.698397        1.229144
C          1.178518        1.305794        1.521862
C          2.250099        1.709273        0.736626
C          1.986513        2.500600       -0.378170
C          0.691985        2.872784       -0.714509
C          1.414361        0.437354        2.726984
F          2.512436       -0.317902        2.580744
C          3.119421        2.822496       -1.308950
F          2.858028        3.879361       -2.084324
C         -6.721025       -0.477359        0.393238
F          1.584017        1.167275        3.839874
F          0.378975       -0.383697        2.950693
F          4.256671        3.065546       -0.647522
F          3.365528        1.781089       -2.133435
H         -1.839468        0.454583       -0.016795
H         -1.805178        3.808342       -0.609790
H         -2.753520       -0.581302        2.442379
H         -4.103840       -1.632019        1.982760
H         -1.979058       -2.816791        1.583235
H         -1.368179       -1.497441        0.611851
H         -3.770512       -3.294216       -0.034337
H         -2.235410       -3.269319       -0.904230
H         -3.934367       -1.993688       -2.186385
H         -2.677155       -0.921663       -1.642806
H         -4.505672        0.642581        1.182519
H         -4.807197        0.165615       -1.259085
H         -6.379660        0.040013        1.291910
H         -7.014906        0.285202       -0.349952
H         -7.608059       -1.054808        0.666909
H         -6.506735       -1.617482       -2.089821
H         -7.214666       -2.636942       -0.814644
H         -5.615661       -3.023523       -1.448936
H         -0.933580        1.392345        1.877228
H          3.262706        1.392100        0.966725
H          0.502665        3.456837       -1.609544
N         -0.050889       -1.418712       -1.677308
O         -0.543762       -2.088727       -2.558782
O         -0.333822       -0.257426       -1.431639
C          1.030171       -2.063894       -0.838902
C          2.194252       -1.167293       -0.625842
H          2.120883       -0.192412       -1.106036
O          1.190656       -1.394735        0.363118
C          3.566702       -1.664117       -0.349083
C          6.163363       -2.557470        0.119772
C          4.599715       -1.294191       -1.212934
C          3.838708       -2.462927        0.763288
C          5.136408       -2.908829        0.993495
C          5.894727       -1.746370       -0.980935
H          4.389198       -0.645111       -2.058599
H          3.037236       -2.706014        1.454463
H          5.348450       -3.524931        1.861576
H          6.695350       -1.458779       -1.654881
H          7.174904       -2.906232        0.302695
C          1.019289       -3.558689       -0.888169
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H          1.090715       -3.907264       -1.918300
H          0.096192       -3.941399       -0.443564
H          1.872323       -3.930761       -0.319468

RS epoxide:Catalyst, binary complex 66; Energy = -2449.844821; 6-31G(d) basis set.
N          2.054284       -1.828332        0.326660
C          1.728116       -3.109015        0.094710
S          2.838891       -4.348864       -0.149269
C          3.411227       -1.311324        0.486692
C          3.955324       -0.796109       -0.866561
C          3.066708        0.368798       -1.327813
C          3.045626        1.512142       -0.307764
C          2.608178        1.027007        1.079501
C          3.417161       -0.194014        1.533690
N          5.356974       -0.388586       -0.717697
C          5.883924        0.190323       -1.947053
N          0.383103       -3.394529        0.046825
C         -0.707713       -2.557415        0.340490
C         -1.868160       -2.652668       -0.433751
C         -2.967242       -1.849734       -0.143802
C         -2.928906       -0.914690        0.885112
C         -1.774014       -0.836204        1.654730
C         -0.683390       -1.664411        1.418330
C         -4.207609       -2.012948       -0.984400
F         -5.244698       -1.340263       -0.481321
C         -1.680662        0.117274        2.813990
F         -0.589156        0.901229        2.704573
C          6.196644       -1.508840       -0.303811
F         -4.009390       -1.587958       -2.238418
F         -4.557174       -3.306823       -1.064719
F         -2.745514        0.910458        2.915430
F         -1.551033       -0.546074        3.972918
H          1.312146       -1.139019        0.305099
H          0.180615       -4.323230       -0.301317
H          3.036508       -0.581179        2.485420
H          4.460157        0.103092        1.685165
H          2.715514        1.832573        1.813465
H          1.532846        0.785203        1.078210
H          4.054569        1.935582       -0.230140
H          2.383624        2.317605       -0.650964
H          3.378253        0.730057       -2.311422
H          2.054975       -0.029166       -1.476798
H          3.999501       -2.161246        0.832256
H          3.873632       -1.625522       -1.596920
H          5.982866       -1.800032        0.727384
H          6.067226       -2.396574       -0.948219
H          7.244702       -1.201955       -0.342022
H          6.953401        0.376835       -1.821448
H          5.407467        1.149802       -2.160474
H          5.749504       -0.471498       -2.822295
H         -1.911457       -3.356819       -1.260140
H         -3.772624       -0.263384        1.080670
H          0.176824       -1.626792        2.080447
N         -2.900031        1.079813       -1.825376
O         -4.022266        1.182450       -1.374676
O         -2.605252        0.645977       -2.921227
C         -1.752312        1.568523       -0.984770
C         -1.871221        2.978171       -0.551274
H         -2.774065        3.506354       -0.858165
O         -2.127636        1.870511        0.313803
C         -0.649123        3.787645       -0.281476
C          1.652295        5.285294        0.194925
C         -0.215014        4.719674       -1.226479
C          0.065670        3.608258        0.902435
C          1.211718        4.363071        1.140912
C          0.938132        5.461631       -0.989430
H         -0.775828        4.860586       -2.146997
H         -0.285188        2.882850        1.628480
H          1.759204        4.230308        2.069156
H          1.278292        6.180244       -1.728363
H          2.548396        5.868986        0.380813
C         -0.466958        0.853580       -1.260908
H         -0.599628       -0.227006       -1.142861
H          0.276587        1.220414       -0.551271
H         -0.127052        1.055472       -2.278035
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RS epoxide:Catalyst, binary complex 67; Energy = -2449.848539; 6-31G(d) basis set.

N	3.375133	-1.183964	1.015116
C	2.106120	-1.468880	1.367081
S	1.724814	-1.951547	2.934845
C	3.800984	-0.459580	-0.178756
C	5.144473	0.226944	0.130446
C	5.520089	1.131966	-1.052203
C	5.643878	0.308771	-2.338117
C	4.354450	-0.463423	-2.623990
C	3.957641	-1.335451	-1.429592
N	5.118508	0.846761	1.454649
C	4.167649	1.940510	1.592762
N	1.191596	-1.330313	0.354103
C	-0.190896	-1.610446	0.368653
C	-1.031458	-1.203273	1.407372
C	-2.403928	-1.368924	1.273971
C	-2.962958	-1.947528	0.138780
C	-2.112396	-2.364394	-0.876027
C	-0.737079	-2.200490	-0.770217
C	-3.313190	-0.894107	2.372294
F	-3.673202	-1.880335	3.201708
C	-2.694766	-2.915318	-2.145935
F	-2.981783	-1.935808	-3.017543
C	6.439118	1.239679	1.917359
F	-2.738358	0.064087	3.113843
F	-4.450427	-0.376128	1.867336
F	-1.847726	-3.751500	-2.761593
F	-3.835114	-3.582440	-1.918629
H	4.004104	-1.081008	1.807807
H	1.565860	-1.213675	-0.581048
H	4.721555	-2.098161	-1.231359
H	3.032875	-1.880744	-1.656399
H	3.539833	0.245301	-2.823270
H	4.469289	-1.084661	-3.518048
H	5.889304	0.962179	-3.181624
H	6.475826	-0.401139	-2.232918
H	4.746961	1.900499	-1.183726
H	6.462883	1.648209	-0.839390
H	3.064850	0.325717	-0.401475
H	5.900417	-0.571675	0.197796
H	7.132160	0.399856	1.809449
H	6.854579	2.105464	1.374429
H	6.383079	1.504238	2.977541
H	4.422284	2.821144	0.979815
H	4.143057	2.251129	2.641289
H	3.161195	1.611435	1.317139
H	-0.616615	-0.744138	2.294929
H	-4.037574	-2.062779	0.043499
H	-0.087971	-2.513969	-1.582775
N	0.902926	1.438844	-1.227239
O	1.783976	2.207885	-0.892463
O	1.018549	0.553378	-2.053456
C	-0.429846	1.613911	-0.545162
C	-1.525324	2.038479	-1.449849
H	-1.266283	2.179884	-2.499667
O	-1.360646	0.697517	-0.993477
C	-2.700206	2.788290	-0.927843
C	-4.881383	4.205495	0.066829
C	-3.578568	2.178419	-0.031378
C	-2.920062	4.104264	-1.336083
C	-4.008230	4.811871	-0.834948
C	-4.667501	2.887484	0.464802
H	-3.411290	1.145850	0.259363
H	-2.241034	4.573043	-2.043857
H	-4.176797	5.836548	-1.150785
H	-5.346863	2.405317	1.160863
H	-5.731007	4.759204	0.454107
C	-0.280693	1.953729	0.909623
H	0.397255	1.245216	1.395965
H	-1.259842	1.896772	1.387764
H	0.122707	2.961269	1.020496

RS epoxide:Catalyst, binary complex 68; Energy = -2449.855506; 6-31G(d) basis set.

N	-1.876862	0.699240	1.050022

C	-1.157701	0.104797	2.015768
S	-1.801506	-1.005843	3.096873
C	-1.726129	2.095634	0.614014
C	-2.835586	2.387729	-0.407975
C	-2.782695	3.858221	-0.848966
C	-2.885022	4.807671	0.345538
C	-1.771117	4.515972	1.351156
C	-1.821223	3.057361	1.807094
N	-2.808219	1.407660	-1.493555
C	-1.798092	1.658772	-2.510491
N	0.171468	0.473114	2.113213
C	1.104933	0.615543	1.071070
C	2.408378	0.960791	1.436497
C	3.413970	0.993769	0.480806
C	3.146968	0.727674	-0.854761
C	1.842651	0.400390	-1.209816
C	0.820712	0.329614	-0.270895
C	4.834359	1.189017	0.925867
F	4.919552	1.979497	2.003563
C	1.549800	0.131088	-2.659713
F	1.299084	1.270356	-3.328423
C	-4.110783	1.186970	-2.100158
F	5.389706	0.009729	1.257426
F	5.593758	1.724232	-0.037454
F	2.586965	-0.458385	-3.269421
F	0.479968	-0.659364	-2.826837
H	-2.804339	0.297857	0.924425
H	0.579330	0.169009	2.990192
H	-2.768570	2.862639	2.327918
H	-1.013511	2.841891	2.513984
H	-0.798018	4.719659	0.883431
H	-1.850054	5.176856	2.220200
H	-2.834084	5.846980	0.005143
H	-3.859656	4.678191	0.834950
H	-1.835307	4.046466	-1.371341
H	-3.587496	4.047477	-1.568822
H	-0.751418	2.226099	0.126487
H	-3.788561	2.231234	0.121363
H	-4.497934	2.070938	-2.636038
H	-4.031744	0.367388	-2.821912
H	-4.831705	0.892493	-1.332373
H	-2.057789	2.494219	-3.181777
H	-1.672898	0.758604	-3.121445
H	-0.831919	1.883409	-2.048776
H	2.639374	1.171716	2.476779
H	3.937390	0.750881	-1.596717
H	-0.176867	0.018933	-0.568508
N	-3.512341	-2.501992	0.531624
O	-3.891750	-3.400983	1.244183
O	-4.053535	-1.412407	0.417555
C	-2.245178	-2.718967	-0.266545
C	-1.152098	-3.312345	0.544651
H	-1.405493	-3.516472	1.583703
O	-1.929715	-4.064143	-0.387514
C	0.290664	-3.084420	0.260884
C	3.003329	-2.591661	-0.187331
C	0.841720	-3.291747	-1.006477
C	1.112267	-2.664856	1.310335
C	2.463747	-2.416380	1.084825
C	2.192123	-3.038903	-1.229764
H	0.213897	-3.671990	-1.806867
H	0.679822	-2.526476	2.299074
H	3.098732	-2.079884	1.899565
H	2.612069	-3.190970	-2.219259
H	4.054588	-2.382066	-0.362371
C	-2.148161	-1.828299	-1.463701
H	-2.928609	-2.105999	-2.179872
H	-1.176088	-1.970082	-1.932870
H	-2.279694	-0.776590	-1.192322

RS epoxide:Catalyst, binary complex 69; Energy = -2449.848240; 6-31G(d) basis set.

N	-3.844556	0.285723	-0.102623
C	-2.981070	1.295996	0.112567
S	-3.510360	2.778820	0.721533
C	-3.525639	-1.087719	-0.471106

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C         -4.748750       -1.963407       -0.143197
C         -4.394382       -3.435021       -0.404016
C         -4.001294       -3.638638       -1.870006
C         -2.843541       -2.717457       -2.258495
C         -3.170231       -1.253272       -1.955497
N         -5.288394       -1.641551        1.177341
C         -4.409139       -1.979360        2.286866
N         -1.677831        1.012185       -0.177754
C         -0.568531        1.872817       -0.033407
C          0.555477        1.391428        0.636852
C          1.703023        2.168658        0.720598
C          1.738775        3.444283        0.168349
C          0.606439        3.920565       -0.482284
C         -0.542735        3.145813       -0.600181
C          2.936618        1.644325        1.398949
F          3.463926        2.558361        2.227148
C          0.600666        5.310380       -1.055431
F         -0.048979        5.355640       -2.227783
C         -6.621273       -2.181776        1.386856
F          2.692146        0.539735        2.122903
F          3.898184        1.333173        0.514470
F         -0.007774        6.180169       -0.237585
F          1.844338        5.766407       -1.264153
H         -4.753185        0.409202        0.334486
H         -1.437743        0.052767       -0.408534
H         -4.027916       -0.919122       -2.553424
H         -2.325491       -0.611428       -2.226172
H         -1.948605       -3.000871       -1.689048
H         -2.599598       -2.833324       -3.319613
H         -3.731841       -4.685163       -2.047354
H         -4.868630       -3.421165       -2.508210
H         -3.557061       -3.730009        0.243131
H         -5.246727       -4.073179       -0.145385
H         -2.673552       -1.448191        0.128143
H         -5.536905       -1.676060       -0.857122
H         -7.267202       -1.903809        0.548756
H         -6.638032       -3.280159        1.490753
H         -7.041720       -1.752867        2.301399
H         -4.278568       -3.066151        2.422535
H         -4.834457       -1.572280        3.208665
H         -3.423657       -1.525895        2.146747
H          0.520874        0.418625        1.114130
H          2.632705        4.054431        0.241307
H         -1.411779        3.519210       -1.129023
N          0.236440       -2.019991        0.108622
O         -0.118855       -1.404022       -0.883777
O         -0.501918       -2.625484        0.856549
C          1.714192       -2.029027        0.424064
C          2.574274       -2.217333       -0.772915
H          2.053250       -2.348025       -1.721075
O          2.346811       -0.949127       -0.168078
C          3.940996       -2.792811       -0.658426
C          6.484799       -3.905756       -0.457461
C          4.210263       -4.028355       -1.248835
C          4.947483       -2.106296        0.023093
C          6.218122       -2.666528        0.120703
C          5.480419       -4.585729       -1.144019
H          3.426197       -4.551770       -1.789999
H          4.730412       -1.132899        0.454630
H          7.003154       -2.131290        0.645262
H          5.686556       -5.548075       -1.601548
H          7.476749       -4.339257       -0.378207
C          2.021491       -2.436963        1.831292
H          1.526789       -1.770834        2.541641
H          3.100359       -2.373546        1.976439
H          1.688211       -3.459744        2.011030

RS epoxide:Catalyst, binary complex 70; Energy = -2449.846901; 6-31G(d) basis set.
N         -0.142600        0.718793        0.402069
C         -0.321877       -0.412278       -0.306576
S         -1.839193       -1.100492       -0.564939
C          0.818061        1.779640        0.079481
C          0.355347        2.551177       -1.172632
C          1.309880        3.722985       -1.447476
C          1.410524        4.653060       -0.236658
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C	1.877209	3.879917	0.997886
C	0.949375	2.701306	1.292891
N	0.155296	1.627066	-2.285305
C	1.369598	1.222538	-2.969934
N	0.793500	-1.055923	-0.787176
C	2.091108	-1.104871	-0.260349
C	3.116631	-1.576750	-1.087868
C	4.416637	-1.657795	-0.608276
C	4.737775	-1.255223	0.684315
C	3.710937	-0.791757	1.496150
C	2.395301	-0.730314	1.051180
C	5.485272	-2.216012	-1.506910
F	6.705318	-1.799394	-1.145270
C	3.988806	-0.316639	2.895217
F	3.277585	-1.006021	3.797927
C	-0.859060	2.065831	-3.226834
F	5.498720	-3.557013	-1.478878
F	5.292450	-1.854718	-2.783912
F	5.280796	-0.430404	3.221395
F	3.646838	0.975670	3.040681
H	-1.007919	1.074084	0.804815
H	0.568720	-1.769420	-1.469481
H	-0.051900	3.073323	1.556257
H	1.316562	2.124110	2.148734
H	2.894646	3.500968	0.828292
H	1.925819	4.538313	1.871032
H	2.096402	5.479659	-0.450077
H	0.426554	5.097807	-0.035056
H	2.310321	3.332856	-1.680552
H	0.967491	4.271157	-2.333480
H	1.795825	1.333014	-0.123989
H	-0.634547	2.960549	-0.931075
H	-0.575772	2.979472	-3.780503
H	-1.032168	1.272304	-3.960978
H	-1.796452	2.249063	-2.695739
H	1.790321	2.009132	-3.620388
H	1.151443	0.348686	-3.594105
H	2.140532	0.930636	-2.248516
H	2.894820	-1.860303	-2.113090
H	5.759012	-1.295001	1.043134
H	1.610497	-0.378803	1.713484
N	-3.396680	1.691571	0.431636
O	-2.864891	1.639182	1.526973
O	-2.943849	2.277359	-0.529640
C	-4.697530	0.953413	0.245402
C	-4.808904	-0.269058	1.069339
H	-3.942622	-0.500873	1.685541
O	-5.451150	0.959450	1.414381
C	-5.668826	-1.409656	0.651673
C	-7.234354	-3.572550	-0.149017
C	-5.065783	-2.627462	0.330427
C	-7.056488	-1.279974	0.584462
C	-7.836498	-2.361509	0.184420
C	-5.848858	-3.703883	-0.074280
H	-3.985040	-2.727205	0.396945
H	-7.516189	-0.334544	0.857549
H	-8.916223	-2.258757	0.137437
H	-5.376011	-4.647543	-0.327701
H	-7.843729	-4.415099	-0.460808
C	-5.330999	1.196153	-1.087341
H	-4.657112	0.867907	-1.880739
H	-5.552333	2.257237	-1.221396
H	-6.256435	0.621842	-1.138416

RS epoxide:Catalyst, binary complex 71; Energy = -2449.838172; 6-31G(d) basis set.

N	2.046282	-1.811677	0.339953
C	1.713785	-3.090686	0.107606
S	2.817263	-4.335310	-0.148869
C	3.410569	-1.284626	0.422025
C	3.869804	-0.835112	-0.993663
C	3.103350	0.430577	-1.414086
C	3.008076	1.549670	-0.361504
C	2.587222	1.040968	1.021060
C	3.437917	-0.156304	1.454892
N	5.313475	-0.737235	-1.195816

C	6.038424	-1.924352	-0.783379
N	0.367673	-3.374885	0.074333
C	-0.720048	-2.535093	0.369814
C	-1.888666	-2.639585	-0.391021
C	-2.983337	-1.830634	-0.101202
C	-2.933952	-0.882856	0.915543
C	-1.771735	-0.796730	1.673081
C	-0.684243	-1.628703	1.435949
C	-4.229479	-1.996482	-0.932525
F	-4.038146	-1.576685	-2.189658
C	-1.666298	0.169611	2.820587
F	-0.569219	0.943543	2.698037
C	6.017701	0.478499	-0.845194
F	-4.581682	-3.289860	-1.005391
F	-5.262197	-1.319392	-0.426332
F	-2.724627	0.972376	2.916694
F	-1.538019	-0.481022	3.986930
H	1.305855	-1.120806	0.299607
H	0.161554	-4.304566	-0.269131
H	3.100325	-0.542055	2.423526
H	4.478783	0.162626	1.582118
H	2.676853	1.846965	1.756861
H	1.519999	0.768983	1.033068
H	3.971332	2.058384	-0.253227
H	2.300932	2.312943	-0.712289
H	3.537494	0.814321	-2.343990
H	2.085146	0.110718	-1.671768
H	4.029557	-2.118589	0.758098
H	3.548369	-1.649732	-1.658481
H	5.578560	1.339496	-1.353369
H	6.066406	0.695651	0.236976
H	7.048933	0.384268	-1.201705
H	7.005596	-1.955260	-1.296744
H	5.468035	-2.817367	-1.056828
H	6.237307	-1.967828	0.302747
H	-1.941186	-3.354152	-1.207907
H	-3.774526	-0.227252	1.110159
H	0.182803	-1.584010	2.088471
N	-2.928556	1.090321	-1.819442
O	-4.040236	1.202649	-1.345793
O	-2.660074	0.659054	-2.922995
C	-1.758511	1.561218	-1.000408
C	-1.840506	2.974753	-0.574018
H	-2.736825	3.521399	-0.867259
O	-2.105503	1.878274	0.302450
C	-0.594962	3.757351	-0.329682
C	1.742945	5.211295	0.103421
C	0.089772	3.630466	0.878533
C	-0.110616	4.612305	-1.322188
C	1.060522	5.332360	-1.106465
C	1.253411	4.365208	1.095353
H	-0.295202	2.959010	1.638389
H	-0.646929	4.710313	-2.262662
H	1.438830	5.991101	-1.881692
H	1.777309	4.274991	2.042209
H	2.653095	5.778204	0.272529
C	-0.491148	0.822037	-1.295825
H	-0.643367	-0.256984	-1.189854
H	0.264257	1.166872	-0.587695
H	-0.156078	1.030288	-2.313481

RS epoxide:Catalyst, binary complex 72; Energy = -2449.842423; 6-31G(d) basis set.

N	-1.012505	1.106172	1.198985
C	-0.376106	0.612955	2.286131
S	-1.161925	0.280655	3.734945
C	-0.553230	2.188740	0.314318
C	-1.810933	2.859918	-0.272176
C	-1.404025	4.024589	-1.188340
C	-0.569110	5.059495	-0.434111
C	0.674790	4.399179	0.156061
C	0.298920	3.225433	1.060716
N	-2.712404	1.870332	-0.881908
C	-2.278702	1.427369	-2.203396
N	0.975742	0.392857	2.201292
C	1.792358	0.142451	1.088985

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C          3.175698        0.247520        1.264594
C          4.035109       -0.035960        0.211059
C          3.547516       -0.406655       -1.036013
C          2.170077       -0.507875       -1.199122
C          1.291041       -0.254387       -0.155081
C          5.517266        0.132324        0.400037
F          6.208075       -0.742780       -0.342365
C          1.642533       -0.909900       -2.548505
F          0.311881       -0.745592       -2.641259
C         -4.086316        2.359524       -0.944697
F          5.921774        1.359393        0.038481
F          5.877843       -0.040226        1.678736
F          2.203869       -0.178360       -3.521872
F          1.906004       -2.193523       -2.831042
H         -2.025741        1.030333        1.261180
H          1.394449        0.200816        3.103587
H         -0.279530        3.582791        1.923648
H          1.206033        2.758147        1.454473
H          1.315095        4.036894       -0.659950
H          1.266875        5.123160        0.724970
H         -0.289458        5.879767       -1.103158
H         -1.169094        5.495843        0.375695
H         -0.814692        3.638624       -2.030574
H         -2.302922        4.486144       -1.612044
H          0.041898        1.781010       -0.515885
H         -2.360640        3.280001        0.583822
H         -4.191268        3.263573       -1.567864
H         -4.726480        1.583546       -1.373288
H         -4.446603        2.581536        0.063639
H         -2.365459        2.212315       -2.971818
H         -2.902527        0.583263       -2.514522
H         -1.237985        1.089765       -2.173733
H          3.577791        0.547406        2.227881
H          4.224001       -0.611928       -1.859137
H          0.225077       -0.374771       -0.295894
N         -4.788748       -0.861884       -0.484373
O         -5.580829       -0.224451        0.175209
O         -4.740642       -0.901108       -1.700974
C         -3.803959       -1.709670        0.278314
C         -2.394826       -1.418214        0.005060
H         -2.204740       -0.621867       -0.715799
O         -3.078760       -0.946212        1.180885
C         -1.296812       -2.404612        0.209099
C          0.896067       -4.089209        0.548312
C         -0.802037       -2.652409        1.489595
C         -0.703340       -3.010560       -0.901431
C          0.388715       -3.854795       -0.729443
C          0.299001       -3.490651        1.654448
H         -1.265170       -2.167023        2.344002
H         -1.084706       -2.806079       -1.898359
H          0.851088       -4.320187       -1.593495
H          0.691521       -3.669390        2.650910
H          1.755934       -4.739164        0.678592
C         -4.407060       -3.011073        0.708597
H         -5.237677       -2.822182        1.393058
H         -3.640646       -3.596879        1.219389
H         -4.767193       -3.565478       -0.161548

RS epoxide:Catalyst, binary complex 73; Energy = -2449.851738; 6-31G(d) basis set.
N         -1.704280       -1.528095       -0.859352
C         -1.128922       -2.674286       -1.220978
S         -1.957743       -4.062443       -1.704003
C         -3.116392       -1.331576       -0.571765
C         -3.287550       -0.569590        0.750817
C         -4.781721       -0.594187        1.155005
C         -5.717272       -0.635414       -0.067577
C         -5.097870        0.137910       -1.232410
C         -3.809488       -0.558432       -1.711153
N         -2.348652       -1.023302        1.782058
C         -2.444678       -2.434872        2.126899
N          0.248935       -2.686481       -1.219300
C          1.154853       -1.909798       -0.478592
C          2.488166       -1.905552       -0.909839
C          3.453375       -1.216122       -0.192519
C          3.128412       -0.501793        0.955704
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C	1.803279	-0.502517	1.363821
C	0.810450	-1.199841	0.678535
C	4.872640	-1.246329	-0.684871
F	4.930520	-1.113768	-2.021494
C	1.400082	0.236553	2.607992
F	1.059693	-0.606651	3.595378
C	-2.431721	-0.194029	2.975723
F	5.609318	-0.262401	-0.152178
F	5.478467	-2.404280	-0.385783
F	2.376119	1.026594	3.070598
F	0.324302	1.017311	2.392654
H	-1.125381	-0.702322	-0.738634
H	0.633317	-3.506101	-1.672419
H	-3.102710	0.182228	-2.104833
H	-4.020208	-1.262758	-2.522815
H	-5.804508	0.231405	-2.062474
H	-4.870727	1.157410	-0.894462
H	-5.887989	-1.673722	-0.379144
H	-6.696663	-0.224861	0.196580
H	-4.979905	-1.457245	1.801749
H	-4.993515	0.302530	1.748334
H	-3.551979	-2.331149	-0.488557
H	-3.004807	0.470724	0.552358
H	-3.366313	-0.348634	3.541391
H	-1.590157	-0.423369	3.635957
H	-2.370832	0.860992	2.689728
H	-3.389637	-2.704072	2.628051
H	-1.624550	-2.679538	2.810708
H	-2.336560	-3.060671	1.235225
H	2.760679	-2.437958	-1.816905
H	3.881199	0.060821	1.494349
H	-0.211901	-1.181724	1.063360
N	-2.584379	3.269968	-0.628319
O	-3.011005	2.770327	0.394628
O	-3.100079	4.186934	-1.232130
C	-1.284310	2.727213	-1.188222
C	-0.306618	2.339344	-0.140537
H	-0.633340	2.498359	0.884476
O	-1.112611	1.389603	-0.843978
C	1.160733	2.307248	-0.377811
C	3.920713	2.320186	-0.788794
C	1.997469	2.994537	0.503422
C	1.713612	1.591921	-1.442638
C	3.088936	1.608722	-1.652034
C	3.373821	3.003360	0.295228
H	1.570623	3.516335	1.356136
H	1.067774	1.005283	-2.090555
H	3.515932	1.041946	-2.473803
H	4.018466	3.541148	0.983275
H	4.994133	2.320824	-0.948126
C	-1.002679	3.198945	-2.579949
H	-0.998883	4.288414	-2.614340
H	-1.770907	2.827439	-3.262811
H	-0.028271	2.826953	-2.894858

RS epoxide:Catalyst, binary complex 74; Energy = -2449.848499; 6-31G(d) basis set.

N	-2.048399	-1.154745	0.493968
C	-0.758804	-0.846287	0.634140
S	-0.282331	0.532957	1.492816
C	-2.680748	-2.190560	-0.313709
C	-4.202550	-2.016406	-0.114968
C	-4.951314	-3.128006	-0.861162
C	-4.629006	-3.084638	-2.356388
C	-3.119864	-3.177706	-2.589001
C	-2.366033	-2.092638	-1.814526
N	-4.531078	-1.845285	1.298114
C	-4.426647	-3.057451	2.094163
N	0.121616	-1.734838	0.063924
C	1.521241	-1.602366	0.009358
C	2.326325	-2.693983	0.319894
C	3.712463	-2.581597	0.231602
C	4.314646	-1.388143	-0.137043
C	3.495277	-0.306048	-0.451975
C	2.113612	-0.407730	-0.408236
C	4.537310	-3.793267	0.561567

F	4.270899	-4.243249	1.796793
C	4.102252	1.024028	-0.796963
F	5.354202	0.902376	-1.254575
C	-5.811129	-1.187728	1.502102
F	4.272562	-4.805555	-0.280460
F	5.850036	-3.545252	0.493513
F	3.385194	1.673006	-1.724650
F	4.151458	1.825530	0.282768
H	-2.701661	-0.616691	1.062189
H	-0.237444	-2.664545	-0.121177
H	-2.671685	-1.096759	-2.154524
H	-1.291265	-2.175872	-2.001259
H	-2.764798	-4.167068	-2.267549
H	-2.890865	-3.092222	-3.656060
H	-5.146187	-3.895066	-2.880342
H	-5.001259	-2.141440	-2.777664
H	-4.658669	-4.105703	-0.453937
H	-6.029494	-3.020854	-0.696196
H	-2.381271	-3.188317	0.053253
H	-4.443437	-1.052578	-0.587838
H	-6.673605	-1.803507	1.193559
H	-5.927629	-0.958255	2.565644
H	-5.827470	-0.247401	0.945174
H	-3.447296	-3.523938	1.951879
H	-5.205500	-3.801877	1.857363
H	-4.519958	-2.795649	3.152195
H	1.877326	-3.628590	0.645365
H	5.393605	-1.302178	-0.187393
H	1.489776	0.428803	-0.697421
N	-3.017925	1.737402	-0.168455
O	-3.702330	1.309650	0.744317
O	-2.865411	1.189008	-1.240028
C	-2.315585	3.059604	0.048965
C	-1.034470	3.190437	-0.674060
H	-0.724224	2.313718	-1.239965
O	-2.251685	3.775348	-1.142954
C	0.037933	4.123173	-0.226174
C	2.071474	5.859216	0.569683
C	-0.171093	5.503241	-0.246233
C	1.272382	3.614613	0.184103
C	2.284378	4.482187	0.582727
C	0.843530	6.368142	0.153653
H	-1.125766	5.889188	-0.590966
H	1.434912	2.540593	0.210754
H	3.241023	4.078815	0.896692
H	0.676197	7.440603	0.132943
H	2.863688	6.534085	0.878904
C	-2.689058	3.726264	1.333874
H	-3.760046	3.938910	1.359300
H	-2.129989	4.659486	1.412925
H	-2.432097	3.077404	2.172708

RS epoxide:Catalyst, binary complex 75; Energy = -2449.838909; 6-31G(d) basis set.

N	3.278893	0.716039	-1.043130
C	2.030755	1.195746	-1.192639
S	1.469052	1.636571	-2.722479
C	3.960841	0.313000	0.183655
C	5.171296	-0.571260	-0.185350
C	5.900226	-0.991546	1.098051
C	6.315704	0.208829	1.950564
C	5.107827	1.079806	2.296078
C	4.389089	1.524643	1.022723
N	4.868657	-1.742233	-1.006009
C	4.920685	-1.566968	-2.446698
N	1.290244	1.240949	-0.042387
C	-0.017244	1.733798	0.143250
C	-0.508775	2.860866	-0.518229
C	-1.800703	3.296988	-0.245059
C	-2.610386	2.652112	0.682412
C	-2.095519	1.547784	1.351439
C	-0.810495	1.089969	1.095485
C	-2.344497	4.477128	-1.001559
F	-3.261352	5.142695	-0.283259
C	-2.968890	0.821300	2.335060
F	-3.696944	1.681818	3.064646

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C          3.685467       -2.483020       -0.616059
F         -1.378970        5.345029       -1.331321
F         -2.940409        4.099004       -2.142176
F         -3.845686        0.012607        1.714444
F         -2.262032        0.067562        3.183136
H          3.815649        0.716969       -1.900909
H          1.632677        0.687795        0.736268
H          5.059141        2.143259        0.410990
H          3.514648        2.142016        1.257426
H          4.413758        0.505571        2.925280
H          5.413715        1.955437        2.877189
H          6.814304       -0.134966        2.862682
H          7.047373        0.812243        1.395846
H          5.241310       -1.644023        1.687264
H          6.767542       -1.592228        0.809760
H          3.279335       -0.318399        0.773812
H          5.862825        0.055515       -0.769028
H          3.649336       -2.635270        0.465806
H          2.748883       -1.978314       -0.923820
H          3.702111       -3.469120       -1.091283
H          4.006685       -1.121773       -2.879599
H          5.053349       -2.545810       -2.920868
H          5.779806       -0.946347       -2.717844
H          0.108936        3.391982       -1.229901
H         -3.610813        3.014191        0.893889
H         -0.426731        0.225171        1.627330
N          0.644239       -2.510536        0.711800
O          1.170771       -1.571309        1.285690
O          1.137756       -3.604954        0.553193
C         -0.712218       -2.265127        0.092278
C         -1.797745       -3.108618        0.612208
H         -1.527046       -3.828214        1.384533
O         -1.605548       -1.736625        1.009502
C         -3.009292       -3.421554       -0.193792
C         -5.252698       -4.042392       -1.723693
C         -3.894871       -2.411755       -0.571157
C         -3.252484       -4.743217       -0.571670
C         -4.371054       -5.051067       -1.339288
C         -5.015244       -2.726085       -1.336119
H         -3.712185       -1.392934       -0.244115
H         -2.566366       -5.528770       -0.265093
H         -4.556938       -6.079178       -1.633570
H         -5.705919       -1.940170       -1.625091
H         -6.127199       -4.285029       -2.319118
C         -0.569179       -1.678577       -1.279958
H         -0.102807       -0.690136       -1.226300
H         -1.559190       -1.581278       -1.728426
H          0.045884       -2.332878       -1.903259

RS epoxide:Catalyst, binary complex 76; Energy = -2449.848581; 6-31G(d) basis set.
N         -2.049837       -1.158835        0.495439
C         -0.761081       -0.846097        0.633872
S         -0.288966        0.536018        1.490417
C         -2.680073       -2.199191       -0.307919
C         -4.202103       -2.028934       -0.107369
C         -4.948688       -3.145310       -0.848606
C         -4.628691       -3.106172       -2.344474
C         -3.119635       -3.195441       -2.579036
C         -2.368115       -2.105236       -1.809547
N         -4.528849       -1.853942        1.305673
C         -4.419118       -3.062921        2.105821
N          0.121677       -1.732656        0.063987
C          1.521320       -1.598340        0.012612
C          2.113164       -0.404439       -0.402394
C          3.496302       -0.299755       -0.434614
C          4.313605       -1.378174       -0.109594
C          3.710937       -2.574889        0.255624
C          2.326000       -2.689998        0.331952
C          4.102896        1.032332       -0.772513
F          3.393878        1.678509       -1.708327
C          4.560281       -3.780481        0.544303
F          3.992269       -4.577096        1.461258
C         -5.810626       -1.199710        1.509602
F          4.136956        1.834069        0.307640
F          5.360253        0.914752       -1.215908
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F          4.745849       -4.525051       -0.557266
F          5.773201       -3.437236        0.995688
H         -2.704060       -0.621721        1.063393
H         -0.235409       -2.663283       -0.120333
H         -2.677585       -1.111499       -2.152283
H         -1.293400       -2.185445       -1.997879
H         -2.761028       -4.182526       -2.254532
H         -2.892494       -3.113088       -3.646734
H         -5.144266       -3.919892       -2.864892
H         -5.004362       -2.165518       -2.768402
H         -4.652544       -4.120705       -0.438380
H         -6.026942       -3.040772       -0.682465
H         -2.376944       -3.194812        0.061873
H         -4.446594       -1.067366       -0.582985
H         -6.671677       -1.819248        1.204655
H         -5.926013       -0.966954        2.572553
H         -5.830876       -0.261376        0.949451
H         -3.438633       -3.526926        1.963267
H         -5.196153       -3.810556        1.873258
H         -4.511114       -2.797625        3.163098
H          1.490144        0.431374       -0.695395
H          5.393371       -1.287618       -0.143579
H          1.875685       -3.621692        0.661153
N         -3.024346        1.728785       -0.179575
O         -3.710803        1.301972        0.732093
O         -2.866712        1.177668       -1.248995
C         -2.326484        3.053647        0.036244
C         -1.043335        3.186054       -0.682846
H         -0.728674        2.308587       -1.245133
O         -2.260681        3.766025       -1.157588
C          0.024946        4.123286       -0.234497
C          2.051253        5.867785        0.561373
C         -0.188199        5.502648       -0.259075
C          1.259886        3.619650        0.180439
C          2.268275        4.491449        0.578974
C          0.822787        6.371770        0.140861
H         -1.143120        5.884773       -0.607346
H          1.425524        2.546197        0.210778
H          3.225335        4.091874        0.896475
H          0.652258        7.443656        0.116658
H          2.840637        6.545967        0.870601
C         -2.706382        3.723227        1.317764
H         -3.778067        3.932832        1.338738
H         -2.150317        4.658329        1.395830
H         -2.450557        3.077874        2.159632

RS epoxide:Catalyst, binary complex 77; Energy = -2449.839010; 6-31G(d) basis set.
N          1.297733       -2.406715       -0.980118
C          1.155230       -2.005467       -2.265041
S          2.011127       -2.719549       -3.521890
C          1.298266       -1.545818        0.219583
C          0.553091       -2.259692        1.375892
C          1.383029       -3.468410        1.834896
C          2.798287       -3.084938        2.272117
C          3.536119       -2.392863        1.126988
C          2.740014       -1.189831        0.617595
N          0.294940       -1.289124        2.454243
C         -0.015654       -1.911846        3.738282
N          0.281768       -0.981363       -2.535651
C         -0.902933       -0.636221       -1.847027
C         -1.656505       -1.586983       -1.156092
C         -2.813074       -1.191318       -0.496644
C         -3.249375        0.130279       -0.518538
C         -2.510569        1.057778       -1.242177
C         -1.347715        0.685800       -1.907065
C         -3.627968       -2.219666        0.240332
F         -4.600559       -2.728278       -0.525871
C         -2.994281        2.477634       -1.364838
F         -3.725428        2.848642       -0.312230
C         -0.830056       -0.427444        2.103556
F         -2.868776       -3.246681        0.652788
F         -4.212026       -1.689957        1.324542
F         -1.970402        3.336852       -1.489462
F         -3.760415        2.629161       -2.456546
H          1.941646       -3.188236       -0.925427
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H          0.338572       -0.667277       -3.498050
H          3.242770       -0.722241       -0.234221
H          2.675268       -0.440438        1.414787
H          4.528029       -2.060295        1.449157
H          3.710213       -3.111994        0.313115
H          2.751810       -2.401322        3.129065
H          3.342650       -3.977267        2.598204
H          0.853430       -4.012166        2.621472
H          1.443214       -4.168858        0.990929
H          0.782551       -0.621925       -0.049601
H         -0.408087       -2.644689        0.992632
H         -1.769362       -0.997986        2.002813
H         -0.977582        0.313854        2.893060
H         -0.657574        0.103891        1.159401
H         -0.269534       -1.122998        4.451517
H          0.843155       -2.454325        4.136043
H         -0.874220       -2.604086        3.674991
H         -1.332350       -2.621961       -1.131164
H         -4.138187        0.431523        0.024729
H         -0.788954        1.425179       -2.473391
N         -0.490567        2.723698        2.111611
O         -1.340715        2.849160        1.253365
O         -0.703651        2.679815        3.306970
C          0.967376        2.643351        1.684001
C          1.202700        2.791348        0.232741
H          0.311289        2.880606       -0.386089
O          1.364694        3.872680        1.158516
C          2.424905        2.280257       -0.447491
C          4.653884        1.273424       -1.797645
C          3.711174        2.614765       -0.019787
C          2.265705        1.465681       -1.568001
C          3.371675        0.955560       -2.241046
C          4.819369        2.107056       -0.692311
H          3.837768        3.291589        0.820108
H          1.266666        1.221837       -1.910674
H          3.229741        0.304694       -3.099866
H          5.817368        2.371926       -0.357434
H          5.522005        0.879784       -2.316771
C          1.816995        1.931029        2.689191
H          1.834659        2.489264        3.626635
H          2.830745        1.845843        2.296150
H          1.424839        0.923708        2.868887

RS epoxide:Catalyst, binary complex 78; Energy = -2449.849569; 6-31G(d) basis set.
N          2.756179        1.043179       -0.196741
C          2.513621        2.357887       -0.294860
S          3.683989        3.531961       -0.597124
C          4.016884        0.416290       -0.612711
C          4.225112       -0.908205        0.148138
C          5.473891       -1.624172       -0.389749
C          5.426093       -1.839529       -1.901728
C          5.257271       -0.504420       -2.624479
C          3.995949        0.203016       -2.132943
N          4.313404       -0.802534        1.604594
C          3.059734       -0.784786        2.331492
N          1.205063        2.772133       -0.150025
C          0.058606        2.093742        0.282524
C          0.096339        1.054381        1.218470
C         -1.088596        0.488594        1.673528
C         -2.329833        0.946882        1.248949
C         -2.358696        1.961371        0.299934
C         -1.187356        2.526930       -0.191072
C         -1.012311       -0.706943        2.578302
F         -2.105635       -0.842955        3.333718
C         -3.676249        2.450048       -0.239048
F         -3.678904        2.439536       -1.581143
C          5.201428        0.232581        2.101213
F         -0.903671       -1.842838        1.846626
F          0.052485       -0.668825        3.384936
F         -4.695013        1.691225        0.177003
F         -3.925788        3.711715        0.139783
H          1.960862        0.411362       -0.255165
H          1.085468        3.750503       -0.381239
H          3.115280       -0.405252       -2.382282
H          3.872445        1.177730       -2.617418
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H	6.132486	0.130157	-2.428980
H	5.204437	-0.650490	-3.708516
H	6.335778	-2.349756	-2.236177
H	4.580815	-2.495438	-2.152505
H	6.366136	-1.030689	-0.148396
H	5.568838	-2.573345	0.145862
H	4.818265	1.116704	-0.357834
H	3.358874	-1.551588	-0.065884
H	5.374729	0.069916	3.170382
H	6.170576	0.190018	1.597440
H	4.789809	1.251012	1.977947
H	2.667153	0.236446	2.476740
H	3.201712	-1.213936	3.331109
H	2.307309	-1.387381	1.810604
H	1.040012	0.711450	1.622161
H	-3.249046	0.510460	1.619898
H	-1.236379	3.310198	-0.942833
N	0.417949	-2.108837	-0.637289
O	0.972033	-2.906263	0.084716
O	0.905210	-1.065989	-1.041953
C	-1.002554	-2.411877	-1.065206
C	-1.835451	-1.203320	-1.196200
H	-1.336831	-0.252233	-1.007165
O	-1.272290	-1.889359	-2.321570
C	-3.316705	-1.235833	-1.024141
C	-6.079460	-1.138756	-0.676802
C	-3.890163	-1.714732	0.155470
C	-4.128225	-0.709000	-2.029172
C	-5.508164	-0.662681	-1.854774
C	-5.270602	-1.664515	0.328490
H	-3.252306	-2.113335	0.941158
H	-3.675842	-0.332464	-2.942298
H	-6.137602	-0.250678	-2.637098
H	-5.712808	-2.037731	1.246844
H	-7.155590	-1.098162	-0.540660
C	-1.446862	-3.797685	-0.715608
H	-0.791107	-4.531165	-1.190410
H	-2.464407	-3.929817	-1.085209
H	-1.424146	-3.950888	0.364177

RS epoxide:Catalyst, binary complex 79; Energy = -2449.850910; 6-31G(d) basis set.

N	2.876973	0.774782	-0.288379
C	2.691918	2.071663	-0.577589
S	3.889689	3.112462	-1.149517
C	4.062422	0.020836	-0.708619
C	4.360240	-1.123893	0.280126
C	5.540503	-1.956046	-0.243806
C	5.304609	-2.483223	-1.659411
C	5.030219	-1.328404	-2.622369
C	3.841776	-0.504722	-2.133020
N	4.608712	-0.724947	1.665438
C	3.432132	-0.489237	2.480130
N	1.427925	2.590388	-0.396966
C	0.266317	2.027406	0.144976
C	0.293832	1.134802	1.224044
C	-0.896325	0.654148	1.750587
C	-2.133289	1.058211	1.255171
C	-2.150234	1.950181	0.191147
C	-0.970761	2.430136	-0.369110
C	-0.870123	-0.320665	2.893738
F	-1.596533	0.117416	3.928112
C	-3.453613	2.352359	-0.443452
F	-4.507300	1.854996	0.208648
C	5.561226	0.358758	1.834463
F	-1.404150	-1.507002	2.529290
F	0.368071	-0.563912	3.331019
F	-3.588846	3.682985	-0.497661
F	-3.517411	1.905389	-1.712748
H	2.045156	0.194654	-0.195247
H	1.340002	3.524847	-0.776595
H	2.935449	-1.127306	-2.135157
H	3.649276	0.349372	-2.792052
H	5.918586	-0.685268	-2.682752
H	4.836638	-1.701643	-3.633491
H	6.170390	-3.066785	-1.990070

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H          4.442224       -3.164386       -1.657459
H          6.448743       -1.338628       -0.246908
H          5.713331       -2.772893        0.463256
H          4.900910        0.723367       -0.710350
H          3.479111       -1.782675        0.299777
H          5.157204        1.341079        1.529244
H          5.838434        0.425090        2.891907
H          6.473731        0.168785        1.263631
H          3.050575        0.542716        2.391392
H          3.676659       -0.652939        3.536820
H          2.633104       -1.184366        2.204859
H          1.234621        0.834878        1.667984
H         -3.059361        0.688297        1.681362
H         -1.007490        3.109645       -1.216262
N          0.079006       -1.308943       -0.872018
O          0.360588       -0.460886       -1.691768
O          0.775838       -1.610348        0.084672
C         -1.260862       -2.001687       -0.996225
C         -2.338742       -1.058004       -1.350599
H         -2.030696       -0.030340       -1.536886
O         -1.739882       -1.959024       -2.293649
C         -3.760565       -1.266875       -0.955321
C         -6.444290       -1.504669       -0.241344
C         -4.109604       -1.574776        0.360279
C         -4.758775       -1.074389       -1.912608
C         -6.097004       -1.198378       -1.556380
C         -5.451061       -1.691782        0.716387
H         -3.332062       -1.715002        1.106444
H         -4.481812       -0.826129       -2.933464
H         -6.870079       -1.050944       -2.303585
H         -5.717934       -1.930851        1.740935
H         -7.489747       -1.595785        0.036160
C         -1.350645       -3.277834       -0.216429
H         -0.601499       -3.984103       -0.583307
H         -2.344581       -3.698987       -0.372720
H         -1.184851       -3.102332        0.845700

RS epoxide:Catalyst, binary complex 80; Energy = -2449.854116; 6-31G(d) basis set.
N         -1.785456       -0.476676       -0.829597
C         -1.378470        0.233976       -1.886053
S         -2.351093        1.092442       -2.971770
C         -3.159942       -0.846736       -0.460581
C         -4.052785        0.361223       -0.116328
C         -5.459204       -0.124467        0.270175
C         -6.081783       -0.976438       -0.836466
C         -5.199831       -2.192323       -1.118500
C         -3.793419       -1.753021       -1.525112
N         -3.404773        1.225156        0.881100
C         -3.579666        0.782010        2.258380
N         -0.019199        0.310165       -2.083988
C          1.043610       -0.351089       -1.454989
C          0.988560       -1.697118       -1.080056
C          2.124860       -2.307024       -0.557660
C          3.323100       -1.619113       -0.410783
C          3.360739       -0.278036       -0.782228
C          2.238745        0.359016       -1.289440
C          2.020489       -3.720903       -0.059452
F          1.601581       -3.743235        1.218295
C          4.601199        0.530885       -0.525819
F          5.709566       -0.210488       -0.632091
C         -3.796440        2.620440        0.743272
F          1.144371       -4.439446       -0.771328
F          3.200378       -4.351018       -0.097942
F          4.710919        1.563697       -1.369562
F          4.592316        1.044158        0.720365
H         -1.083497       -0.757943       -0.150028
H          0.234974        1.044321       -2.733572
H         -3.841925       -1.206003       -2.472339
H         -3.141947       -2.620529       -1.679299
H         -5.147935       -2.816669       -0.215596
H         -5.634318       -2.812218       -1.909599
H         -7.089806       -1.291332       -0.546512
H         -6.181090       -0.378378       -1.752293
H         -5.406572       -0.728148        1.186313
H         -6.089841        0.743821        0.496645
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H         -3.030510       -1.441177        0.453004
H         -4.141843        0.956296       -1.029187
H         -3.615998        2.951212       -0.283924
H         -4.856731        2.800853        0.992552
H         -3.187012        3.235280        1.415634
H         -4.603804        0.935828        2.636295
H         -2.898494        1.341153        2.910876
H         -3.335802       -0.280970        2.354308
H          0.083980       -2.277597       -1.229341
H          4.202146       -2.112171       -0.010352
H          2.282168        1.409418       -1.566087
N         -0.661999       -0.677342        2.654343
O         -0.858107       -1.505126        1.772119
O         -1.213606       -0.653512        3.726256
C          0.382838        0.375404        2.352522
C         -0.165928        1.555973        1.650399
H         -1.236935        1.522552        1.429229
O          0.160954        1.537217        3.056201
C          0.627908        2.437673        0.757780
C          2.044698        4.046198       -1.029585
C          1.935549        2.832397        1.056193
C          0.019231        2.886528       -0.416338
C          0.727045        3.686300       -1.310556
C          2.643892        3.624570        0.157965
H          2.388157        2.538521        1.998420
H         -1.011901        2.606001       -0.628829
H          0.244806        4.029228       -2.221395
H          3.665446        3.911856        0.385704
H          2.600474        4.665650       -1.726678
C          1.745881       -0.249231        2.304140
H          2.112689       -0.373171        3.327283
H          2.440736        0.379154        1.747814
H          1.686521       -1.227243        1.824774

RS epoxide:Catalyst, binary complex 81; Energy = -2449.843132; 6-31G(d) basis set.
N         -0.171309        1.640732        1.110969
C          0.124233        1.207263        2.348663
S         -0.962772        1.313330        3.631860
C          0.726225        2.084282        0.040923
C         -0.139834        2.801861       -1.011861
C          0.745486        3.201060       -2.201497
C          1.886293        4.118323       -1.754738
C          2.709687        3.468224       -0.639958
C          1.816466        3.045891        0.528437
N         -1.336782        2.023267       -1.329092
C         -1.088890        0.878315       -2.193565
N          1.376176        0.671178        2.538053
C          2.027270       -0.120149        1.551597
C          1.300449       -1.066402        0.829534
C          1.922413       -1.780894       -0.186656
C          3.268290       -1.585035       -0.481545
C          3.988088       -0.663668        0.270459
C          3.379715        0.071183        1.284374
C          1.112292       -2.797553       -0.943576
F          0.907797       -3.904843       -0.226178
C          5.420887       -0.365889       -0.072610
F          6.155956       -0.148852        1.025913
C         -2.417691        2.845515       -1.851922
F         -0.101497       -2.304543       -1.259462
F          1.708835       -3.156884       -2.086460
F          5.989127       -1.364285       -0.758238
F          5.514396        0.740527       -0.829472
H         -1.147000        1.872078        0.944714
H          1.575097        0.448220        3.507053
H          1.326591        3.923939        0.970330
H          2.411097        2.584253        1.320187
H          3.232488        2.583018       -1.029878
H          3.481812        4.157964       -0.284166
H          2.525659        4.367265       -2.607911
H          1.466541        5.063409       -1.384603
H          1.169025        2.297612       -2.659434
H          0.134108        3.692338       -2.967245
H          1.203800        1.217804       -0.436883
H         -0.502547        3.725128       -0.534907
H         -2.631400        3.659457       -1.152721
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H         -2.195819        3.279841       -2.842154
H         -3.319286        2.232363       -1.941848
H         -0.772453        1.163173       -3.210487
H         -2.010150        0.294826       -2.283424
H         -0.323122        0.225926       -1.759622
H          0.253498       -1.239339        1.064936
H          3.745800       -2.139246       -1.281554
H          3.946139        0.804241        1.851348
N         -2.026732       -3.296838        0.469112
O         -1.285592       -2.888691        1.344276
O         -1.961320       -4.381206       -0.066922
C         -3.151103       -2.399131        0.004833
C         -2.817047       -0.978335       -0.138304
H         -1.801317       -0.678972        0.125346
O         -2.885357       -1.879284       -1.258710
C         -3.843205        0.097628       -0.066274
C         -5.697882        2.172974        0.096302
C         -3.756157        1.034301        0.965514
C         -4.862448        0.196276       -1.013595
C         -5.790310        1.233926       -0.927826
C         -4.680116        2.070076        1.044663
H         -2.974343        0.944303        1.718566
H         -4.912957       -0.528713       -1.821438
H         -6.580147        1.312097       -1.668600
H         -4.604075        2.795044        1.849194
H         -6.417959        2.983100        0.157299
C         -4.488100       -3.006994        0.297795
H         -4.598401       -3.935594       -0.266312
H         -5.269707       -2.304017        0.005803
H         -4.579516       -3.218087        1.366260

RS epoxide:Catalyst, binary complex 82; Energy = -2449.842989; 6-31G(d) basis set.
N          3.338429       -0.576586        1.317071
C          3.113543        0.137660        2.427588
S          4.307375        0.452018        3.568284
C          2.408832       -1.356206        0.495354
C          3.279029       -2.296454       -0.364434
C          2.380091       -3.106494       -1.308058
C          1.402421       -3.957601       -0.495989
C          0.558100       -3.074258        0.422729
C          1.424286       -2.189993        1.325404
N          4.380668       -1.561204       -0.984075
C          3.967088       -0.661502       -2.052687
N          1.829739        0.610989        2.621243
C          1.020568        1.227234        1.645316
C         -0.329025        1.434435        1.944349
C         -1.142471        2.122144        1.051052
C         -0.648181        2.595017       -0.160055
C          0.692940        2.374377       -0.450323
C          1.531809        1.709384        0.437665
C         -2.572990        2.362450        1.450730
F         -2.636407        3.092229        2.576550
C          1.302522        2.900938       -1.722013
F          0.421902        3.573243       -2.468078
C          5.458109       -2.430135       -1.429435
F         -3.268335        3.008360        0.513226
F         -3.211095        1.207101        1.714488
F          2.320122        3.735356       -1.449676
F          1.810377        1.912865       -2.472914
H          4.315999       -0.743422        1.092058
H          1.688117        0.954178        3.564526
H          2.003212       -2.811429        2.022140
H          0.786160       -1.538643        1.929760
H         -0.083145       -2.432579       -0.196432
H         -0.097013       -3.692076        1.047256
H          0.757021       -4.539771       -1.162108
H          1.968770       -4.678068        0.110043
H          1.819730       -2.422936       -1.959357
H          2.998572       -3.740954       -1.953092
H          1.835762       -0.695557       -0.168754
H          3.752927       -3.002137        0.336091
H          5.779415       -3.073417       -0.605123
H          5.177975       -3.069002       -2.284282
H          6.309353       -1.815393       -1.736653
H          3.650611       -1.195336       -2.964361
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H	4.807507	-0.012362	-2.315807
H	3.138293	-0.027384	-1.728327
H	-0.734116	1.069721	2.884921
H	-1.292105	3.114621	-0.859358
H	2.586017	1.588148	0.204659
N	-0.940377	0.161019	-2.174436
O	-0.888478	1.105894	-2.932442
O	0.016264	-0.422641	-1.698494
C	-2.331594	-0.293382	-1.795623
C	-2.534114	-0.608803	-0.375912
H	-1.654273	-0.536514	0.266597
O	-2.924349	0.646735	-0.958700
C	-3.636077	-1.497841	0.088126
C	-5.682834	-3.179482	0.953634
C	-3.333678	-2.760970	0.598071
C	-4.962588	-1.071580	0.023209
C	-5.983337	-1.914102	0.455862
C	-4.356354	-3.601313	1.025877
H	-2.298128	-3.084914	0.658003
H	-5.181271	-0.077043	-0.353342
H	-7.014479	-1.578204	0.408876
H	-4.117979	-4.584743	1.418829
H	-6.479940	-3.834781	1.290516
C	-3.083496	-0.822896	-2.976706
H	-2.543105	-1.660490	-3.425332
H	-3.205499	-0.030308	-3.718100
H	-4.063774	-1.167068	-2.642683

RS epoxide:Catalyst, binary complex 83; Energy = -2449.851783; 6-31G(d) basis set.

N	2.944173	0.019111	0.264171
C	3.706615	-1.077712	0.398987
S	5.393288	-1.072088	0.520796
C	3.455566	1.381999	0.389754
C	2.626767	2.361764	-0.465040
C	3.173227	3.783828	-0.268686
C	3.203283	4.205449	1.200819
C	4.022886	3.219122	2.032120
C	3.478385	1.802040	1.864829
N	2.549160	2.057241	-1.896308
C	1.418757	1.245230	-2.299701
N	3.036709	-2.270825	0.436684
C	1.661796	-2.423728	0.107327
C	1.246607	-2.254306	-1.214431
C	-0.104723	-2.324749	-1.525168
C	-1.051812	-2.593192	-0.541603
C	-0.625101	-2.768232	0.766722
C	0.724997	-2.680784	1.102157
C	-0.571976	-1.980945	-2.909439
F	-0.974626	-0.697279	-2.971199
C	-1.616786	-2.923771	1.881191
F	-1.293287	-3.931177	2.701948
C	3.786256	1.573383	-2.483452
F	0.396344	-2.132280	-3.820380
F	-1.614821	-2.732640	-3.284712
F	-1.636987	-1.805829	2.642465
F	-2.859484	-3.130981	1.443247
H	1.932242	-0.074855	0.348635
H	3.625035	-3.089541	0.523518
H	2.454292	1.744578	2.259590
H	4.086258	1.077335	2.417750
H	5.070258	3.245794	1.701868
H	4.015011	3.503065	3.089758
H	3.607809	5.219206	1.292895
H	2.175583	4.235905	1.590009
H	4.191579	3.832742	-0.679809
H	2.558845	4.464781	-0.865378
H	4.484104	1.364023	0.015579
H	1.594413	2.344168	-0.080863
H	3.693862	1.594237	-3.574229
H	4.620053	2.225459	-2.207520
H	4.042601	0.542291	-2.180483
H	1.479979	0.194763	-1.971851
H	1.344559	1.248143	-3.393100
H	0.492811	1.666533	-1.896549
H	1.985797	-2.051328	-1.983144

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H         -2.108012       -2.628435       -0.783871
H          1.051672       -2.785263        2.132747
N         -0.651770        0.597218        1.270571
O         -0.116695        0.240850        0.233325
O         -0.067265        0.873301        2.294633
C         -2.161683        0.719908        1.264677
C         -2.735804        0.975569       -0.079784
H         -2.022255        1.053489       -0.898642
O         -2.739509       -0.311955        0.537251
C         -4.041979        1.665767       -0.254623
C         -6.457400        3.007827       -0.608674
C         -5.228591        1.098749        0.211546
C         -4.067348        2.897953       -0.909958
C         -5.273049        3.569775       -1.081854
C         -6.434025        1.771999        0.033609
H         -5.199784        0.127658        0.697427
H         -3.143050        3.327877       -1.287655
H         -5.289269        4.528303       -1.590680
H         -7.356995        1.327920        0.392868
H         -7.399184        3.529339       -0.747150
C         -2.729554        1.133217        2.584890
H         -3.807756        1.253466        2.472989
H         -2.294359        2.079817        2.908265
H         -2.524985        0.369874        3.337190

RS epoxide:Catalyst, binary complex 84; Energy = -2449.842736; 6-31G(d) basis set.
N          2.854367        1.570216       -0.454137
C          1.796158        2.406050       -0.324119
S          1.818563        3.974734       -0.918212
C          3.289030        0.580473        0.548950
C          3.800608       -0.698367       -0.155912
C          5.108540       -0.364684       -0.889669
C          6.180973        0.197319        0.047688
C          5.674834        1.459870        0.747948
C          4.357371        1.181532        1.473221
N          3.963414       -1.760123        0.849036
C          4.770706       -2.879343        0.377090
N          0.688759        1.918465        0.325155
C          0.218179        0.586757        0.298652
C          0.439637       -0.258588       -0.790958
C         -0.111220       -1.536693       -0.791624
C         -0.900133       -1.993053        0.257994
C         -1.119802       -1.136617        1.331693
C         -0.550724        0.132109        1.371260
C          0.137280       -2.406646       -1.992872
F          1.450370       -2.679191       -2.125148
C         -1.998146       -1.545559        2.481446
F         -1.386853       -1.336756        3.656555
C          2.667574       -2.291844        1.262192
F         -0.506900       -3.571704       -1.917565
F         -0.244870       -1.791134       -3.119001
F         -3.127109       -0.805367        2.506484
F         -2.355952       -2.826616        2.423371
H          3.607802        2.018125       -0.963972
H         -0.015554        2.628216        0.516183
H          3.958556        2.094635        1.929255
H          4.533634        0.453739        2.272700
H          6.416756        1.828942        1.463094
H          5.541821        2.263200        0.009041
H          6.437803       -0.551832        0.807099
H          7.093635        0.413162       -0.517606
H          5.472697       -1.239734       -1.434554
H          4.878045        0.379586       -1.664040
H          2.417019        0.345824        1.155862
H          3.055417       -1.008402       -0.912765
H          2.155219       -2.810508        0.433085
H          2.813317       -3.006066        2.077286
H          2.002997       -1.504678        1.628717
H          4.379600       -3.318373       -0.558900
H          4.764458       -3.659100        1.143468
H          5.808754       -2.581919        0.217127
H          1.021580        0.088688       -1.639767
H         -1.356023       -2.976246        0.224754
H         -0.713143        0.782880        2.225879
N         -3.713211       -1.601366       -0.868489
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O         -3.109910       -1.967596       -1.854964
O         -3.991506       -2.297718        0.090298
C         -4.071308       -0.135432       -0.759000
C         -2.920008        0.725594       -1.082737
H         -2.024414        0.207027       -1.424933
O         -4.018960        0.514275       -1.980034
C         -2.701384        2.077354       -0.491983
C         -2.023119        4.554004        0.600895
C         -2.246854        3.107603       -1.317930
C         -2.818850        2.291653        0.883063
C         -2.478410        3.528342        1.428626
C         -1.912550        4.343851       -0.773192
H         -2.139032        2.932495       -2.384728
H         -3.147509        1.480700        1.527723
H         -2.565677        3.688824        2.498802
H         -1.542282        5.134452       -1.416548
H         -1.745206        5.513110        1.026120
C         -5.214430        0.139234        0.170354
H         -4.999768       -0.227019        1.173176
H         -6.114031       -0.356470       -0.204173
H         -5.385652        1.216348        0.191921

RS epoxide:Catalyst, binary complex 85; Energy = -2449.851035; 6-31G(d) basis set.
N          3.441513       -1.335817        0.329037
C          3.059445       -2.616456        0.258443
S          4.013760       -3.886527        0.804331
C          3.094676       -0.183107       -0.513052
C          4.284744        0.791719       -0.365461
C          4.057603        2.063738       -1.189380
C          3.859412        1.707509       -2.663817
C          2.689025        0.738391       -2.821692
C          2.882587       -0.533573       -1.990394
N          4.604764        0.983291        1.050874
C          3.606669        1.742449        1.794561
N          1.819030       -2.879887       -0.299347
C          0.614055       -2.229907        0.010968
C         -0.536804       -2.644158       -0.671130
C         -1.778746       -2.138744       -0.315060
C         -1.913632       -1.190802        0.695383
C         -0.758127       -0.754898        1.335027
C          0.496793       -1.266101        1.018437
C         -2.997480       -2.583055       -1.075590
F         -2.826190       -3.789200       -1.632027
C         -0.862784        0.318532        2.382630
F         -1.950700        0.164194        3.146510
C          5.933709        1.537205        1.258583
F         -4.077947       -2.645307       -0.289439
F         -3.287620       -1.731014       -2.077813
F          0.205593        0.345597        3.187460
F         -0.953889        1.543238        1.821870
H          4.256540       -1.157031        0.913300
H          1.712296       -3.861966       -0.526765
H          3.758125       -1.093807       -2.346531
H          2.012704       -1.186611       -2.107486
H          1.771952        1.242042       -2.490303
H          2.546765        0.467654       -3.873249
H          3.684334        2.613791       -3.252841
H          4.775095        1.242789       -3.054925
H          3.174043        2.595882       -0.819209
H          4.918820        2.731207       -1.070060
H          2.182329        0.304362       -0.141501
H          5.153580        0.267663       -0.794850
H          6.182571        1.481052        2.322583
H          6.669435        0.948816        0.702588
H          6.020672        2.591565        0.947111
H          3.547656        2.798488        1.485335
H          3.864840        1.712157        2.857145
H          2.612304        1.301217        1.677767
H         -0.456581       -3.389960       -1.456122
H         -2.891763       -0.812005        0.978690
H          1.367851       -0.955315        1.584263
N         -0.067774        3.016091       -0.635320
O         -0.117162        4.224720       -0.614639
O          0.886804        2.340045       -0.287410
C         -1.305875        2.260241       -1.059555
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C	-2.493121	2.680131	-0.277011
H	-2.313286	3.474695	0.447073
O	-2.261575	3.087230	-1.624711
C	-3.621556	1.766769	0.030379
C	-5.650365	-0.021078	0.712617
C	-3.997649	1.609391	1.366197
C	-4.286624	1.051335	-0.967240
C	-5.294518	0.155960	-0.623354
C	-5.006897	0.713924	1.706879
H	-3.483207	2.170529	2.141088
H	-4.019399	1.207369	-2.008375
H	-5.794564	-0.413084	-1.400486
H	-5.285807	0.587253	2.748204
H	-6.431017	-0.727481	0.977006
C	-1.005508	0.941020	-1.703796
H	-0.596027	1.120872	-2.702770
H	-0.281447	0.372926	-1.117695
H	-1.923658	0.361471	-1.801381

RS epoxide:Catalyst, binary complex 86; Energy = -2449.845246; 6-31G(d) basis set.

N	3.697181	0.106631	-1.154952
C	3.761348	-1.079259	-1.774612
S	5.197395	-1.699231	-2.397367
C	2.559619	0.996351	-0.928730
C	3.133260	2.366521	-0.511735
C	1.972801	3.282568	-0.102959
C	0.981147	3.457502	-1.256785
C	0.495351	2.108326	-1.791440
C	1.661366	1.187624	-2.156807
N	4.205954	2.203385	0.469424
C	3.747689	1.771890	1.783414
N	2.587243	-1.789194	-1.911412
C	1.576591	-1.918382	-0.934168
C	0.283298	-2.238206	-1.349004
C	-0.717021	-2.427547	-0.402366
C	-0.460441	-2.283726	0.953132
C	0.824063	-1.935016	1.352235
C	1.847155	-1.765795	0.429582
C	-2.100253	-2.781572	-0.866055
F	-2.464434	-2.062904	-1.936537
C	1.115011	-1.772288	2.817698
F	2.056921	-0.845168	3.037342
C	5.058208	3.376187	0.577739
F	-2.194573	-4.073318	-1.214656
F	-3.015523	-2.567072	0.095837
F	0.017821	-1.408060	3.501811
F	1.552805	-2.914561	3.366854
H	4.591093	0.521515	-0.901499
H	2.676176	-2.569534	-2.551811
H	2.262570	1.622696	-2.966315
H	1.280882	0.228164	-2.515743
H	-0.109665	1.591817	-1.034436
H	-0.152177	2.252681	-2.663320
H	0.130719	4.064135	-0.926412
H	1.469415	4.006941	-2.073295
H	1.454359	2.848819	0.760315
H	2.361796	4.258515	0.210150
H	1.936605	0.619750	-0.104213
H	3.613681	2.790690	-1.407003
H	5.420231	3.663905	-0.413596
H	4.549739	4.243922	1.030974
H	5.923682	3.132150	1.201199
H	3.210812	2.562573	2.332659
H	4.613876	1.471088	2.380382
H	3.080220	0.910984	1.694644
H	0.062721	-2.323178	-2.409290
H	-1.249198	-2.421722	1.683251
H	2.850142	-1.508150	0.758001
N	-0.922718	1.654085	1.367615
O	-0.933640	2.868357	1.378852
O	0.021482	0.948428	1.667495
C	-2.196821	0.940228	0.966910
C	-2.853832	1.473217	-0.230720
H	-2.364115	2.323729	-0.705568
O	-2.050140	0.273045	-0.244035

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C         -4.318122        1.344518       -0.466553
C         -7.070339        1.172048       -0.875090
C         -5.096617        2.503929       -0.489732
C         -4.916425        0.100069       -0.661102
C         -6.291568        0.017626       -0.864484
C         -6.470324        2.416319       -0.689077
H         -4.625664        3.473705       -0.350364
H         -4.302707       -0.793537       -0.667601
H         -6.753704       -0.952237       -1.019603
H         -7.071799        3.319653       -0.703154
H         -8.141893        1.104250       -1.034590
C         -2.824233        0.251880        2.139826
H         -2.090096       -0.404070        2.613368
H         -3.674442       -0.334987        1.788667
H         -3.169416        0.990108        2.868280

RS epoxide:Catalyst, binary complex 87; Energy = -2449.843023; 6-31G(d) basis set.
N         -1.898336       -0.273530       -1.850994
C         -1.362751        0.943094       -1.686126
S         -2.195646        2.406190       -1.647925
C         -3.287620       -0.683939       -1.649301
C         -3.903970       -0.146608       -0.343343
C         -5.271552       -0.824010       -0.149397
C         -6.199920       -0.511044       -1.326807
C         -5.577667       -0.964241       -2.649450
C         -4.188075       -0.354501       -2.845906
N         -2.974184       -0.233120        0.787873
C         -2.844614       -1.573594        1.346100
N          0.009930        0.970698       -1.598150
C          0.897058       -0.070249       -1.278418
C          0.555239       -1.119251       -0.412114
C          1.503279       -2.089667       -0.111890
C          2.806519       -2.010034       -0.594609
C          3.141411       -0.942921       -1.418532
C          2.195213        0.003754       -1.787533
C          1.138116       -3.287863        0.724517
F         -0.140124       -3.267451        1.114380
C          4.557559       -0.753307       -1.882549
F          4.611603       -0.327994       -3.151504
C         -3.324898        0.735547        1.820408
F          1.321900       -4.419077        0.020094
F          1.908253       -3.387236        1.813203
F          5.184014        0.174630       -1.135457
F          5.271578       -1.880316       -1.795511
H         -1.247724       -1.030889       -2.015606
H          0.406285        1.902577       -1.668034
H         -4.256936        0.735049       -2.941141
H         -3.723545       -0.735668       -3.761717
H         -5.495137       -2.060317       -2.650400
H         -6.224479       -0.694727       -3.490667
H         -7.172684       -0.992030       -1.179428
H         -6.380698        0.571507       -1.364012
H         -5.143805       -1.912509       -0.068120
H         -5.719700       -0.483808        0.791313
H         -3.230994       -1.778178       -1.568094
H         -4.086603        0.921202       -0.495247
H         -3.295214        1.742217        1.390142
H         -4.325291        0.562957        2.253553
H         -2.599366        0.688585        2.635989
H         -3.758013       -1.923351        1.855723
H         -2.029067       -1.590471        2.076547
H         -2.597989       -2.290914        0.555301
H         -0.434217       -1.162244        0.037345
H          3.540787       -2.766820       -0.338999
H          2.466173        0.819725       -2.451172
N         -0.056216       -0.283230        3.341890
O          0.531493       -1.236268        2.864021
O         -1.040725       -0.335666        4.046475
C          0.532248        1.066334        3.024344
C          0.079295        1.631310        1.750035
H         -0.689371        1.079807        1.195111
O         -0.397309        2.086564        3.037802
C          0.956953        2.542342        0.960695
C          2.535304        4.153560       -0.678362
C          0.476046        3.779526        0.528644
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C	2.232564	2.120999	0.581751
C	3.020297	2.921878	-0.242578
C	1.267214	4.583997	-0.286870
H	-0.521311	4.096510	0.817218
H	2.599540	1.151358	0.912897
H	4.002996	2.575517	-0.548136
H	0.888384	5.541577	-0.628955
H	3.145484	4.779676	-1.321853
C	1.858403	1.253043	3.703862
H	1.712556	1.241226	4.787614
H	2.271682	2.218346	3.409612
H	2.547627	0.454370	3.423026

RS epoxide:Catalyst, binary complex 88; Energy = -2449.845466; 6-31G(d) basis set.

N	-1.416571	-1.335678	0.941116
C	-1.143163	-1.101213	2.237317
S	-1.397386	-2.202197	3.491229
C	-1.751584	-2.667145	0.433175
C	-2.496349	-2.583696	-0.914563
C	-2.806867	-4.008473	-1.400702
C	-1.559667	-4.887045	-1.500844
C	-0.823004	-4.940960	-0.163481
C	-0.487583	-3.529054	0.311321
N	-3.718758	-1.778792	-0.930370
C	-3.535317	-0.397504	-1.329619
N	-0.620906	0.130705	2.538332
C	-0.590711	1.260257	1.693188
C	0.593528	1.971046	1.509969
C	0.606774	3.082061	0.667759
C	-0.534465	3.473446	-0.020362
C	-1.714506	2.765039	0.186730
C	-1.759817	1.689555	1.061863
C	1.895567	3.835315	0.490916
F	2.441199	4.151354	1.673137
C	-2.939382	3.132963	-0.603757
F	-2.907703	2.581353	-1.826322
C	-4.540614	-1.894843	0.261096
F	2.813663	3.098016	-0.166596
F	1.728936	4.964675	-0.200743
F	-4.062768	2.711142	-0.008629
F	-3.037201	4.458188	-0.774049
H	-1.015595	-0.694215	0.256985
H	-0.320574	0.231467	3.499284
H	0.195559	-3.049197	-0.403879
H	0.018549	-3.544209	1.282210
H	-1.458044	-5.432599	0.586014
H	0.091257	-5.538463	-0.246575
H	-1.835080	-5.893336	-1.834161
H	-0.885918	-4.473348	-2.265317
H	-3.520276	-4.470695	-0.703827
H	-3.314019	-3.929215	-2.366823
H	-2.411625	-3.125182	1.177159
H	-1.809076	-2.124157	-1.643293
H	-4.099963	-1.410101	1.151089
H	-5.512987	-1.430745	0.068499
H	-4.717367	-2.947937	0.499938
H	-4.514694	0.072500	-1.470486
H	-2.995229	-0.348878	-2.279895
H	-2.977063	0.208130	-0.600327
H	1.494216	1.655298	2.030172
H	-0.508178	4.322026	-0.694654
H	-2.691777	1.169525	1.256805
N	0.704479	0.700167	-1.672013
O	1.218609	1.664401	-2.193664
O	-0.488278	0.548703	-1.466249
C	1.593145	-0.456256	-1.291038
C	2.635488	-0.160746	-0.302150
H	2.693702	0.871686	0.035996
O	1.393439	-0.817432	0.034849
C	3.880718	-0.967670	-0.195361
C	6.237599	-2.442099	-0.032846
C	5.109127	-0.347249	-0.429871
C	3.832512	-2.322467	0.134849
C	5.012611	-3.056829	0.215613
C	6.285148	-1.086396	-0.353141

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H          5.140801        0.712358       -0.671328
H          2.872893       -2.787405        0.343700
H          4.974947       -4.109165        0.478793
H          7.239205       -0.603129       -0.537979
H          7.156347       -3.016665        0.030159
C          1.625208       -1.483075       -2.382672
H          0.622765       -1.889256       -2.544036
H          2.302985       -2.289047       -2.095926
H          1.983033       -1.025388       -3.308416

RS epoxide:Catalyst, binary complex 89; Energy = -2449.845480; 6-31G(d) basis set.
N          3.890118       -0.249744        0.312384
C          3.192964        0.887486        0.131756
S          3.980952        2.319021       -0.296214
C          3.382759       -1.602210        0.522277
C          4.325544       -2.614091       -0.160907
C          3.812063       -4.038301        0.092696
C          3.635418       -4.336342        1.582169
C          2.677813       -3.331557        2.221748
C          3.183572       -1.905650        2.012144
N          4.536173       -2.399080       -1.592241
C          5.592685       -1.471543       -1.963502
N          1.845284        0.764627        0.292232
C          0.855429        1.752936        0.101146
C         -0.294159        1.387851       -0.598527
C         -1.343967        2.286121       -0.732540
C         -1.253155        3.568449       -0.202778
C         -0.095924        3.926417        0.479648
C          0.953960        3.030405        0.651041
C         -2.607235        1.887853       -1.440893
F         -2.995860        2.829489       -2.312964
C          0.042843        5.324130        1.015926
F         -1.149876        5.856014        1.322527
C          3.331709       -2.139557       -2.359428
F         -2.471520        0.739419       -2.123625
F         -3.626102        1.719987       -0.581628
F          0.799208        5.358197        2.121204
F          0.617161        6.139868        0.120274
H          4.892076       -0.129252        0.236086
H          1.477463       -0.143310        0.559337
H          4.145563       -1.767841        2.524618
H          2.486086       -1.175402        2.439829
H          1.686483       -3.427895        1.759058
H          2.557521       -3.532470        3.291368
H          3.266329       -5.358507        1.717147
H          4.610404       -4.280528        2.086253
H          2.843769       -4.165932       -0.410243
H          4.513124       -4.736536       -0.373923
H          2.414404       -1.695351        0.013659
H          5.311927       -2.526654        0.320609
H          2.926284       -1.122370       -2.202391
H          3.560898       -2.240897       -3.425253
H          2.550593       -2.864066       -2.113183
H          5.300228       -0.409013       -1.904463
H          5.891213       -1.669200       -2.999264
H          6.469560       -1.633457       -1.328618
H         -0.357436        0.405430       -1.053068
H         -2.068648        4.274957       -0.317165
H          1.837943        3.313828        1.208130
N         -0.401464       -2.100442        0.055416
O          0.241810       -2.866963       -0.630338
O          0.026932       -1.498866        1.027731
C         -1.850287       -1.882186       -0.315775
C         -2.770253       -1.905851        0.851155
H         -2.308681       -2.091979        1.820622
O         -2.325762       -0.703275        0.231026
C         -4.205697       -2.263663        0.696322
C         -6.886163       -2.964893        0.416861
C         -4.693767       -3.414911        1.316274
C         -5.061669       -1.455177       -0.053718
C         -6.400571       -1.809256       -0.191020
C         -6.031908       -3.766451        1.172023
H         -4.028243       -4.033638        1.912829
H         -4.675267       -0.546096       -0.505601
H         -7.066465       -1.177469       -0.770192
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H          -6.408977       -4.663687        1.652370
H          -7.931162       -3.237696        0.308543
C          -2.164883       -2.270810       -1.727345
H          -3.215440       -2.050434       -1.918260
H          -1.982266       -3.335283       -1.877366
H          -1.548952       -1.700211       -2.426533

RS epoxide:Catalyst, binary complex 90; Energy = -2449.856845; 6-31G(d) basis set.
N          -2.463818       -0.641787        0.288624
C          -1.256171       -1.203932        0.096738
S          -0.977294       -2.436855       -1.013312
C          -3.707945       -1.062355       -0.341826
C          -4.848310       -0.395634        0.452008
C          -6.197835       -0.885247       -0.088266
C          -6.334083       -0.524621       -1.571190
C          -5.164896       -1.085059       -2.384632
C          -3.816329       -0.641766       -1.810394
N          -4.624380       -0.521313        1.893717
C          -4.880752       -1.851576        2.424753
N          -0.290167       -0.625566        0.896010
C           1.106085       -0.780806        0.871532
C           1.757622       -1.976502        0.568434
C           3.149251       -1.991652        0.500213
C           3.913090       -0.862517        0.755041
C           3.251349        0.310493        1.107614
C           1.869595        0.354585        1.172543
C           3.829653       -3.249400        0.039464
F           3.173610       -4.348136        0.431384
C           4.061716        1.535904        1.417670
F           3.317637        2.654206        1.388056
C          -5.315358        0.503177        2.659427
F           3.903042       -3.294202       -1.303044
F           5.085362       -3.335819        0.500862
F           4.616303        1.469398        2.637211
F           5.065534        1.693863        0.543113
H          -2.640399       -0.163867        1.176874
H          -0.602955        0.202408        1.398421
H          -3.723331        0.452104       -1.862333
H          -2.992387       -1.078125       -2.380303
H          -5.211301       -2.182709       -2.377779
H          -5.244266       -0.772495       -3.430853
H          -7.285710       -0.897544       -1.964418
H          -6.352912        0.568863       -1.672967
H          -6.271776       -1.974810        0.029846
H          -7.015566       -0.440816        0.491441
H          -3.782472       -2.158447       -0.283028
H          -4.769911        0.680421        0.241936
H          -6.414366        0.417930        2.612689
H          -5.017650        0.427664        3.709734
H          -5.021574        1.490001        2.289917
H          -5.949655       -2.121968        2.415686
H          -4.529243       -1.896492        3.459799
H          -4.329089       -2.600559        1.848553
H           1.193112       -2.875196        0.365323
H           4.994656       -0.889917        0.677219
H           1.371485        1.287231        1.417849
N          -2.047788        2.363345        0.423536
O          -1.993153        1.939206        1.572795
O          -3.044898        2.405469       -0.254897
C          -0.734770        2.789184       -0.194453
C          -0.369936        1.937846       -1.364757
H          -1.094026        1.161971       -1.625964
O          -0.893268        3.263841       -1.477945
C           1.037101        1.680722       -1.761324
C           3.700567        1.078016       -2.318163
C           1.419408        0.360982       -2.013418
C           1.982440        2.706061       -1.841481
C           3.312815        2.401099       -2.112904
C           2.750143        0.059545       -2.284806
H           0.678926       -0.436106       -1.973871
H           1.671428        3.738177       -1.708757
H           4.048541        3.197621       -2.162809
H           3.044227       -0.973576       -2.445412
H           4.742821        0.843998       -2.512641
C           0.153796        3.525195        0.766763
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H         -0.141932        4.578068        0.782590
H          1.192976        3.453848        0.445109
H          0.059797        3.116868        1.772548

RS epoxide:Catalyst, binary complex 91; Energy = -2449.845910; 6-31G(d) basis set.
N         -3.298612       -0.127717        1.130379
C         -2.968820       -0.647537        2.322775
S         -4.119454       -1.015828        3.493132
C         -2.535229        0.692864        0.191088
C         -3.560480        1.352939       -0.755467
C         -2.807652        2.109839       -1.857844
C         -1.909947        3.187091       -1.246449
C         -0.949042        2.588341       -0.219591
C         -1.678828        1.777615        0.853417
N         -4.561773        0.383197       -1.200557
C         -4.059786       -0.606902       -2.143869
N         -1.633055       -0.874409        2.590730
C         -0.658503       -1.363633        1.707834
C          0.679810       -1.349331        2.109841
C          1.665844       -1.858878        1.270569
C          1.362378       -2.351053        0.004524
C          0.024659       -2.367458       -0.377191
C         -0.982395       -1.923132        0.469628
C          3.076656       -1.889376        1.790803
F          3.953418       -2.275043        0.864646
C         -0.395422       -2.825843       -1.746572
F          0.540757       -3.545558       -2.361556
C         -5.768108        1.015842       -1.711862
F          3.459849       -0.666362        2.221607
F          3.193895       -2.711722        2.840517
F         -1.514550       -3.566425       -1.689043
F         -0.687170       -1.766638       -2.527573
H         -4.290890       -0.163914        0.905674
H         -1.468531       -1.071347        3.571108
H         -2.333953        2.423481        1.453127
H         -0.947632        1.333514        1.536050
H         -0.238731        1.921488       -0.725940
H         -0.352187        3.375024        0.251273
H         -1.348815        3.704340       -2.032678
H         -2.537289        3.943583       -0.755767
H         -2.191479        1.403917       -2.431749
H         -3.522932        2.555557       -2.558315
H         -1.872344        0.062293       -0.418934
H         -4.111545        2.090557       -0.151966
H         -6.152550        1.728084       -0.976492
H         -5.609979        1.547004       -2.665775
H         -6.530622        0.249316       -1.877744
H         -3.149794       -1.080657       -1.764333
H         -3.834456       -0.181187       -3.135528
H         -4.815058       -1.386988       -2.273888
H          0.946686       -0.952658        3.086664
H          2.139248       -2.716604       -0.659534
H         -2.021706       -2.022621        0.174646
N          2.911643       -0.608223       -2.133580
O          2.047720       -1.194262       -2.758157
O          3.918262       -1.112654       -1.682432
C          2.676578        0.858466       -1.848224
C          3.123475        1.261168       -0.489816
H          3.553205        0.464776        0.116547
O          3.874367        1.532267       -1.671876
C          2.559085        2.419373        0.254072
C          1.572524        4.564169        1.741879
C          2.024487        2.204173        1.526638
C          2.604738        3.712407       -0.269364
C          2.110503        4.780847        0.474455
C          1.528965        3.273359        2.266453
H          2.019590        1.200791        1.942544
H          3.057398        3.877382       -1.242723
H          2.158679        5.786379        0.068438
H          1.117497        3.100875        3.256239
H          1.195664        5.400191        2.322786
C          1.585541        1.454996       -2.681682
H          1.403014        2.477751       -2.346878
H          1.887511        1.466514       -3.732188
H          0.671076        0.867312       -2.587537
```

RS epoxide:Catalyst, binary complex 92; Energy = -2449.849308; 6-31G(d) basis set.

N	1.742538	-1.153461	-0.901321
C	1.163766	-2.204320	-1.509499
S	1.994313	-3.569819	-2.050999
C	3.125675	-1.195378	-0.413820
C	3.735886	0.210991	-0.236198
C	5.182994	0.049801	0.260865
C	5.286354	-0.767881	1.549488
C	4.632968	-2.138905	1.382212
C	3.192582	-1.980010	0.903152
N	3.712791	1.082263	-1.410015
C	2.608883	2.017899	-1.464882
N	-0.200477	-2.173432	-1.687596
C	-1.120033	-1.133378	-1.486673
C	-2.410104	-1.449269	-1.037822
C	-3.335809	-0.437352	-0.846199
C	-3.006799	0.900936	-1.069053
C	-1.733969	1.196932	-1.533181
C	-0.801528	0.191092	-1.774975
C	-4.735659	-0.762645	-0.402284
F	-5.135933	0.051590	0.588695
C	-1.310754	2.624981	-1.743145
F	-2.358618	3.437397	-1.915536
C	3.942497	0.418708	-2.679670
F	-5.611351	-0.605511	-1.405842
F	-4.850868	-2.022515	0.034165
F	-0.621632	3.086645	-0.681179
F	-0.508466	2.750758	-2.806770
H	1.148270	-0.463721	-0.446287
H	-0.569165	-3.055228	-2.021659
H	2.614223	-1.429771	1.661320
H	2.714299	-2.954762	0.759506
H	5.192584	-2.727008	0.642483
H	4.658988	-2.699988	2.322188
H	6.335667	-0.871266	1.845541
H	4.781731	-0.226426	2.362797
H	5.773231	-0.438481	-0.527628
H	5.600633	1.051685	0.395124
H	3.700902	-1.736033	-1.171970
H	3.169691	0.731878	0.551408
H	3.095676	-0.208565	-3.011129
H	4.124483	1.175917	-3.448807
H	4.832472	-0.215192	-2.621795
H	1.631242	1.555335	-1.673605
H	2.797976	2.752565	-2.254970
H	2.526469	2.552621	-0.513936
H	-2.668724	-2.479077	-0.812915
H	-3.733378	1.687375	-0.894047
H	0.161317	0.433859	-2.209501
N	0.980248	2.931528	2.076703
O	0.061268	3.721615	2.087672
O	2.161051	3.207163	1.984037
C	0.670898	1.453197	2.170008
C	-0.623494	1.039977	1.608488
H	-1.256959	1.844040	1.241224
O	0.615225	0.918489	0.878513
C	-1.312566	-0.229549	1.965603
C	-2.706614	-2.583187	2.510441
C	-0.681964	-1.467201	1.820567
C	-2.643940	-0.174778	2.380279
C	-3.337438	-1.349147	2.655970
C	-1.378580	-2.641157	2.092773
H	0.342033	-1.516172	1.459824
H	-3.144956	0.786535	2.461994
H	-4.378514	-1.300999	2.958524
H	-0.885344	-3.599966	1.966387
H	-3.253614	-3.498578	2.713077
C	1.468714	0.782590	3.243793
H	1.299465	1.287202	4.198645
H	2.533207	0.827021	3.002562
H	1.151056	-0.257072	3.336245

RS epoxide:Catalyst, binary complex 93; Energy = -2449.849370; 6-31G(d) basis set.

N	-1.786081	-1.556051	-0.405666

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C         -1.241733       -2.706582       -0.833445
S         -2.115609       -4.067398       -1.307938
C         -3.232031       -1.311537       -0.416363
C         -3.667839       -0.332371        0.691364
C         -5.193274       -0.168643        0.626996
C         -5.657232        0.330072       -0.742321
C         -5.189155       -0.611105       -1.852292
C         -3.673910       -0.802244       -1.793955
N         -3.240863       -0.667292        2.049123
C         -2.109469        0.115689        2.504731
N          0.133143       -2.770068       -0.902691
C          1.117905       -1.983797       -0.288409
C          0.904200       -1.316102        0.919988
C          1.933707       -0.570763        1.487762
C          3.196671       -0.519651        0.913967
C          3.413878       -1.239807       -0.256150
C          2.390744       -1.948204       -0.869531
C          1.659353        0.173627        2.765770
F          2.785353        0.576288        3.362912
C          4.789460       -1.300271       -0.860360
F          5.578698       -0.312725       -0.420016
C         -3.171205       -2.080232        2.368193
F          0.914340        1.277653        2.551750
F          0.977204       -0.580505        3.637602
F          5.398679       -2.457713       -0.564732
F          4.745795       -1.219315       -2.200833
H         -1.203305       -0.722296       -0.386862
H          0.455248       -3.609691       -1.368034
H         -3.169856        0.156830       -1.987534
H         -3.337489       -1.513220       -2.556126
H         -5.675928       -1.588357       -1.732376
H         -5.481667       -0.228622       -2.835945
H         -6.747073        0.436210       -0.760739
H         -5.236921        1.331662       -0.915222
H         -5.669609       -1.133954        0.852526
H         -5.487283        0.527166        1.418564
H         -3.700413       -2.284214       -0.237971
H         -3.225487        0.643833        0.459884
H         -2.347210       -2.624316        1.874360
H         -3.054059       -2.195457        3.450278
H         -4.109074       -2.569404        2.085580
H         -1.238685        0.090194        1.828147
H         -1.783155       -0.241231        3.486336
H         -2.399034        1.167601        2.598668
H         -0.043840       -1.418849        1.434910
H          3.992065        0.059806        1.366873
H          2.574744       -2.478256       -1.799926
N         -2.405379        3.288484       -0.398860
O         -2.984442        4.151454       -1.025179
O         -2.714108        2.890524        0.706491
C         -1.179521        2.677632       -1.049190
C         -0.123637        2.285283       -0.082065
H         -0.347220        2.484398        0.963927
O         -1.022436        1.343613       -0.676281
C          1.311076        2.208575       -0.463099
C          4.006143        2.189772       -1.184086
C          2.242584        2.930738        0.286993
C          1.738237        1.449212       -1.553288
C          3.081157        1.451506       -1.918949
C          3.586048        2.921522       -0.074400
H          1.913924        3.498409        1.153337
H          1.020538        0.846988       -2.104142
H          3.408154        0.856453       -2.765445
H          4.304780        3.486993        0.510227
H          5.054079        2.180546       -1.465666
C         -1.008309        3.094551       -2.476042
H         -0.955046        4.181425       -2.544708
H         -1.855675        2.747380       -3.072057
H         -0.087303        2.665727       -2.868513

RS epoxide:Catalyst, binary complex 94; Energy = -2449.860446; 6-31G(d) basis set.
N         -2.286104       -0.776925       -1.059631
C         -1.114016       -1.432669       -1.009341
S         -0.966589       -3.067297       -0.625686
C         -3.587158       -1.372935       -0.793481
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C	-4.446169	-0.409458	0.037683
C	-5.780283	-1.100914	0.365562
C	-6.517108	-1.501641	-0.916607
C	-5.652039	-2.415454	-1.786498
C	-4.302041	-1.763978	-2.090423
N	-3.697124	0.121959	1.182638
C	-3.248111	-0.886736	2.131804
N	-0.048952	-0.630821	-1.345590
C	1.314567	-0.782313	-1.057844
C	1.790925	-1.491161	0.051853
C	3.149839	-1.490960	0.326876
C	4.059126	-0.785209	-0.457175
C	3.569288	-0.065708	-1.536257
C	2.214426	-0.069233	-1.850180
C	3.665868	-2.256806	1.512657
F	2.701140	-2.522794	2.401936
C	4.486986	0.840817	-2.300849
F	4.474775	2.082008	-1.773986
C	-4.411733	1.193363	1.860851
F	4.208451	-3.428154	1.149329
F	4.627964	-1.570854	2.155267
F	5.756401	0.417706	-2.270927
F	4.124666	0.963626	-3.584568
H	-2.280653	0.236155	-1.178639
H	-0.283913	0.259724	-1.772487
H	-4.447603	-0.862593	-2.701978
H	-3.654722	-2.444296	-2.654088
H	-5.480773	-3.363319	-1.258700
H	-6.169689	-2.660550	-2.719627
H	-7.462823	-1.994410	-0.667573
H	-6.770538	-0.595273	-1.483430
H	-5.591982	-1.998497	0.970045
H	-6.406616	-0.432544	0.966420
H	-3.402086	-2.286548	-0.220462
H	-4.671184	0.463190	-0.594166
H	-5.265151	0.840242	2.463673
H	-3.722038	1.716190	2.534063
H	-4.778812	1.913801	1.123776
H	-4.074449	-1.432072	2.617960
H	-2.677846	-0.389248	2.923653
H	-2.586270	-1.610476	1.644657
H	1.102875	-2.013326	0.702764
H	5.115911	-0.774190	-0.212997
H	1.852980	0.502122	-2.700739
N	-2.623776	3.071096	-0.109532
O	-3.229081	3.917387	0.514076
O	-3.122703	2.263897	-0.870091
C	-1.128994	3.005924	0.105336
C	-0.671787	1.680691	0.594166
H	-1.471982	0.950426	0.760038
O	-0.548489	2.106879	-0.774851
C	0.596786	1.473487	1.340805
C	2.961160	0.971348	2.735551
C	0.567189	0.748458	2.532665
C	1.819520	1.926112	0.835662
C	2.995525	1.679493	1.534780
C	1.746922	0.500014	3.229139
H	-0.379176	0.366396	2.906835
H	1.854073	2.437123	-0.122289
H	3.941325	2.019486	1.123564
H	1.719266	-0.074128	4.149571
H	3.881178	0.766023	3.272420
C	-0.511860	4.345647	0.360974
H	0.543132	4.211535	0.600117
H	-1.011441	4.832424	1.198119
H	-0.603217	4.976005	-0.527487

RS epoxide:Catalyst, binary complex 95; Energy = -2449.852931; 6-31G(d) basis set.

N	-2.924599	-1.433029	0.995363
C	-2.297153	-2.538714	1.419822
S	-3.126515	-3.894737	1.967308
C	-2.501851	-0.031070	0.992408
C	-3.799447	0.804379	0.923880
C	-3.444175	2.289939	0.810857
C	-2.631366	2.737414	2.027416

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C         -1.379797        1.875418        2.203350
C         -1.702584        0.377196        2.234863
N         -4.701885        0.271790       -0.096491
C         -4.246709        0.486971       -1.464526
N         -0.914960       -2.540650        1.410259
C         -0.073323       -2.075667        0.383232
C         -0.548889       -1.668164       -0.870715
C          0.354013       -1.280181       -1.851409
C          1.728370       -1.320667       -1.637657
C          2.189097       -1.741642       -0.397009
C          1.305294       -2.098535        0.615604
C         -0.147145       -0.868078       -3.208957
F          0.006946       -1.863814       -4.098660
C          3.667606       -1.861949       -0.147700
F          4.095007       -3.114151       -0.375737
C         -6.072508        0.729040        0.070404
F         -1.450135       -0.556282       -3.191599
F          0.524847        0.183867       -3.685596
F          4.373952       -1.054148       -0.950030
F          3.985402       -1.567284        1.119051
H         -3.924263       -1.539087        0.831729
H         -0.538467       -3.322701        1.934176
H         -2.297689        0.135741        3.125494
H         -0.779390       -0.207982        2.302297
H         -0.690761        2.079037        1.372329
H         -0.846135        2.154910        3.118466
H         -2.348722        3.790353        1.925854
H         -3.253616        2.656812        2.929121
H         -2.866810        2.463319       -0.105283
H         -4.361997        2.883740        0.731230
H         -1.897361        0.189973        0.099727
H         -4.314525        0.647065        1.884644
H         -6.202660        1.802744       -0.145907
H         -6.720869        0.168913       -0.609941
H         -6.403680        0.537219        1.095135
H         -4.886139       -0.086373       -2.142146
H         -3.218994        0.136843       -1.591553
H         -4.283952        1.545319       -1.769595
H         -1.612281       -1.675161       -1.083102
H          2.417604       -1.002297       -2.411905
H          1.684824       -2.402023        1.587263
N         -0.371747        2.704387       -1.098658
O         -0.873800        1.700626       -1.565873
O         -0.960570        3.739027       -0.851119
C          1.092151        2.655346       -0.732483
C          1.475962        1.388210       -0.064062
H          0.673191        0.660077        0.075055
O          1.759694        1.662601       -1.432304
C          2.616032        1.299691        0.885562
C          4.717422        1.082660        2.701364
C          2.362585        0.931087        2.208360
C          3.924086        1.546619        0.469533
C          4.972181        1.436812        1.379152
C          3.410838        0.828938        3.115796
H          1.342071        0.721284        2.522482
H          4.114766        1.795846       -0.570206
H          5.990538        1.619336        1.050769
H          3.209953        0.545048        4.144051
H          5.536574        0.994580        3.408082
C          1.708154        4.004164       -0.530440
H          1.651539        4.588348       -1.451895
H          2.753898        3.867798       -0.252615
H          1.190093        4.542593        0.263626

RS epoxide:Catalyst, binary complex 96; Energy = -2449.849330; 6-31G(d) basis set.
N          3.048664       -0.527566       -0.750609
C          1.744965       -0.776360       -0.953145
S          1.183960       -1.154531       -2.500625
C          3.730445       -0.230560        0.503363
C          5.173477       -0.778391        0.445350
C          5.892655       -0.454046        1.761944
C          5.867364        1.040627        2.086180
C          4.431276        1.562868        2.138707
C          3.707912        1.271023        0.825029
N          5.292756       -2.200837        0.132311
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C	5.300473	-2.552308	-1.279043
N	0.971820	-0.681348	0.175805
C	-0.386138	-0.976498	0.377182
C	-1.107416	-1.897663	-0.388610
C	-2.455128	-2.097156	-0.116536
C	-3.105478	-1.440145	0.921340
C	-2.364220	-0.565642	1.704608
C	-1.022361	-0.325150	1.438442
C	-3.242270	-2.989183	-1.033601
F	-3.687549	-2.311972	-2.107440
C	-3.003535	0.105264	2.887188
F	-2.561942	1.363020	3.052272
C	4.399333	-3.073098	0.872501
F	-2.505205	-4.006832	-1.495671
F	-4.318852	-3.507028	-0.425860
F	-4.336934	0.155157	2.775099
F	-2.728214	-0.549310	4.027454
H	3.584412	-0.441491	-1.606209
H	1.372133	-0.126621	0.923036
H	4.197896	1.802703	-0.001439
H	2.673434	1.636909	0.841656
H	3.898460	1.075636	2.967466
H	4.417249	2.638420	2.341844
H	6.378270	1.225568	3.036720
H	6.421819	1.590415	1.313541
H	5.412998	-1.005598	2.582175
H	6.917825	-0.827356	1.684870
H	3.214180	-0.784405	1.299829
H	5.695833	-0.235217	-0.356757
H	3.349549	-3.010781	0.531637
H	4.727368	-4.109460	0.743552
H	4.433008	-2.845771	1.941770
H	4.297614	-2.587501	-1.737031
H	5.748913	-3.545212	-1.395828
H	5.917544	-1.840667	-1.836134
H	-0.629033	-2.436565	-1.194069
H	-4.159917	-1.602019	1.111605
H	-0.477084	0.403116	2.033742
N	1.291894	3.048582	-1.865125
O	2.013604	2.093690	-1.663458
O	1.512162	3.949327	-2.650552
C	-0.010788	3.115230	-1.095650
C	-0.730421	1.819747	-1.053669
H	-0.246819	0.999824	-1.588417
O	0.042331	2.323150	0.044573
C	-2.199729	1.699000	-0.856138
C	-4.940816	1.349454	-0.471791
C	-2.846736	2.336104	0.206558
C	-2.924922	0.864721	-1.707701
C	-4.295578	0.698780	-1.520362
C	-4.212577	2.161315	0.397117
H	-2.266379	2.921741	0.913019
H	-2.411770	0.325202	-2.500569
H	-4.851649	0.041365	-2.180449
H	-4.703898	2.640930	1.237922
H	-6.006624	1.209669	-0.319126
C	-0.593997	4.493702	-1.052494
H	0.074607	5.167413	-0.510392
H	-1.559065	4.460308	-0.547999
H	-0.731415	4.873662	-2.064447

RS epoxide:Catalyst, binary complex 97; Energy = -2449.842414; 6-31G(d) basis set.

N	-1.889323	0.439560	-1.274345
C	-1.104173	1.374970	-1.821679
S	-1.643400	2.803229	-2.528996
C	-3.350882	0.429963	-1.306168
C	-3.765775	-0.908031	-0.661427
C	-5.274113	-1.141223	-0.862766
C	-6.068603	0.178450	-0.778601
C	-5.338247	1.188662	0.107841
C	-4.006047	1.601768	-0.541003
N	-2.876657	-1.996775	-1.089194
C	-3.014828	-2.392165	-2.485066
N	0.256124	1.153814	-1.779051
C	1.060640	0.138780	-1.250537

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C          2.402578        0.154316       -1.665184
C          3.307316       -0.768052       -1.170700
C          2.916635       -1.744356       -0.259280
C          1.592206       -1.752301        0.151086
C          0.661126       -0.827113       -0.316259
C          4.748819       -0.682184       -1.591559
F          5.334844       -1.886095       -1.582747
C          1.162630       -2.737512        1.202429
F          1.899246       -3.855345        1.162690
C         -2.950852       -3.153760       -0.207709
F          4.877584       -0.171440       -2.822755
F          5.458706        0.104368       -0.764988
F          1.314099       -2.220439        2.439692
F         -0.120281       -3.087837        1.075642
H         -1.544583       -0.521251       -1.190809
H          0.761289        1.887311       -2.261945
H         -3.308719        1.964275        0.221664
H         -4.170628        2.424136       -1.239445
H         -5.953285        2.079390        0.268361
H         -5.159607        0.746430        1.094632
H         -6.184387        0.609318       -1.781251
H         -7.078579       -0.015433       -0.404953
H         -5.453040       -1.617612       -1.833007
H         -5.624399       -1.840612       -0.095820
H         -3.675237        0.462494       -2.357079
H         -3.567387       -0.794631        0.413016
H         -2.789441       -2.834166        0.825024
H         -3.918886       -3.676934       -0.278037
H         -2.160702       -3.861056       -0.476549
H         -3.950316       -2.934126       -2.694709
H         -2.180520       -3.049846       -2.747187
H         -2.970957       -1.513583       -3.135945
H          2.734557        0.899087       -2.382699
H          3.622699       -2.478763        0.110781
H         -0.337996       -0.869305        0.100773
N         -1.822134        0.233004        2.372643
O         -1.623187       -0.955865        2.179396
O         -2.889626        0.795077        2.285890
C         -0.594673        1.047458        2.720305
C         -0.077401        1.773839        1.552277
H         -0.693102        1.719391        0.652455
O         -0.801253        2.406016        2.631304
C          1.360623        2.087214        1.316254
C          4.007094        2.622168        0.611062
C          1.673334        3.234739        0.582842
C          2.377163        1.203561        1.684504
C          3.697288        1.474398        1.336471
C          2.994085        3.503934        0.236460
H          0.875253        3.903844        0.269982
H          2.135112        0.278236        2.199904
H          4.480760        0.774171        1.607947
H          3.231638        4.396262       -0.334123
H          5.035689        2.821379        0.326663
C          0.121955        0.488683        3.915438
H          0.416507       -0.545849        3.743580
H         -0.545918        0.537379        4.780497
H          0.999867        1.103203        4.117124

RS epoxide:Catalyst, binary complex 98; Energy = -2449.847544; 6-31G(d) basis set.
N         -2.749285       -0.956788       -0.412549
C         -2.659281       -2.286576       -0.525128
S         -3.937177       -3.314182       -0.927916
C         -3.930758       -0.175997       -0.791354
C         -4.183493        0.965089        0.216443
C         -5.371220        1.810726       -0.265228
C         -5.166703        2.345984       -1.682731
C         -4.941449        1.195352       -2.663592
C         -3.750219        0.347789       -2.221628
N         -4.391503        0.550587        1.603771
C         -3.190194        0.300729        2.377322
N         -1.428519       -2.868606       -0.305068
C         -0.191866       -2.352022        0.097123
C         -0.042389       -1.265839        0.966668
C          1.234187       -0.878060        1.363817
C          2.370685       -1.556104        0.946338
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C	2.211133	-2.634598	0.081737
C	0.954593	-3.027240	-0.349413
C	1.414467	0.267377	2.318817
F	2.417486	1.070539	1.920560
C	3.446431	-3.322491	-0.429737
F	4.111886	-2.531785	-1.293410
C	-5.348517	-0.525465	1.794928
F	0.310082	1.030229	2.401507
F	1.709745	-0.146191	3.553443
F	4.296098	-3.603814	0.565562
F	3.165192	-4.461880	-1.068015
H	-1.893602	-0.410157	-0.360268
H	-1.432756	-3.850940	-0.550818
H	-2.835040	0.955198	-2.258747
H	-3.604696	-0.509049	-2.889586
H	-5.841732	0.567155	-2.700501
H	-4.774526	1.574552	-3.677247
H	-6.031002	2.946880	-1.984913
H	-4.292475	3.011612	-1.699215
H	-6.285936	1.202823	-0.247851
H	-5.514592	2.624298	0.451942
H	-4.778579	-0.866479	-0.769246
H	-3.297620	1.614389	0.217233
H	-4.966427	-1.510210	1.470694
H	-5.595096	-0.595178	2.859856
H	-6.275621	-0.322096	1.252586
H	-2.793683	-0.721680	2.243159
H	-3.411041	0.422341	3.444797
H	-2.412851	1.024150	2.109011
H	-0.905527	-0.751457	1.372116
H	3.357170	-1.246174	1.277537
H	0.852182	-3.864749	-1.032207
N	-0.454401	2.294422	0.104534
O	-1.111228	2.854276	0.951602
O	-0.844814	1.369181	-0.589687
C	0.957074	2.809387	-0.144290
C	1.783267	1.939963	-1.016725
H	1.319735	1.004941	-1.327122
O	1.102254	3.102537	-1.496366
C	3.270156	1.955433	-1.035018
C	6.058937	1.869864	-1.089237
C	3.938047	0.730584	-1.021572
C	4.003772	3.139955	-1.123669
C	5.394841	3.093917	-1.143917
C	5.327662	0.685010	-1.039236
H	3.366443	-0.191919	-1.025696
H	3.484812	4.090100	-1.208518
H	5.961411	4.017110	-1.213636
H	5.832608	-0.276043	-1.030308
H	7.143789	1.839532	-1.106875
C	1.405028	3.776107	0.905972
H	1.220361	3.362779	1.897221
H	0.861588	4.717720	0.804442
H	2.474223	3.955086	0.792652

RS epoxide:Catalyst, binary complex 99; Energy = -2449.843914; 6-31G(d) basis set.

N	2.357853	-0.666086	-0.310696
C	1.025231	-0.616543	-0.430405
S	0.281179	0.638468	-1.289651
C	3.169489	-1.600108	0.462306
C	4.615705	-1.543714	-0.076994
C	5.498778	-2.497800	0.737888
C	5.443225	-2.201517	2.237474
C	4.004898	-2.254569	2.754319
C	3.120889	-1.290378	1.964326
N	4.766520	-1.796837	-1.507885
C	4.612394	-0.652655	-2.393266
N	0.339011	-1.649601	0.149795
C	-1.063280	-1.811117	0.152848
C	-1.898144	-0.769050	0.561806
C	-3.272365	-0.949026	0.554955
C	-3.842021	-2.168194	0.193958
C	-2.998782	-3.207547	-0.168909
C	-1.615584	-3.035606	-0.205207
C	-4.149620	0.223268	0.890894

F	-3.591284	1.012403	1.818688
C	-3.551686	-4.552091	-0.548534
F	-3.154143	-5.503671	0.311141
C	4.040209	-2.945561	-2.013962
F	-4.362564	0.990811	-0.193333
F	-5.349491	-0.159974	1.343635
F	-4.889214	-4.560628	-0.568252
F	-3.123467	-4.929298	-1.762721
H	2.840452	0.145341	-0.687057
H	0.874615	-2.451230	0.460043
H	3.467196	-0.259248	2.102948
H	2.082258	-1.322718	2.314496
H	3.617788	-3.278471	2.653398
H	3.967471	-2.005367	3.819556
H	6.073828	-2.911478	2.782686
H	5.854830	-1.200558	2.424749
H	5.171297	-3.532385	0.564685
H	6.520398	-2.419690	0.355150
H	2.801153	-2.623043	0.284666
H	4.976959	-0.519293	0.101114
H	2.950796	-2.771516	-2.089691
H	4.405793	-3.184296	-3.017797
H	4.212229	-3.821507	-1.381681
H	3.562738	-0.407676	-2.629960
H	5.119155	-0.865234	-3.341380
H	5.082426	0.229354	-1.948665
H	-1.465670	0.170754	0.882006
H	-4.917291	-2.303114	0.202117
H	-0.973728	-3.850406	-0.529116
N	2.584513	2.493531	0.189450
O	2.542646	1.978274	1.285638
O	3.328327	2.148781	-0.715191
C	1.637819	3.638091	-0.088593
C	0.354660	3.535045	0.637480
H	0.236136	2.643661	1.251109
O	1.420059	4.387321	1.063105
C	-0.891498	4.184011	0.144515
C	-3.253833	5.373010	-0.738511
C	-1.981674	3.389302	-0.218646
C	-0.990591	5.574347	0.073634
C	-2.169921	6.166318	-0.369644
C	-3.158493	3.984819	-0.661199
H	-1.902484	2.306139	-0.171303
H	-0.145452	6.182992	0.381278
H	-2.244038	7.248257	-0.419860
H	-4.002552	3.361851	-0.936788
H	-4.174584	5.835242	-1.080999
C	1.868317	4.293342	-1.412114
H	2.874063	4.716152	-1.463296
H	1.131567	5.087931	-1.536013
H	1.746959	3.558774	-2.209988

RS epoxide:Catalyst, binary complex 100; Energy = -2449.848086; 6-31G(d) basis set.

N	2.416294	-0.278137	0.614516
C	1.212541	-0.180391	1.210461
S	0.974750	0.499044	2.726231
C	3.688881	0.046553	1.246612
C	4.785094	-0.665195	0.431683
C	6.141824	-0.449700	1.114299
C	6.457041	1.047010	1.204869
C	5.341328	1.803205	1.931357
C	3.977869	1.549434	1.282606
N	4.402081	-2.050058	0.144827
C	4.469414	-2.940655	1.293098
N	0.203721	-0.701993	0.426633
C	-1.180298	-0.740370	0.671387
C	-1.868745	0.327207	1.259540
C	-3.248425	0.263150	1.378146
C	-3.974744	-0.827273	0.906579
C	-3.281853	-1.866359	0.303349
C	-1.895133	-1.837768	0.192870
C	-3.995638	1.398207	2.021130
F	-5.122940	1.684248	1.346084
C	-4.049713	-2.988993	-0.330615
F	-3.323796	-4.111221	-0.418881

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C          5.107578       -2.601482       -0.999722
F         -4.367532        1.095341        3.273907
F         -3.266211        2.518359        2.080518
F         -5.168790       -3.275472        0.345991
F         -4.424845       -2.667840       -1.584353
H          2.538445       -0.987768       -0.113002
H          0.506783       -1.225765       -0.389400
H          3.970150        1.928302        0.252046
H          3.184476        2.059928        1.834383
H          5.305061        1.476833        2.979748
H          5.554548        2.877057        1.942327
H          7.415852        1.201299        1.711161
H          6.563962        1.451889        0.189345
H          6.117259       -0.879379        2.125063
H          6.928044       -0.974265        0.558819
H          3.672383       -0.329601        2.280014
H          4.809575       -0.165080       -0.546750
H          6.189060       -2.734175       -0.825142
H          4.685477       -3.581961       -1.241968
H          4.965223       -1.944320       -1.862267
H          5.501323       -3.142590        1.625135
H          4.007722       -3.897319        1.029967
H          3.911655       -2.517253        2.133961
H         -1.331090        1.205091        1.590578
H         -5.056331       -0.853463        0.988803
H         -1.372051       -2.667588       -0.273670
N          2.397253        0.375304       -2.385878
O          3.336160        1.070937       -2.083496
O          2.362916       -0.846419       -2.317838
C          1.116922        1.034970       -2.840364
C          0.396131        1.663929       -1.721736
H          0.910800        1.666125       -0.758407
O          1.138317        2.405515       -2.713780
C         -1.090506        1.776438       -1.687660
C         -3.867123        1.967607       -1.475489
C         -1.676021        2.935170       -1.174626
C         -1.902762        0.710311       -2.080782
C         -3.286970        0.804716       -1.977494
C         -3.060990        3.030305       -1.071103
H         -1.044638        3.758836       -0.852538
H         -1.452006       -0.209002       -2.446220
H         -3.906282       -0.040981       -2.260938
H         -3.510473        3.929756       -0.662675
H         -4.945747        2.038592       -1.378217
C          0.578540        0.419834       -4.100681
H          1.299853        0.575118       -4.908052
H         -0.354355        0.920663       -4.360117
H          0.406298       -0.649646       -3.977108

RS epoxide:Catalyst, binary complex 101; Energy = -2449.846376; 6-31G(d) basis set.
N          0.394942       -0.378451       -0.287613
C          0.231544       -0.994933       -1.464152
S          1.406060       -1.993989       -2.147961
C         -0.371590        0.724275        0.296163
C          0.277812        1.098841        1.638889
C         -0.595612        2.158714        2.326221
C         -0.712004        3.404830        1.442608
C         -1.270353        3.054462        0.060811
C         -0.429688        1.962937       -0.605510
N          0.607639       -0.094214        2.413621
C         -0.544907       -0.818670        2.923426
N         -0.957047       -0.768414       -2.132507
C         -2.212184       -0.784218       -1.462210
C         -2.458869       -1.716512       -0.450299
C         -3.667196       -1.682654        0.232243
C         -4.650262       -0.749887       -0.091856
C         -4.400736        0.152569       -1.116465
C         -3.188803        0.144000       -1.804462
C         -3.902785       -2.629494        1.377191
F         -3.165670       -3.739704        1.265072
C         -5.402772        1.222599       -1.449724
F         -6.622353        0.931261       -0.984064
C          1.572258        0.177796        3.467105
F         -3.581334       -2.056792        2.550071
F         -5.188536       -2.992778        1.460826
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F         -5.041663        2.401393       -0.917349
F         -5.500151        1.406631       -2.773085
H          1.195072       -0.675565        0.268728
H         -0.955080       -1.163775       -3.066888
H          0.593606        2.331877       -0.763502
H         -0.832184        1.702755       -1.589426
H         -2.308492        2.703146        0.153704
H         -1.294073        3.943688       -0.577160
H         -1.339351        4.159224        1.928482
H          0.287026        3.847229        1.320821
H         -1.595890        1.746552        2.518452
H         -0.160241        2.419588        3.297343
H         -1.400478        0.401703        0.499391
H          1.242669        1.567634        1.412612
H          1.153809        0.772882        4.297232
H          1.927130       -0.771320        3.881078
H          2.425397        0.715181        3.043412
H         -1.090394       -0.274914        3.713639
H         -0.209590       -1.772838        3.341287
H         -1.248607       -1.038507        2.115120
H         -1.700179       -2.452361       -0.197697
H         -5.594256       -0.733806        0.441772
H         -2.994869        0.866969       -2.591589
N          3.253038        2.648634        0.204438
O          2.994382        3.501787       -0.621144
O          3.268178        2.818631        1.408667
C          3.589879        1.265070       -0.315727
C          4.607539        0.558252        0.502507
H          4.995184        1.115759        1.354248
O          3.208419        0.289402        0.598995
C          5.482311       -0.505837       -0.057291
C          7.168686       -2.468093       -1.089855
C          6.866959       -0.332213       -0.011641
C          4.940764       -1.668080       -0.608616
C          5.787280       -2.645373       -1.124550
C          7.708083       -1.310491       -0.531840
H          7.285245        0.567864        0.431997
H          3.862129       -1.803268       -0.634126
H          5.363216       -3.548641       -1.551872
H          8.783994       -1.171412       -0.496553
H          7.826113       -3.232825       -1.491659
C          3.330896        1.093507       -1.778015
H          2.266769        1.223230       -1.993429
H          3.617669        0.082895       -2.069039
H          3.903730        1.824959       -2.349650

RS epoxide:Catalyst, binary complex 102; Energy = -2449.845624; 6-31G(d) basis set.
N          3.602512       -1.329707        0.451797
C          3.147966       -2.570428        0.167185
S          4.042186       -3.953121        0.468036
C          3.486734       -0.177220       -0.466997
C          3.901492        1.102152        0.288438
C          4.018820        2.286213       -0.685791
C          4.935848        1.971008       -1.867037
C          4.416658        0.755926       -2.632012
C          4.358401       -0.450315       -1.699432
N          2.990323        1.333873        1.430358
C          2.470415        2.689011        1.584377
N          1.894309       -2.674249       -0.411096
C          0.696423       -2.055432       -0.005629
C         -0.493587       -2.645310       -0.458338
C         -1.722976       -2.153539       -0.046178
C         -1.811484       -1.070496        0.822181
C         -0.624509       -0.485813        1.246966
C          0.626789       -0.950242        0.848894
C         -2.983027       -2.763350       -0.593589
F         -2.829707       -4.065969       -0.868153
C         -0.674527        0.706042        2.159357
F         -0.651049        1.866110        1.465886
C          3.575417        0.900845        2.692895
F         -4.007313       -2.640361        0.257840
F         -3.355953       -2.168821       -1.743753
F         -1.793368        0.724380        2.898034
F          0.364197        0.740794        3.001703
H          4.521135       -1.384141        0.884231
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H          1.747923       -3.617235       -0.753203
H          5.375631       -0.696160       -1.361318
H          3.972049       -1.338659       -2.212863
H          3.411098        0.972339       -3.018011
H          5.052838        0.531150       -3.494270
H          4.995514        2.845172       -2.523638
H          5.955182        1.768097       -1.510034
H          3.027883        2.543144       -1.070948
H          4.394960        3.157538       -0.140643
H          2.439681       -0.071216       -0.765440
H          4.923509        0.924878        0.677662
H          2.829615        1.000520        3.486254
H          3.866230       -0.150446        2.643208
H          4.461791        1.498363        2.973152
H          1.940726        3.010529        0.686631
H          3.250664        3.430298        1.828569
H          1.751581        2.679358        2.407150
H         -0.453496       -3.507855       -1.117867
H         -2.775428       -0.705187        1.160949
H          1.517309       -0.440682        1.210550
N         -0.027772        2.424282       -1.253744
O          0.892683        1.642096       -1.097180
O          0.046463        3.627110       -1.129954
C         -1.379027        1.821281       -1.565224
C         -2.458807        2.425107       -0.743301
H         -2.140812        3.221668       -0.072657
O         -2.255666        2.740781       -2.119272
C         -3.665347        1.669168       -0.327105
C         -5.802874        0.136079        0.596919
C         -3.999122        1.676036        1.029058
C         -4.433662        0.928605       -1.227628
C         -5.494933        0.158563       -0.762367
C         -5.062604        0.906560        1.491543
H         -3.410210        2.269795        1.722031
H         -4.204428        0.966809       -2.288465
H         -6.080284       -0.429465       -1.461998
H         -5.310471        0.907664        2.548324
H         -6.626050       -0.473654        0.955747
C         -1.286081        0.446747       -2.151403
H         -0.996799        0.529026       -3.203422
H         -0.540490       -0.145155       -1.622993
H         -2.250913       -0.054225       -2.083923

RS epoxide:Catalyst, binary complex 103; Energy = -2449.853385; 6-31G(d) basis set.
N         -2.087703       -1.776525       -0.121764
C         -1.009811       -2.086015        0.616923
S         -1.043348       -2.489279        2.244244
C         -3.457700       -1.831523        0.363650
C         -4.307434       -0.829274       -0.427067
C         -5.744299       -0.852046        0.123274
C         -6.340218       -2.260958        0.043348
C         -5.470341       -3.275978        0.785858
C         -4.035740       -3.245648        0.258898
N         -3.651337        0.484174       -0.476291
C         -3.321813        1.037427        0.832953
N          0.145269       -2.100055       -0.146271
C          1.414295       -1.637942        0.206445
C          2.479876       -1.943428       -0.648696
C          3.745949       -1.431987       -0.393743
C          3.989920       -0.615097        0.704875
C          2.919861       -0.310074        1.538564
C          1.642823       -0.804076        1.306111
C          4.842650       -1.662295       -1.393302
F          4.687417       -2.815460       -2.055887
C          3.092659        0.674905        2.659467
F          2.588371        1.880182        2.317423
C         -4.396596        1.443388       -1.276187
F          4.861009       -0.679699       -2.310604
F          6.049772       -1.680388       -0.814457
F          2.449097        0.293234        3.767497
F          4.378904        0.864153        2.974857
H         -1.921824       -1.177305       -0.931004
H         -0.015313       -2.177370       -1.145120
H         -4.012281       -3.560133       -0.793210
H         -3.394435       -3.929996        0.823712
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H	-5.465268	-3.037213	1.857943
H	-5.887016	-4.283506	0.686599
H	-7.358736	-2.259207	0.445532
H	-6.415974	-2.557337	-1.012206
H	-5.744737	-0.512951	1.167897
H	-6.369366	-0.153582	-0.442992
H	-3.452929	-1.545228	1.422985
H	-4.348824	-1.181027	-1.471477
H	-5.333732	1.781774	-0.804490
H	-3.777230	2.332322	-1.444289
H	-4.640415	1.001165	-2.247993
H	-4.192922	1.128260	1.502449
H	-2.906977	2.040095	0.693169
H	-2.556416	0.427742	1.324202
H	2.315127	-2.580343	-1.513579
H	4.980448	-0.218599	0.896061
H	0.822397	-0.533949	1.960000
N	0.420338	0.103756	-2.553948
O	-0.557883	-0.628010	-2.620571
O	1.334877	0.114281	-3.346300
C	0.484499	1.099558	-1.422164
C	-0.800824	1.807316	-1.196455
H	-1.630892	1.522841	-1.842549
O	-0.349402	0.735673	-0.373486
C	-0.835671	3.170314	-0.602371
C	-0.933648	5.741811	0.468448
C	-1.410631	4.211459	-1.333507
C	-0.318426	3.415903	0.671539
C	-0.368683	4.700635	1.202866
C	-1.455412	5.495947	-0.799469
H	-1.822828	4.015631	-2.320659
H	0.109190	2.597610	1.244443
H	0.031157	4.886846	2.194543
H	-1.902638	6.302750	-1.371338
H	-0.973387	6.742611	0.886699
C	1.863342	1.640513	-1.188149
H	1.893421	2.111645	-0.205477
H	2.113099	2.376931	-1.954696
H	2.603281	0.837779	-1.224384

RS epoxide:Catalyst, binary complex 104; Energy = -2449.854493; 6-31G(d) basis set.

N	-1.116062	-2.039693	0.004962
C	-0.425198	-3.187260	-0.122667
S	-1.117229	-4.716686	-0.283165
C	-2.561259	-1.968203	-0.221628
C	-3.199852	-0.770158	0.509967
C	-4.706072	-0.744582	0.207881
C	-5.000702	-0.700374	-1.291196
C	-4.359211	-1.890863	-2.002343
C	-2.857696	-1.932246	-1.726752
N	-2.981874	-0.709549	1.956804
C	-1.870818	0.128960	2.359473
N	0.944475	-3.085404	-0.120993
C	1.724817	-1.970560	0.234392
C	2.799837	-1.588891	-0.573463
C	3.570963	-0.491957	-0.212532
C	3.276125	0.252511	0.928084
C	2.198825	-0.132340	1.715873
C	1.446750	-1.258266	1.400271
C	4.737114	-0.069252	-1.062856
F	4.752992	-0.690029	-2.244069
C	1.796082	0.726430	2.880964
F	2.854573	1.303799	3.463128
C	-2.979620	-1.993449	2.634967
F	4.706460	1.254823	-1.294158
F	5.903789	-0.326713	-0.453121
F	0.980443	1.722118	2.481847
F	1.137020	0.031701	3.814649
H	-0.604806	-1.169138	-0.144813
H	1.419643	-3.938718	-0.385538
H	-2.374734	-1.045780	-2.162702
H	-2.394530	-2.808986	-2.190751
H	-4.816016	-2.821464	-1.639265
H	-4.542060	-1.846517	-3.081161
H	-6.082100	-0.681928	-1.463541

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H         -4.596351        0.233394       -1.709910
H         -5.171844       -1.639362        0.644956
H         -5.134445        0.120745        0.722136
H         -2.980107       -2.892425        0.188634
H         -2.770188        0.153670        0.090791
H         -2.090673       -2.611223        2.415095
H         -3.016423       -1.822497        3.715478
H         -3.868974       -2.568906        2.360789
H         -1.856823        0.214724        3.451335
H         -1.996028        1.132686        1.939975
H         -0.886540       -0.242899        2.037518
H          3.001215       -2.123365       -1.496119
H          3.872598        1.120225        1.192804
H          0.642725       -1.586336        2.049857
N          1.102024        0.418619       -2.158958
O          2.126857        0.656705       -2.762630
O          0.462873       -0.614772       -2.227330
C          0.584684        1.494281       -1.231968
C         -0.894234        1.577578       -1.186159
H         -1.422315        0.885095       -1.841730
O         -0.122219        0.925192       -0.173233
C         -1.626735        2.813729       -0.806204
C         -3.043852        5.122312       -0.152833
C         -1.420518        3.432119        0.429127
C         -2.553252        3.344187       -1.705960
C         -3.256152        4.499864       -1.381153
C         -2.129909        4.585256        0.751622
H         -0.719589        2.997649        1.136516
H         -2.723518        2.851665       -2.660035
H         -3.973820        4.909834       -2.084328
H         -1.972916        5.060716        1.714443
H         -3.597091        6.020221        0.103061
C          1.547873        2.618559       -1.016745
H          1.143296        3.288677       -0.258427
H          1.684855        3.168802       -1.949479
H          2.517769        2.237986       -0.695574

RS epoxide:Catalyst, binary complex 105; Energy = -2449.855629; 6-31G(d) basis set.
N         -2.194933       -0.981136       -0.876780
C         -1.001751       -1.602934       -0.800226
S         -0.791646       -3.093104       -0.040164
C         -3.467351       -1.572286       -0.478142
C         -4.360795       -0.533705        0.217172
C         -5.647137       -1.234809        0.686752
C         -6.388505       -1.866553       -0.494950
C         -5.494460       -2.859311       -1.239577
C         -4.187759       -2.196160       -1.678026
N         -3.625734        0.204489        1.247906
C         -3.077342       -0.615224        2.319909
N          0.011856       -0.891715       -1.405374
C          1.389619       -0.868680       -1.113973
C          2.025817        0.372180       -1.270216
C          3.353782        0.529844       -0.917410
C          4.095942       -0.536780       -0.416539
C          3.468293       -1.767937       -0.306336
C          2.133886       -1.958455       -0.661283
C          4.005915        1.874333       -1.066145
F          4.847596        2.126067       -0.051882
C          4.210170       -2.907658        0.330575
F          5.530382       -2.831863        0.108262
C         -4.382973        1.325398        1.785175
F          4.725611        1.959091       -2.195661
F          3.107318        2.873173       -1.101353
F          4.040993       -2.903127        1.666357
F          3.790019       -4.098481       -0.112502
H         -2.232739       -0.015183       -1.202125
H         -0.297860       -0.029185       -1.842711
H         -4.393499       -1.410829       -2.418564
H         -3.516807       -2.924029       -2.147070
H         -5.261994       -3.704914       -0.578275
H         -6.016619       -3.270872       -2.109552
H         -7.301137       -2.360954       -0.145921
H         -6.701875       -1.071814       -1.186031
H         -5.393379       -2.014258        1.418076
H         -6.296950       -0.513730        1.194827
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H	-3.231840	-2.373594	0.227555
H	-4.646854	0.218448	-0.532839
H	-5.184581	1.019819	2.477761
H	-3.703524	1.987501	2.335751
H	-4.827952	1.896711	0.964689
H	-3.849291	-1.087135	2.950506
H	-2.464426	0.022719	2.967079
H	-2.429787	-1.398747	1.912936
H	1.451955	1.231686	-1.601783
H	5.128483	-0.404909	-0.111330
H	1.676342	-2.931181	-0.557460
N	-2.785056	3.029230	-0.512071
O	-3.361857	2.143286	-1.109853
O	-3.307366	3.990711	0.012626
C	-1.279088	2.932576	-0.373689
C	-0.888057	1.775606	0.457690
H	-1.727551	1.143868	0.770975
O	-0.797351	1.803046	-1.004084
C	0.376563	1.586056	1.219060
C	2.810370	0.939767	2.430789
C	0.624988	0.282789	1.664718
C	1.340011	2.574969	1.431347
C	2.550054	2.250681	2.037907
C	1.841840	-0.045667	2.251816
H	-0.125990	-0.491183	1.512448
H	1.158499	3.600712	1.133659
H	3.299113	3.021925	2.185369
H	2.040545	-1.072301	2.544307
H	3.768210	0.686505	2.875551
C	-0.615820	4.261318	-0.607227
H	0.445934	4.093030	-0.788138
H	-0.753942	4.925693	0.246462
H	-1.049030	4.733551	-1.492832

RS epoxide:Catalyst, binary complex 106; Energy = -2449.842745; 6-31G(d) basis set.

N	3.468550	-1.195975	-0.385997
C	3.039448	-2.079489	-1.319349
S	4.078085	-3.127195	-2.109361
C	2.982486	0.192531	-0.277420
C	3.124241	0.689036	1.180265
C	4.619150	0.775990	1.529269
C	5.388186	1.696766	0.578188
C	5.230230	1.233584	-0.872317
C	3.749904	1.109215	-1.239420
N	2.438614	1.981529	1.310195
C	2.764333	2.668641	2.554548
N	1.692000	-2.089772	-1.618765
C	0.596485	-1.963937	-0.744989
C	-0.682579	-2.064537	-1.298601
C	-1.804294	-1.993066	-0.481004
C	-1.689102	-1.807871	0.891084
C	-0.408618	-1.715035	1.429753
C	0.728327	-1.806794	0.638822
C	-3.168387	-2.069002	-1.107756
F	-4.080169	-2.561511	-0.271672
C	-0.274220	-1.546578	2.918891
F	1.001646	-1.398423	3.300698
C	0.989901	1.823932	1.239544
F	-3.595530	-0.840806	-1.482516
F	-3.164283	-2.822386	-2.214166
F	-0.944642	-0.460815	3.345632
F	-0.777048	-2.595078	3.579888
H	4.465789	-1.301607	-0.234444
H	1.501793	-2.653544	-2.439622
H	3.624425	0.740640	-2.265232
H	3.281047	2.095984	-1.171368
H	5.719065	1.936272	-1.554590
H	5.741101	0.270265	-1.013943
H	5.003180	2.720127	0.669533
H	6.446327	1.721412	0.858551
H	4.749261	1.081877	2.570782
H	5.041109	-0.236939	1.479976
H	1.932660	0.182057	-0.571801
H	2.658613	-0.049504	1.860904
H	0.665574	1.407606	0.280688

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H          0.600265        1.179597        2.050731
H          0.525535        2.809941        1.331582
H          3.810496        2.980185        2.571333
H          2.565207        2.048363        3.447639
H          2.150827        3.570371        2.625416
H         -0.799639       -2.215307       -2.368459
H         -2.572495       -1.746500        1.519188
H          1.709770       -1.779878        1.094480
N         -4.638770        0.826476        0.487360
O         -5.621150        1.029206       -0.189904
O         -4.486519       -0.099149        1.264866
C         -3.466915        1.756796        0.325567
C         -3.132412        2.021682       -1.089102
H         -3.778427        1.550791       -1.828234
O         -3.815789        2.963424       -0.266919
C         -1.733768        2.311680       -1.504669
C          0.875714        2.785204       -2.355867
C         -1.128246        3.538498       -1.237578
C         -1.028590        1.316573       -2.185622
C          0.277869        1.548496       -2.603258
C          0.174858        3.774447       -1.669771
H         -1.689173        4.304692       -0.710069
H         -1.516061        0.368450       -2.393806
H          0.824313        0.771542       -3.131702
H          0.641259        4.735656       -1.478073
H          1.883127        2.979689       -2.708777
C         -2.510365        1.741557        1.475976
H         -1.767902        2.522093        1.305572
H         -3.034951        1.941379        2.413391
H         -2.008134        0.776992        1.554340

RS epoxide:Catalyst, binary complex 107; Energy = -2449.838432; 6-31G(d) basis set.
N          2.784100       -2.727304       -0.180671
C          1.472447       -2.829531        0.109083
S          0.676794       -4.294368       -0.152088
C          3.748956       -1.644947        0.039562
C          3.437556       -0.309815       -0.685899
C          4.656344        0.612505       -0.505341
C          5.010209        0.837785        0.967447
C          5.259896       -0.487917        1.685127
C          4.053782       -1.414146        1.528884
N          3.046390       -0.389836       -2.089282
C          1.640251       -0.668605       -2.345847
N          0.873874       -1.702431        0.600084
C         -0.503521       -1.462130        0.758698
C         -1.461951       -1.954137       -0.134621
C         -2.802256       -1.641035        0.059090
C         -3.218370       -0.822351        1.104375
C         -2.251732       -0.313779        1.962664
C         -0.906068       -0.631505        1.806094
C         -3.819735       -2.196887       -0.899305
F         -4.213572       -3.429304       -0.558626
C         -2.643709        0.643075        3.052276
F         -3.925180        0.502787        3.406010
C          3.899353       -1.216829       -2.925150
F         -4.916552       -1.427175       -0.951495
F         -3.324485       -2.271242       -2.146872
F         -1.891882        0.483375        4.147865
F         -2.482701        1.921460        2.655978
H          3.174571       -3.614715       -0.470738
H          1.468492       -0.944503        0.918626
H          3.189834       -0.959107        2.033557
H          4.231176       -2.382752        2.007419
H          6.146562       -0.977691        1.259642
H          5.466210       -0.318441        2.746408
H          5.890613        1.484646        1.039538
H          4.189735        1.364132        1.470918
H          5.523799        0.174231       -1.017555
H          4.445345        1.563624       -1.005531
H          4.669149       -2.033039       -0.415383
H          2.602093        0.180981       -0.176404
H          3.754614       -2.297688       -2.751931
H          3.671316       -1.016010       -3.976515
H          4.952639       -0.974274       -2.760906
H          1.363999       -1.729093       -2.225156
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H	1.407560	-0.379453	-3.376679
H	1.008942	-0.068122	-1.679652
H	-1.159903	-2.565705	-0.974843
H	-4.265176	-0.573474	1.235311
H	-0.169834	-0.239387	2.501209
N	1.782136	2.440141	1.075561
O	2.610341	3.202355	1.515404
O	1.573176	1.306560	1.487707
C	0.971032	2.929000	-0.102828
C	-0.480080	2.779333	0.039644
H	-0.839523	2.327087	0.963559
O	0.202944	4.031509	0.241274
C	-1.371015	2.650262	-1.143908
C	-3.058921	2.295554	-3.327629
C	-1.637528	3.723511	-1.991440
C	-1.946185	1.403860	-1.388312
C	-2.786730	1.222069	-2.479974
C	-2.485125	3.541325	-3.082416
H	-1.191208	4.692058	-1.785741
H	-1.723718	0.577960	-0.719422
H	-3.227634	0.247207	-2.664749
H	-2.701557	4.377320	-3.740184
H	-3.720608	2.161149	-4.177570
C	1.785012	2.958370	-1.361278
H	2.597427	3.680903	-1.246117
H	1.134588	3.272572	-2.180087
H	2.202482	1.974782	-1.602261

RS epoxide:Catalyst, binary complex 108; Energy = -2449.854891; 6-31G(d) basis set.

N	1.746326	1.569876	-0.306468
C	0.483982	1.823792	0.073818
S	0.086184	2.976320	1.239135
C	2.920393	2.292853	0.157810
C	4.149596	1.376558	0.090540
C	5.373051	2.139082	0.627604
C	5.616548	3.423054	-0.170941
C	4.380149	4.322474	-0.149536
C	3.152430	3.568324	-0.660214
N	3.882203	0.078210	0.720403
C	3.596878	0.149061	2.146496
N	-0.426260	1.019922	-0.570053
C	-1.814542	0.923144	-0.391445
C	-2.382875	-0.346220	-0.534697
C	-3.753684	-0.519618	-0.409548
C	-4.589636	0.557235	-0.136205
C	-4.015727	1.817269	-0.014943
C	-2.646060	2.019147	-0.148510
C	-4.346814	-1.884166	-0.612205
F	-5.443352	-2.066340	0.133381
C	-4.897461	3.015576	0.202699
F	-5.185450	3.628471	-0.957473
C	4.916430	-0.903921	0.437259
F	-4.703699	-2.083979	-1.890438
F	-3.477054	-2.861683	-0.297047
F	-6.065634	2.678160	0.767346
F	-4.312761	3.927245	0.989300
H	1.922520	0.828949	-0.982345
H	-0.028978	0.252491	-1.107022
H	3.294182	3.289830	-1.713727
H	2.253508	4.189896	-0.599076
H	4.193030	4.659026	0.879282
H	4.547834	5.221294	-0.751928
H	6.486234	3.954033	0.230351
H	5.855111	3.160547	-1.210742
H	5.209022	2.397137	1.682592
H	6.258615	1.494870	0.586964
H	2.731395	2.586998	1.195676
H	4.333583	1.153358	-0.971631
H	5.854239	-0.732214	0.991134
H	4.552034	-1.903282	0.709781
H	5.140763	-0.903921	-0.634558
H	4.456282	0.485414	2.749197
H	3.316836	-0.848257	2.501526
H	2.749044	0.814146	2.333921
H	-1.737249	-1.196549	-0.730230

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H         -5.657705        0.416563       -0.014355
H         -2.226167        3.011327       -0.053203
N          2.958870       -1.728012       -2.094209
O          3.911801       -2.395589       -2.433924
O          2.893488       -0.514365       -2.157624
C          1.791959       -2.478470       -1.504104
C          1.463011       -2.046065       -0.123765
H          2.085488       -1.236315        0.275898
O          0.700666       -1.650332       -1.279765
C          0.808969       -2.964026        0.846350
C         -0.372738       -4.655219        2.723081
C         -0.473641       -3.467005        0.625344
C          1.499760       -3.314165        2.007888
C          0.912792       -4.162603        2.940311
C         -1.065083       -4.304872        1.566428
H         -1.012113       -3.199367       -0.277949
H          2.499639       -2.923775        2.179505
H          1.455988       -4.432076        3.840265
H         -2.070604       -4.675472        1.394784
H         -0.834648       -5.308101        3.456799
C          1.601780       -3.839816       -2.097433
H          1.372247       -3.755958       -3.162647
H          0.772771       -4.331549       -1.587935
H          2.507276       -4.433135       -1.971796

RS epoxide:Catalyst, binary complex 109; Energy = -2449.843535; 6-31G(d) basis set.
N          2.528657       -0.548715       -1.519051
C          1.622706       -1.446459       -1.106887
S          1.935879       -2.984805       -0.504080
C          3.963952       -0.512138       -1.231005
C          4.281137       -0.682761        0.266445
C          5.790449       -0.476539        0.476245
C          6.598561       -1.480141       -0.349472
C          6.267769       -1.341152       -1.835776
C          4.766171       -1.505386       -2.082216
N          3.406132        0.140702        1.110055
C          3.774883        1.548921        1.157648
N          0.309104       -1.054876       -1.257368
C         -0.221008        0.239385       -1.145755
C          0.431285        1.269391       -0.463440
C         -0.189123        2.511429       -0.347663
C         -1.453815        2.747409       -0.865156
C         -2.104180        1.699700       -1.516257
C         -1.499133        0.463212       -1.672910
C          0.543085        3.591186        0.398512
F         -0.089750        4.767221        0.344943
C         -3.501852        1.927425       -2.019423
F         -3.925407        0.930283       -2.808684
C          3.300684       -0.413440        2.452715
F          0.693617        3.277749        1.699159
F          1.779138        3.771545       -0.093809
F         -4.373264        2.021555       -0.999624
F         -3.596241        3.067458       -2.715139
H          2.156999        0.278616       -1.969386
H         -0.361455       -1.808688       -1.134261
H          4.449570       -2.521875       -1.824688
H          4.524620       -1.344351       -3.138338
H          6.589692       -0.349419       -2.183899
H          6.821749       -2.079211       -2.424922
H          7.670382       -1.331380       -0.181013
H          6.359432       -2.499407       -0.018066
H          6.074761        0.542278        0.177743
H          6.029746       -0.575231        1.541626
H          4.269421        0.500321       -1.527929
H          4.049616       -1.722105        0.520401
H          4.265419       -0.443665        2.988170
H          2.615417        0.196812        3.047885
H          2.896304       -1.428472        2.395015
H          4.726398        1.736811        1.682634
H          2.989394        2.107451        1.676807
H          3.854572        1.958207        0.144948
H          1.390297        1.078280        0.019846
H         -1.926304        3.717891       -0.762740
H         -2.008537       -0.340950       -2.194042
N         -4.170423       -3.528325       -0.077304
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O	-5.369400	-3.451149	-0.261241
O	-3.511467	-4.545295	-0.098026
C	-3.449783	-2.236784	0.234623
C	-2.407606	-2.369332	1.273507
H	-2.253451	-3.366152	1.683697
O	-2.108523	-2.306164	-0.127567
C	-2.016908	-1.188751	2.097936
C	-1.307838	1.062566	3.579180
C	-2.935788	-0.611426	2.976477
C	-0.733693	-0.655674	1.981462
C	-0.387260	0.475755	2.714721
C	-2.579549	0.509993	3.719921
H	-3.933776	-1.033361	3.067588
H	-0.010152	-1.121546	1.315062
H	0.599637	0.909963	2.593130
H	-3.298978	0.959316	4.397074
H	-1.034371	1.950399	4.140852
C	-4.245565	-1.006247	-0.072032
H	-4.479974	-0.957637	-1.138602
H	-3.657058	-0.132874	0.211746
H	-5.180914	-1.006932	0.489303

RS epoxide:Catalyst, binary complex 110; Energy = -2449.847135; 6-31G(d) basis set.

N	-2.464403	0.507672	-0.686474
C	-1.138292	0.567871	-0.826012
S	-0.286609	-0.659019	-1.624841
C	-3.356116	1.370728	0.078093
C	-4.778192	0.792566	-0.079747
C	-5.786376	1.731724	0.595562
C	-5.467026	1.874989	2.086305
C	-4.028165	2.350677	2.294049
C	-3.026507	1.441493	1.577226
N	-5.051287	0.425837	-1.468727
C	-5.212831	1.557427	-2.369286
N	-0.543983	1.690883	-0.315144
C	0.840802	1.881949	-0.140024
C	1.602200	0.908713	0.511897
C	2.960958	1.111087	0.690874
C	3.579476	2.285862	0.263008
C	2.803996	3.256676	-0.351337
C	1.440377	3.060175	-0.567791
C	3.772547	0.078212	1.420845
F	3.253533	-1.152939	1.281671
C	3.413264	4.559715	-0.785305
F	2.995381	4.912819	-2.010123
C	-6.161616	-0.504668	-1.594581
F	5.034531	0.038387	0.973830
F	3.829444	0.332337	2.736347
F	3.066942	5.558954	0.042567
F	4.750031	4.507225	-0.809448
H	-2.938490	-0.213733	-1.223664
H	-1.136159	2.494810	-0.143915
H	-3.064887	0.421373	1.974414
H	-2.005547	1.796910	1.744489
H	-3.927975	3.375350	1.908594
H	-3.789213	2.390708	3.361472
H	-6.170425	2.567987	2.559439
H	-5.598677	0.901036	2.575931
H	-5.749947	2.719565	0.116050
H	-6.801817	1.343878	0.456591
H	-3.339613	2.390918	-0.344954
H	-4.770770	-0.156358	0.476266
H	-7.138855	-0.056331	-1.346189
H	-6.210805	-0.864789	-2.626483
H	-5.995449	-1.363809	-0.938221
H	-6.127310	2.141382	-2.172118
H	-5.263302	1.186993	-3.397163
H	-4.350237	2.226547	-2.299025
H	1.110661	0.012856	0.874785
H	4.644173	2.434221	0.404106
H	0.855356	3.814281	-1.086123
N	-1.613994	-2.025054	1.111033
O	-2.783648	-1.963625	0.784732
O	-1.047249	-1.222243	1.826761
C	-0.825666	-3.224998	0.621758

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C          0.636756       -3.092241        0.728596
H          1.009670       -2.145622        1.109015
O         -0.142059       -3.819599        1.683399
C          1.561622       -3.858306       -0.149798
C          3.313247       -5.238733       -1.820325
C          1.650130       -5.248149       -0.071457
C          2.361305       -3.157025       -1.054850
C          3.230368       -3.849197       -1.891982
C          2.526017       -5.935949       -0.906916
H          1.041237       -5.779982        0.653909
H          2.295737       -2.072572       -1.098946
H          3.846357       -3.301928       -2.598630
H          2.597001       -7.017279       -0.840483
H          3.995325       -5.776923       -2.471385
C         -1.582087       -4.061816       -0.358939
H         -2.480590       -4.475147        0.103255
H         -0.935901       -4.874888       -0.692141
H         -1.864389       -3.450499       -1.218152

RS epoxide:Catalyst, binary complex 111; Energy = -2449.845068; 6-31G(d) basis set.
N          1.916223       -0.058520        1.134607
C          1.585696        0.377467        2.355421
S          2.694694        0.981537        3.471637
C          3.279491       -0.300527        0.676293
C          3.253595       -1.350259       -0.447353
C          4.696831       -1.842657       -0.698096
C          5.734815       -0.729758       -0.450054
C          5.143417        0.641883       -0.784582
C          3.969389        0.975355        0.157839
N          2.244821       -2.389481       -0.211064
C          2.453925       -3.169419        1.004313
N          0.254126        0.340398        2.696549
C         -0.842518       -0.198867        1.998925
C         -0.758272       -1.378301        1.256026
C         -1.875717       -1.832602        0.559893
C         -3.092310       -1.170447        0.621225
C         -3.174657       -0.025493        1.408293
C         -2.071419        0.464879        2.087482
C         -1.719426       -3.032975       -0.328255
F         -1.241447       -2.677910       -1.539005
C         -4.446123        0.774920        1.398254
F         -5.524429       -0.011067        1.283592
C          2.097025       -3.270029       -1.364160
F         -0.848899       -3.920426        0.180901
F         -2.875481       -3.667384       -0.534673
F         -4.587123        1.502867        2.515088
F         -4.465437        1.627919        0.364290
H          1.199836       -0.452128        0.534661
H          0.052806        0.840001        3.553765
H          3.220904        1.585112       -0.363030
H          4.308136        1.555664        1.020636
H          5.908669        1.420410       -0.715653
H          4.801285        0.634012       -1.827098
H          6.048553       -0.735315        0.600810
H          6.634365       -0.921319       -1.042650
H          4.914097       -2.700698       -0.052066
H          4.771171       -2.197180       -1.731820
H          3.839982       -0.689711        1.535470
H          2.916442       -0.832652       -1.358322
H          1.935368       -2.669954       -2.266165
H          2.977137       -3.913221       -1.528110
H          1.224149       -3.911108       -1.218196
H          1.596238       -3.836348        1.138237
H          2.513795       -2.510568        1.876835
H          3.360994       -3.793348        0.976594
H          0.160122       -1.955402        1.215634
H         -3.952734       -1.525915        0.065311
H         -2.149971        1.380533        2.666172
N         -1.920078       -0.135661       -2.912826
O         -3.101412       -0.011987       -2.665706
O         -1.447923       -0.772719       -3.833554
C         -0.944962        0.587534       -2.015957
C         -1.285481        2.010548       -1.752040
H         -2.179935        2.393741       -2.243090
O         -1.547009        0.961287       -0.827411
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C	-0.235101	2.988522	-1.349754
C	1.767090	4.779145	-0.598116
C	0.403350	2.851377	-0.115356
C	0.120312	4.035327	-2.201839
C	1.121452	4.925925	-1.825324
C	1.403982	3.742968	0.259639
H	0.107440	2.044591	0.549190
H	-0.382348	4.150644	-3.158672
H	1.398234	5.737189	-2.491202
H	1.898678	3.619975	1.219360
H	2.548457	5.475089	-0.309346
C	0.430880	-0.000137	-2.010988
H	0.419398	-0.980168	-1.521895
H	1.089971	0.676308	-1.461298
H	0.802536	-0.114912	-3.029850

RS epoxide:Catalyst, binary complex 112; Energy = -2449.846151; 6-31G(d) basis set.

N	3.002833	-0.116875	-0.170594
C	1.920795	-0.876218	-0.399898
S	1.935342	-2.552915	-0.453109
C	4.346892	-0.612304	0.090926
C	5.378901	0.350931	-0.528089
C	6.793517	-0.161799	-0.224970
C	7.026538	-0.349031	1.275898
C	5.989663	-1.299338	1.876933
C	4.573719	-0.797430	1.595391
N	5.219476	0.610485	-1.959710
C	4.284058	1.661052	-2.316741
N	0.793522	-0.104606	-0.632665
C	-0.533858	-0.526877	-0.804696
C	-1.334361	0.171552	-1.709125
C	-2.689217	-0.124789	-1.814725
C	-3.271542	-1.120348	-1.044423
C	-2.463599	-1.808740	-0.145265
C	-1.110394	-1.526277	-0.012600
C	-3.520476	0.699964	-2.754737
F	-4.827360	0.438902	-2.638474
C	-3.057176	-2.876069	0.732512
F	-2.766486	-4.105101	0.286258
C	4.998392	-0.572879	-2.772932
F	-3.354228	2.016715	-2.517579
F	-3.177905	0.499109	-4.034279
F	-2.583167	-2.795253	1.986873
F	-4.392507	-2.783117	0.800808
H	2.851644	0.871395	0.023489
H	0.977684	0.844795	-0.943245
H	4.411346	0.166897	2.096817
H	3.819914	-1.493873	1.977982
H	6.112962	-2.298092	1.436735
H	6.142533	-1.405967	2.955777
H	8.040014	-0.724108	1.452844
H	6.955870	0.625732	1.778145
H	6.947545	-1.123412	-0.733022
H	7.510613	0.544620	-0.653509
H	4.423180	-1.587447	-0.400806
H	5.270534	1.323261	-0.022191
H	3.991760	-1.009785	-2.642029
H	5.114751	-0.305731	-3.828255
H	5.738782	-1.343039	-2.540826
H	3.226078	1.343343	-2.296068
H	4.500397	2.003583	-3.335078
H	4.402079	2.513961	-1.641410
H	-0.902281	0.958914	-2.321902
H	-4.332537	-1.327128	-1.110966
H	-0.508399	-2.055457	0.716379
N	1.111616	2.145167	1.405055
O	1.701968	1.410518	2.158494
O	1.571615	2.597777	0.361433
C	-0.333969	2.485818	1.708581
C	-1.139976	1.266275	1.922346
H	-0.581760	0.329718	1.905411
O	-0.687905	2.122109	2.989258
C	-2.602671	1.150638	1.655367
C	-5.326037	0.753578	1.183669
C	-3.247526	1.850329	0.635938

C	-3.326073	0.234804	2.426750
C	-4.681602	0.036521	2.191988
C	-4.608742	1.656962	0.405430
H	-2.688287	2.518762	-0.010394
H	-2.817007	-0.334572	3.199527
H	-5.231952	-0.684976	2.786960
H	-5.097445	2.196148	-0.399828
H	-6.383839	0.596548	0.997420
C	-0.735130	3.830917	1.176684
H	-0.065224	4.594311	1.580866
H	-1.751233	4.039982	1.511169
H	-0.686624	3.861076	0.087939

RS epoxide:Catalyst, binary complex 113; Energy = -2449.840572; 6-31G(d) basis set.

N	3.682894	0.834225	-0.484692
C	2.563037	1.560145	-0.663710
S	2.498204	2.686202	-1.915575
C	3.979175	-0.187355	0.520306
C	5.115886	-1.091683	0.015435
C	5.559460	-2.032087	1.150909
C	5.949452	-1.312105	2.438853
C	4.779343	-0.467484	2.934400
C	4.359123	0.508944	1.840673
N	4.781618	-1.928625	-1.147039
C	5.972362	-2.225728	-1.924910
N	1.568323	1.291117	0.238561
C	0.243057	1.735522	0.343994
C	-0.536541	1.078936	1.311346
C	-1.860065	1.436128	1.510257
C	-2.451276	2.451509	0.765126
C	-1.673879	3.092570	-0.188549
C	-0.340480	2.757347	-0.412563
C	-2.700093	0.726869	2.535229
F	-3.188694	1.590688	3.439279
C	-2.315406	4.121023	-1.078578
F	-2.849648	3.544756	-2.168467
C	3.697622	-1.533327	-2.035146
F	-3.766130	0.136873	1.963057
F	-2.020713	-0.210103	3.200343
F	-3.309522	4.765611	-0.450522
F	-1.439632	5.037019	-1.504770
H	4.420152	1.067630	-1.138844
H	1.762954	0.520443	0.867245
H	5.190701	1.191813	1.621884
H	3.522981	1.137971	2.167998
H	3.937400	-1.124370	3.191961
H	5.044771	0.084888	3.841401
H	6.251127	-2.042702	3.196485
H	6.816626	-0.662506	2.257549
H	4.720828	-2.712841	1.346758
H	6.386079	-2.654155	0.794227
H	3.095088	-0.828071	0.658344
H	5.957196	-0.409435	-0.228763
H	2.777665	-1.341588	-1.482399
H	3.920410	-0.649254	-2.658386
H	3.507428	-2.372205	-2.713363
H	6.348849	-1.341510	-2.472419
H	5.746164	-3.006879	-2.656909
H	6.775990	-2.592363	-1.281002
H	-0.113093	0.269146	1.898795
H	-3.487555	2.730956	0.924139
H	0.234568	3.282074	-1.162044
N	0.034310	-1.126582	-0.813242
O	0.784305	-1.540914	0.056361
O	0.381203	-0.570468	-1.832465
C	-1.446285	-1.339696	-0.615097
C	-1.781497	-2.707299	-0.145882
H	-0.937467	-3.382632	-0.006781
O	-1.746479	-1.572790	0.716947
C	-3.105280	-3.327048	-0.421726
C	-5.562880	-4.520223	-0.965250
C	-4.271788	-2.801760	0.135786
C	-3.168041	-4.455889	-1.240657
C	-4.396246	-5.048100	-1.515523
C	-5.497948	-3.400989	-0.138225

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H         -4.206923       -1.937442        0.789955
H         -2.255184       -4.870787       -1.660550
H         -4.441253       -5.924399       -2.154269
H         -6.404684       -2.995077        0.299109
H         -6.520933       -4.985322       -1.175263
C         -2.299371       -0.444101       -1.459206
H         -2.007679        0.601190       -1.327633
H         -3.337704       -0.572370       -1.150298
H         -2.197594       -0.705314       -2.513622

RS epoxide:Catalyst, binary complex 114; Energy = -2449.843869; 6-31G(d) basis set.
N          3.757619       -0.344071        1.121410
C          3.777790        0.732380        1.940042
S          5.152121        1.167921        2.806570
C          2.608753       -1.232965        0.860565
C          3.100391       -2.451821        0.044011
C          1.942652       -3.440771       -0.159326
C          1.304444       -3.876529        1.158620
C          0.813702       -2.660641        1.941808
C          1.961026       -1.680944        2.179685
N          3.730046       -2.164577       -1.242145
C          5.134657       -1.799546       -1.217583
N          2.628483        1.468156        2.072557
C          1.628085        1.705992        1.102837
C          0.331178        1.981824        1.531976
C         -0.650924        2.302164        0.598757
C         -0.369662        2.321335       -0.758633
C          0.923225        2.019141       -1.173908
C          1.929711        1.740234       -0.260858
C         -2.036594        2.602213        1.097908
F         -2.864678        2.971586        0.115064
C          1.194088        1.911611       -2.646591
F          0.528642        2.842574       -3.344005
C          2.980888       -1.283786       -2.118040
F         -2.585043        1.532874        1.705213
F         -2.023134        3.587041        2.009104
F          2.495273        2.035900       -2.934184
F          0.794953        0.715998       -3.119966
H          4.657609       -0.811554        1.118614
H          2.693131        2.157596        2.812274
H          2.734966       -2.159395        2.796852
H          1.610003       -0.803051        2.732827
H          0.022626       -2.155501        1.370570
H          0.378988       -2.962300        2.900785
H          0.480178       -4.571265        0.963933
H          2.042778       -4.420954        1.763731
H          1.175163       -2.977024       -0.791907
H          2.337320       -4.298845       -0.711666
H          1.870038       -0.700476        0.254202
H          3.862748       -2.962728        0.654349
H          1.923441       -1.555695       -2.146913
H          3.054787       -0.224515       -1.818173
H          3.380866       -1.363064       -3.134776
H          5.317851       -0.740913       -0.962765
H          5.566755       -1.972266       -2.209772
H          5.674203       -2.432328       -0.505084
H          0.096393        1.955259        2.592819
H         -1.147895        2.543475       -1.479205
H          2.944953        1.549326       -0.593434
N         -0.984010       -1.262334       -1.556930
O         -0.689987       -2.042384       -2.439969
O         -0.204639       -0.759746       -0.771315
C         -2.446676       -0.915147       -1.399711
C         -2.861392       -0.736934        0.011018
H         -2.082966       -0.875334        0.760642
O         -2.605038        0.356746       -0.863697
C         -4.271356       -0.945160        0.439932
C         -6.898540       -1.341888        1.270289
C         -5.224270        0.050780        0.228951
C         -4.628906       -2.135172        1.075465
C         -5.942747       -2.333519        1.486681
C         -6.537627       -0.150696        0.645141
H         -4.922379        0.980208       -0.244481
H         -3.879167       -2.903696        1.246404
H         -6.221001       -3.260514        1.977984
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H         -7.278767        0.626217        0.486279
H         -7.922924       -1.496688        1.594358
C         -3.307346       -1.368057       -2.536062
H         -3.262718       -2.452768       -2.641458
H         -2.975910       -0.908592       -3.469963
H         -4.334116       -1.064844       -2.325424

RS epoxide:Catalyst, binary complex 115; Energy = -2449.842338; 6-31G(d) basis set.
N         -1.075344        1.436137       -0.030591
C         -1.069255        1.060553       -1.319558
S         -2.423785        1.355998       -2.301553
C         -0.008161        1.610695        0.961008
C          0.116070        3.093083        1.385735
C          1.223058        3.210426        2.445930
C          0.989164        2.294735        3.648829
C          0.835064        0.838514        3.210687
C         -0.279499        0.714108        2.174914
N          0.346853        4.047227        0.306056
C         -0.845898        4.550756       -0.359303
N          0.023489        0.465617       -1.881261
C          1.167449       -0.109894       -1.270955
C          1.038353       -1.102863       -0.298491
C          2.175695       -1.586550        0.336963
C          3.445413       -1.137589       -0.017674
C          3.559964       -0.192507       -1.028898
C          2.432175        0.328206       -1.655865
C          2.031772       -2.639928        1.401577
F          3.076206       -2.634166        2.240094
C          4.904261        0.355444       -1.420020
F          5.057225        0.362468       -2.751477
C          1.357428        3.659728       -0.660239
F          0.923943       -2.450272        2.134911
F          1.953041       -3.871668        0.876896
F          5.046631        1.624526       -1.006263
F          5.907268       -0.355571       -0.895038
H         -1.977812        1.818817        0.248806
H         -0.053859        0.379800       -2.887613
H         -1.238869        1.017340        2.620889
H         -0.392326       -0.326512        1.851794
H          1.777048        0.481123        2.768401
H          0.622671        0.192176        4.068256
H          1.813186        2.396911        4.362495
H          0.075141        2.607890        4.171531
H          2.189415        2.958329        1.987018
H          1.282187        4.258475        2.753230
H          0.943526        1.328275        0.509163
H         -0.833484        3.380613        1.861964
H          1.007624        2.887593       -1.371249
H          1.646064        4.537527       -1.247361
H          2.256057        3.284059       -0.160144
H         -1.299883        3.842116       -1.071746
H         -0.583098        5.457640       -0.915134
H         -1.597224        4.822200        0.388112
H          0.051619       -1.465896       -0.026934
H          4.327959       -1.516370        0.485040
H          2.530691        1.096895       -2.417255
N         -4.733809        0.944070        0.089045
O         -4.111938        1.510092        0.973872
O         -5.564375        1.462445       -0.620040
C         -4.463696       -0.534214       -0.126313
C         -3.197720       -0.995708        0.449028
H         -2.615946       -0.251418        0.985042
O         -4.464684       -1.229770        1.083089
C         -2.418803       -2.148169       -0.087883
C         -0.716964       -4.164812       -0.993312
C         -2.091579       -2.230053       -1.443472
C         -1.899931       -3.084872        0.810811
C         -1.053973       -4.092324        0.357878
C         -1.241998       -3.239266       -1.892835
H         -2.476808       -1.483575       -2.134070
H         -2.150094       -3.010763        1.866024
H         -0.638723       -4.805981        1.061881
H         -0.982880       -3.295041       -2.945697
H         -0.041327       -4.939991       -1.341354
C         -5.193154       -1.103605       -1.301758
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H         -6.270173       -0.988530       -1.164625
H         -4.947547       -2.164088       -1.374741
H         -4.893147       -0.590283       -2.217784

RS epoxide:Catalyst, binary complex 116; Energy = -2449.839261; 6-31G(d) basis set.
N          3.651100        0.542144       -0.714190
C          3.664957        1.840886       -0.323436
S          4.977536        2.844971       -0.576719
C          3.149131       -0.552141        0.139057
C          2.935236       -1.847763       -0.670522
C          2.467329       -2.931251        0.314298
C          3.494739       -3.174298        1.421318
C          3.757395       -1.899880        2.217999
C          4.150367       -0.756584        1.286774
N          2.015009       -1.626582       -1.805192
C          1.099954       -2.727551       -2.090911
N          2.542136        2.321529        0.324299
C          1.188904        2.135566       -0.017198
C          0.753232        1.281451       -1.032288
C         -0.604701        1.222692       -1.332162
C         -1.547755        1.987963       -0.661618
C         -1.098341        2.819045        0.362590
C          0.246099        2.898035        0.689404
C         -1.071014        0.216048       -2.342832
F         -1.270970       -0.980340       -1.745202
C         -2.124990        3.565101        1.166995
F         -2.970799        4.241024        0.380964
C          2.742417       -1.313856       -3.032849
F         -2.232681        0.564575       -2.903138
F         -0.181804        0.016720       -3.321665
F         -2.865179        2.707501        1.891255
F         -1.569688        4.434802        2.018779
H          4.528308        0.306897       -1.171084
H          2.729057        3.228783        0.736455
H          5.135047       -0.966519        0.844309
H          4.247838        0.185968        1.838793
H          2.848183       -1.629923        2.766210
H          4.544274       -2.059223        2.962432
H          3.136937       -3.970564        2.082632
H          4.433024       -3.528807        0.973253
H          1.512061       -2.622565        0.763671
H          2.289307       -3.866767       -0.221687
H          2.171218       -0.255884        0.535555
H          3.922018       -2.173158       -1.057926
H          3.380688       -0.440516       -2.897653
H          3.368782       -2.159558       -3.368793
H          2.025388       -1.080695       -3.824159
H          1.619487       -3.654606       -2.390476
H          0.451655       -2.422091       -2.915232
H          0.462541       -2.939721       -1.231242
H          1.442439        0.644235       -1.575215
H         -2.602666        1.928579       -0.915548
H          0.567713        3.554185        1.492493
N         -4.047279       -1.095826       -1.302217
O         -4.014652       -1.654837       -2.378094
O         -4.521434        0.003583       -1.091050
C         -3.435495       -1.828843       -0.124670
C         -2.934206       -0.931857        0.939289
H         -3.055065        0.135429        0.761261
O         -4.176726       -1.627692        1.034204
C         -1.839629       -1.306997        1.872558
C          0.227715       -1.873447        3.659599
C         -0.722023       -0.472703        1.941178
C         -1.923885       -2.421872        2.706882
C         -0.886434       -2.707350        3.591384
C          0.304705       -0.750558        2.835989
H         -0.670350        0.409162        1.310044
H         -2.814309       -3.043309        2.678775
H         -0.957104       -3.572993        4.242421
H          1.157022       -0.078221        2.898444
H          1.025800       -2.089100        4.364014
C         -2.940823       -3.197784       -0.470990
H         -2.251038       -3.148683       -1.313178
H         -2.428591       -3.617102        0.395914
H         -3.781722       -3.840903       -0.740315
```

RS epoxide:Catalyst, binary complex 117; Energy = -2449.837866; 6-31G(d) basis set.

N	1.889952	-1.349223	-0.346942
C	0.641606	-0.905963	-0.529557
S	0.351976	0.533004	-1.371657
C	2.363963	-2.454915	0.485134
C	3.850121	-2.686370	0.169838
C	4.435855	-3.705326	1.161063
C	4.235671	-3.323413	2.624799
C	2.747125	-3.149451	2.913745
C	2.160339	-2.103489	1.970459
N	4.138222	-3.175178	-1.190696
C	5.445909	-2.714023	-1.630712
N	-0.346756	-1.707965	-0.020014
C	-1.726803	-1.424262	0.007025
C	-2.195290	-0.176960	0.424898
C	-3.559847	0.066359	0.461200
C	-4.480902	-0.925612	0.134924
C	-4.002334	-2.173569	-0.240539
C	-2.635257	-2.427566	-0.318262
C	-4.047931	1.439968	0.828477
F	-5.213132	1.393100	1.486917
C	-4.972165	-3.252607	-0.633925
F	-4.482713	-4.473791	-0.374627
C	3.168646	-2.985364	-2.259448
F	-3.166556	2.094167	1.599584
F	-4.244175	2.198533	-0.262673
F	-6.135028	-3.132471	0.020352
F	-5.251324	-3.211564	-1.944920
H	2.606931	-0.774690	-0.781071
H	-0.091515	-2.659741	0.216398
H	2.650264	-1.137339	2.141204
H	1.092445	-1.954579	2.163156
H	2.233357	-4.111132	2.776728
H	2.579339	-2.842966	3.951229
H	4.671819	-4.089321	3.274359
H	4.759732	-2.382477	2.839973
H	3.949971	-4.668939	0.958440
H	5.498758	-3.842387	0.939201
H	1.816026	-3.378218	0.233674
H	4.332990	-1.702270	0.332036
H	3.076399	-1.943757	-2.613847
H	3.491465	-3.594161	-3.110430
H	2.178398	-3.337322	-1.963162
H	6.201428	-2.916943	-0.867077
H	5.456475	-1.630384	-1.845650
H	5.735711	-3.249270	-2.540097
H	-1.490674	0.586097	0.727815
H	-5.547046	-0.733899	0.190560
H	-2.279737	-3.404154	-0.633107
N	3.419412	1.435319	-0.164120
O	3.802426	0.846722	-1.162474
O	3.429353	0.971587	0.956829
C	2.862008	2.827065	-0.348445
C	1.748383	3.137742	0.573880
H	1.457290	2.328188	1.241249
O	3.083152	3.602214	0.783835
C	0.705712	4.150761	0.255418
C	-1.289591	6.018654	-0.299082
C	1.034194	5.498315	0.101779
C	-0.625053	3.744180	0.142756
C	-1.620258	4.674396	-0.136812
C	0.036385	6.428293	-0.177122
H	2.067530	5.811927	0.218613
H	-0.875928	2.694542	0.262123
H	-2.650446	4.343487	-0.220614
H	0.294514	7.476491	-0.292109
H	-2.065631	6.747208	-0.512496
C	3.068226	3.374362	-1.724095
H	4.133810	3.451397	-1.952027
H	2.612775	4.364158	-1.773823
H	2.590756	2.718538	-2.453915

RS epoxide:Catalyst, binary complex 118; Energy = -2449.847713; 6-31G(d) basis set.

N	2.340295	-0.846719	-1.191889

```
C          1.250485       -0.138331       -1.565285
S          1.307529        1.406558       -2.200286
C          3.694828       -0.309077       -1.123300
C          4.501520       -1.241413       -0.198638
C          5.921265       -0.687388       -0.024930
C          6.623076       -0.562416       -1.380839
C          5.804440        0.302489       -2.341595
C          4.378585       -0.231738       -2.491243
N          3.761365       -1.530082        1.038264
C          3.779475       -0.435517        2.005753
N          0.093470       -0.856875       -1.351607
C         -1.238722       -0.446309       -1.233652
C         -1.638682        0.873469       -0.980541
C         -2.984994        1.139619       -0.771638
C         -3.953908        0.140957       -0.794817
C         -3.540765       -1.160607       -1.041066
C         -2.203224       -1.457113       -1.265089
C         -3.425954        2.533049       -0.424863
F         -4.467887        2.926974       -1.166680
C         -4.539420       -2.281724       -0.990286
F         -5.766887       -1.869616       -1.330225
C          4.194119       -2.768092        1.672400
F         -3.826527        2.594031        0.863897
F         -2.448609        3.433287       -0.571048
F         -4.202028       -3.288292       -1.807994
F         -4.631237       -2.802146        0.247689
H          2.195081       -1.569441       -0.486373
H          0.229201       -1.842905       -1.158045
H          4.396104       -1.239828       -2.927739
H          3.790711        0.406979       -3.154464
H          5.761962        1.330789       -1.958257
H          6.289639        0.349888       -3.321808
H          7.625110       -0.142245       -1.245690
H          6.752714       -1.563279       -1.814838
H          5.870543        0.302638        0.446932
H          6.494645       -1.336867        0.647071
H          3.643042        0.703984       -0.695076
H          4.577992       -2.205521       -0.725503
H          4.139001       -3.592985        0.955988
H          5.222262       -2.714943        2.067442
H          3.526948       -2.993407        2.510908
H          4.764101       -0.316868        2.485774
H          3.042169       -0.636560        2.790318
H          3.506200        0.511935        1.532630
H         -0.911853        1.675170       -0.934570
H         -5.000394        0.374177       -0.629098
H         -1.904701       -2.484227       -1.455426
N          1.194666        2.835022        0.954223
O          2.381893        2.607867        0.856188
O          0.574093        3.670562        0.328080
C          0.380265        1.976641        1.903609
C          0.598639        0.538699        1.652874
H          1.360628        0.319296        0.903819
O          1.175347        1.245519        2.766428
C         -0.358984       -0.581395        1.882111
C         -2.023676       -2.819597        2.086187
C         -1.733895       -0.420643        2.068746
C          0.174272       -1.872466        1.795782
C         -0.652714       -2.987208        1.899384
C         -2.559281       -1.536931        2.174315
H         -2.180512        0.567786        2.074806
H          1.246415       -1.991841        1.631700
H         -0.228769       -3.984381        1.828889
H         -3.630041       -1.403056        2.290484
H         -2.676978       -3.684355        2.145380
C         -0.815362        2.705516        2.445400
H         -0.494497        3.671252        2.844717
H         -1.241194        2.115633        3.257133
H         -1.564965        2.884245        1.675544

RS epoxide:Catalyst, binary complex 119; Energy = -2449.838059; 6-31G(d) basis set.
N          1.890577       -1.348046       -0.358180
C          0.643815       -0.902145       -0.544813
S          0.360338        0.540901       -1.381920
C          2.358763       -2.457804        0.471825
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C          3.846412       -2.689616        0.164136
C          4.424882       -3.714222        1.153758
C          4.216874       -3.339026        2.618151
C          2.726956       -3.163939        2.899320
C          2.147287       -2.112659        1.957552
N          4.142443       -3.171849       -1.197031
C          5.452506       -2.708200       -1.627103
N         -0.348265       -1.704933       -0.043361
C         -1.727594       -1.418290       -0.020135
C         -2.194347       -0.170773        0.401325
C         -3.557246        0.079736        0.423091
C         -4.480800       -0.905679        0.081024
C         -4.004911       -2.153775       -0.293837
C         -2.637640       -2.414055       -0.360873
C         -4.043269        1.455889        0.783055
F         -3.160753        2.113231        1.550292
C         -4.967747       -3.267900       -0.594342
F         -4.522254       -4.049173       -1.588942
C          3.178878       -2.977806       -2.270399
F         -4.239793        2.208816       -0.311949
F         -5.208238        1.413879        1.442413
F         -5.142783       -4.062100        0.473793
F         -6.173482       -2.805059       -0.945595
H          2.610406       -0.772123       -0.785745
H         -0.095701       -2.658268        0.189626
H          2.637958       -1.148158        2.135334
H          1.078600       -1.962766        2.144955
H          2.212397       -4.124104        2.754867
H          2.553692       -2.862048        3.937241
H          4.647987       -4.108794        3.266513
H          4.741305       -2.400063        2.840888
H          3.938558       -4.676050        0.943781
H          5.488775       -3.851913        0.937091
H          1.811186       -3.379316        0.213193
H          4.329504       -1.706967        0.334122
H          3.088665       -1.934836       -2.621294
H          3.506292       -3.583352       -3.121958
H          2.186991       -3.330824       -1.980899
H          6.203681       -2.915281       -0.860254
H          5.464205       -1.623359       -1.835985
H          5.747552       -3.238420       -2.537757
H         -1.488816        0.587953        0.712698
H         -5.545811       -0.704291        0.113580
H         -2.284595       -3.385934       -0.693046
N          3.418542        1.436441       -0.146697
O          3.420521        0.963011        0.970250
O          3.807641        0.856298       -1.147590
C          2.863006        2.830044       -0.322339
C          1.738115        3.129717        0.589966
H          1.439293        2.311834        1.243704
O          3.070047        3.592556        0.820979
C          0.698896        4.146177        0.271302
C         -1.290422        6.020397       -0.283975
C          1.029408        5.494914        0.132716
C         -0.631098        3.741670        0.143579
C         -1.623289        4.675051       -0.136271
C          0.034701        6.428000       -0.146738
H          2.061702        5.807003        0.262167
H         -0.884078        2.691316        0.251516
H         -2.652917        4.345599       -0.231925
H          0.294529        7.477025       -0.249746
H         -2.064127        6.751364       -0.497623
C          3.085237        3.392375       -1.689442
H          4.153377        3.471479       -1.904339
H          2.630740        4.382867       -1.733608
H          2.615954        2.744974       -2.431948

RS epoxide:Catalyst, binary complex 120; Energy = -2449.849176; 6-31G(d) basis set.
N         -1.518383       -0.866180        0.540461
C         -0.277758       -1.325923        0.260044
S          0.049757       -2.941318       -0.074315
C         -2.680379       -1.724797        0.730788
C         -3.683286       -0.974568        1.622782
C         -4.847761       -1.917057        1.958469
C         -5.543237       -2.368608        0.669352
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C	-4.555212	-3.034571	-0.291965
C	-3.361495	-2.121279	-0.581486
N	-3.004977	-0.323198	2.745950
C	-2.402916	-1.244942	3.699607
N	0.665451	-0.329335	0.284974
C	2.066545	-0.429789	0.185360
C	2.824194	0.418204	1.001955
C	4.207566	0.405792	0.926484
C	4.871699	-0.452478	0.054352
C	4.110653	-1.279989	-0.757945
C	2.717878	-1.271790	-0.714391
C	5.019442	1.349458	1.766601
F	6.075811	0.732404	2.317556
C	4.779125	-2.178622	-1.760084
F	4.251793	-3.410161	-1.749725
C	-3.845019	0.651845	3.419808
F	5.505100	2.363637	1.034280
F	4.300091	1.887036	2.761226
F	4.637269	-1.708396	-3.010657
F	6.093819	-2.297124	-1.529058
H	-1.585102	-0.003553	1.082270
H	0.340401	0.602963	0.537715
H	-3.699469	-1.210760	-1.094050
H	-2.633761	-2.620287	-1.227933
H	-4.191624	-3.971654	0.151436
H	-5.057760	-3.301146	-1.227723
H	-6.369210	-3.048692	0.903344
H	-5.982404	-1.489242	0.176348
H	-4.469936	-2.794972	2.499758
H	-5.562274	-1.412420	2.618958
H	-2.352618	-2.644769	1.234100
H	-4.091526	-0.152746	1.016082
H	-4.270197	1.342252	2.684059
H	-4.674698	0.199468	3.989028
H	-3.235251	1.230592	4.120435
H	-3.146337	-1.839204	4.256249
H	-1.819422	-0.670709	4.425516
H	-1.719966	-1.929496	3.187627
H	2.324581	1.085591	1.696613
H	5.955010	-0.474317	0.012708
H	2.146067	-1.918400	-1.366824
N	0.429060	3.373159	-0.777965
O	1.178546	2.501324	-0.380170
O	0.768411	4.426396	-1.271425
C	-1.056280	3.109797	-0.683522
C	-1.444505	1.760693	-1.164835
H	-0.628498	1.135935	-1.531208
O	-1.323041	2.089323	0.224053
C	-2.801681	1.432157	-1.672475
C	-5.317645	0.718451	-2.640597
C	-2.925898	0.846445	-2.933539
C	-3.939055	1.656253	-0.895257
C	-5.194534	1.298342	-1.379087
C	-4.182206	0.495650	-3.417529
H	-2.037806	0.650869	-3.528573
H	-3.830559	2.083425	0.098141
H	-6.075630	1.465830	-0.766853
H	-4.273747	0.036840	-4.396659
H	-6.296149	0.435111	-3.015163
C	-1.882138	4.357808	-0.699862
H	-1.650301	4.971146	0.174299
H	-2.937964	4.088266	-0.683454
H	-1.670860	4.932243	-1.601588

RS epoxide:Catalyst, binary complex 121; Energy = -2449.846133; 6-31G(d) basis set.

N	3.426518	-0.434205	-0.970720
C	3.519712	-1.779879	-1.042574
S	4.965137	-2.558265	-1.404950
C	2.262414	0.403507	-1.308868
C	2.715650	1.880317	-1.336957
C	1.513541	2.768444	-1.689539
C	0.833396	2.354593	-2.995916
C	0.435348	0.879505	-2.969876
C	1.642838	0.000313	-2.653350
N	3.354710	2.377384	-0.121714

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C          4.789522        2.206770        0.000010
N          2.382589       -2.518722       -0.828294
C          1.294184       -2.221728        0.015189
C          1.448549       -1.442346        1.164235
C          0.354198       -1.210041        1.986151
C         -0.885022       -1.782319        1.718909
C         -1.021919       -2.564261        0.579262
C          0.048684       -2.774886       -0.283345
C          0.497624       -0.282722        3.160320
F          0.226498        0.993056        2.809469
C         -2.345439       -3.211987        0.281424
F         -3.367269       -2.489403        0.765223
C          2.677396        2.058746        1.119671
F         -0.355066       -0.594337        4.145090
F          1.735757       -0.290691        3.659958
F         -2.536588       -3.340974       -1.042714
F         -2.436586       -4.436126        0.813309
H          4.324045        0.002323       -1.147261
H          2.498060       -3.495475       -1.072200
H          2.407817        0.108653       -3.434878
H          1.353057       -1.055506       -2.631819
H         -0.329944        0.715287       -2.200394
H         -0.008315        0.579971       -3.925149
H         -0.045686        2.984312       -3.177757
H          1.521605        2.524735       -3.835584
H          0.791713        2.720677       -0.864499
H          1.868943        3.801818       -1.740513
H          1.500698        0.311711       -0.524824
H          3.456537        1.978232       -2.145914
H          1.593795        2.131252        1.004441
H          2.926479        1.046890        1.489807
H          2.979761        2.771439        1.895075
H          5.094229        1.210816        0.370829
H          5.179962        2.942167        0.712667
H          5.273547        2.387936       -0.964764
H          2.421902       -1.028535        1.406777
H         -1.724686       -1.627732        2.386875
H         -0.078253       -3.364068       -1.186693
N         -1.283652        2.978162        1.784286
O         -0.330587        3.539344        1.282806
O         -1.834716        3.300953        2.816305
C         -1.869606        1.799899        1.043904
C         -1.891659        1.982029       -0.426310
H         -1.482955        2.924694       -0.791835
O         -0.924059        1.169266        0.242968
C         -2.904656        1.311721       -1.284867
C         -4.852996        0.106476       -2.870129
C         -2.947051       -0.077464       -1.404361
C         -3.828345        2.098422       -1.974874
C         -4.803140        1.495144       -2.762954
C         -3.922337       -0.679048       -2.193835
H         -2.199499       -0.672187       -0.886908
H         -3.784618        3.181463       -1.892065
H         -5.521982        2.109231       -3.296016
H         -3.952511       -1.759960       -2.278255
H         -5.614109       -0.362789       -3.485559
C         -2.842819        1.007149        1.859296
H         -3.711357        1.618523        2.108380
H         -2.371654        0.679781        2.789257
H         -3.164148        0.139900        1.279738

RS epoxide:Catalyst, binary complex 122; Energy = -2449.842673; 6-31G(d) basis set.
N          2.553757        0.064685       -1.494966
C          1.480010       -0.736134       -1.360315
S          1.539325       -2.400368       -1.107136
C          3.958955       -0.237806       -1.190611
C          4.151991       -0.762583        0.247705
C          5.642589       -1.030656        0.510827
C          6.229044       -1.992686       -0.523460
C          6.070308       -1.415013       -1.930320
C          4.596050       -1.155605       -2.241680
N          3.495301        0.127000        1.217288
C          4.335240        1.215852        1.701597
N          0.295184       -0.042178       -1.489880
C         -1.024780       -0.448136       -1.237751
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C         -1.373392       -1.418495       -0.289516
C         -2.712992       -1.685929       -0.045907
C         -3.730196       -0.993015       -0.695083
C         -3.371523       -0.005772       -1.601175
C         -2.037485        0.258886       -1.889635
C         -3.075280       -2.761532        0.940710
F         -2.126378       -2.934313        1.870320
C         -4.431259        0.879740       -2.185409
F         -5.609341        0.254802       -2.295231
C          2.936899       -0.605320        2.342420
F         -4.222333       -2.477867        1.580228
F         -3.253961       -3.945122        0.334284
F         -4.632497        1.958456       -1.401159
F         -4.095499        1.341252       -3.397153
H          2.373120        1.042287       -1.695978
H          0.374051        0.926016       -1.789072
H          4.050349       -2.103994       -2.254133
H          4.477372       -0.696578       -3.229203
H          6.636280       -0.475163       -1.999301
H          6.490901       -2.095316       -2.678102
H          7.284907       -2.182941       -0.303087
H          5.709129       -2.958408       -0.466474
H          6.206330       -0.089092        0.470840
H          5.761689       -1.430371        1.525380
H          4.452106        0.742287       -1.249246
H          3.634780       -1.724008        0.304498
H          2.220868       -1.351987        1.981262
H          3.701592       -1.118557        2.953075
H          2.410409        0.100295        2.996717
H          5.121488        0.871392        2.394985
H          3.703949        1.943729        2.217317
H          4.813350        1.730149        0.864140
H         -0.605786       -1.941055        0.263803
H         -4.772669       -1.195133       -0.474788
H         -1.782834        1.028382       -2.613600
N          1.662573        2.906141       -0.314038
O          1.188907        2.823297       -1.446502
O          2.838167        2.945214       -0.061245
C          0.650984        2.910677        0.806938
C          0.412086        1.554258        1.322550
H          1.078305        0.774601        0.941907
O          1.181913        2.565122        2.027017
C         -0.906403        1.122765        1.868928
C         -3.346838        0.182259        2.846886
C         -0.935253        0.212931        2.927875
C         -2.106221        1.539909        1.287670
C         -3.322667        1.078240        1.781221
C         -2.151680       -0.254101        3.415581
H         -0.002180       -0.134809        3.363115
H         -2.096059        2.201508        0.426245
H         -4.246476        1.400512        1.310357
H         -2.166979       -0.968009        4.232883
H         -4.293938       -0.192058        3.221626
C         -0.266862        4.096460        0.708013
H          0.323407        5.010112        0.824712
H         -0.995645        4.043592        1.516711
H         -0.778473        4.119883       -0.255333

RS epoxide:Catalyst, binary complex 123; Energy = -2449.842858; 6-31G(d) basis set.
N          3.589507       -1.068115        0.922465
C          3.832273       -0.176126        1.906169
S          5.287149       -0.158461        2.754548
C          2.288487       -1.628863        0.518954
C          2.540787       -2.797423       -0.459630
C          1.194599       -3.398488       -0.891576
C          0.319513       -3.809395        0.294033
C          0.120210       -2.645613        1.264988
C          1.471543       -2.105011        1.726810
N          3.340222       -2.481853       -1.641815
C          4.779238       -2.630799       -1.531871
N          2.845359        0.717590        2.227742
C          1.858529        1.272977        1.381676
C          2.133241        1.592712        0.051420
C          1.148760        2.193995       -0.724725
C         -0.096445        2.511333       -0.193129
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C         -0.356217        2.186839        1.134054
C          0.604678        1.562504        1.919838
C          1.470792        2.509701       -2.161321
F          2.613997        3.206551       -2.253991
C         -1.675780        2.541213        1.763419
F         -1.590373        3.683917        2.461738
C          2.989455       -1.245932       -2.314242
F          1.637609        1.395583       -2.884895
F          0.506621        3.232454       -2.742756
F         -2.640806        2.714106        0.846499
F         -2.090550        1.594732        2.615600
H          4.381902       -1.683887        0.783424
H          3.046450        1.237937        3.073598
H          2.039861       -2.888811        2.247149
H          1.333323       -1.284146        2.437101
H         -0.424004       -1.828347        0.772599
H         -0.475313       -2.958902        2.128877
H         -0.645597       -4.183683       -0.067073
H          0.798380       -4.640712        0.829692
H          0.656637       -2.660319       -1.498582
H          1.407633       -4.254846       -1.538450
H          1.712823       -0.866160       -0.018783
H          3.090429       -3.573153        0.095991
H          1.906240       -1.138286       -2.405242
H          3.377982       -0.353036       -1.791607
H          3.417816       -1.248461       -3.322467
H          5.289679       -1.762000       -1.077652
H          5.204818       -2.757823       -2.533798
H          5.021909       -3.525951       -0.951027
H          3.115702        1.384734       -0.363859
H         -0.843517        3.006182       -0.804780
H          0.384892        1.295467        2.949302
N         -1.203027        0.194911       -1.940351
O         -1.194339        0.835345       -2.970492
O         -0.281708       -0.476902       -1.515080
C         -2.467541        0.239049       -1.115160
C         -2.798311       -1.044416       -0.449404
H         -2.122092       -1.875213       -0.654249
O         -2.178120        0.044013        0.229123
C         -4.189886       -1.382865       -0.045743
C         -6.789613       -2.050222        0.697989
C         -4.836522       -2.458054       -0.656982
C         -4.840692       -0.646402        0.945564
C         -6.139550       -0.983535        1.315445
C         -6.136751       -2.787364       -0.288081
H         -4.321505       -3.036472       -1.419828
H         -4.316847        0.174687        1.427403
H         -6.642860       -0.415620        2.091527
H         -6.638569       -3.621899       -0.767177
H         -7.802406       -2.310731        0.988766
C         -3.450430        1.270255       -1.575958
H         -2.997303        2.262217       -1.599436
H         -4.294162        1.276954       -0.885399
H         -3.802480        1.021752       -2.578454

RS epoxide:Catalyst, binary complex 124; Energy = -2449.845010; 6-31G(d) basis set.
N         -2.878023        0.067285       -0.068309
C         -1.824626       -0.763467       -0.072741
S         -1.865586       -2.336699       -0.657903
C         -4.206778       -0.257086       -0.579164
C         -5.065604       -0.879250        0.547810
C         -5.279597        0.186896        1.632137
C         -5.989311        1.424658        1.077612
C         -5.179393        2.042131       -0.066101
C         -4.866302        1.002215       -1.147504
N         -6.334203       -1.370445       -0.005544
C         -7.251676       -1.807246        1.038865
N         -0.701187       -0.170932        0.481409
C          0.599481       -0.687894        0.589552
C          1.222313       -1.384232       -0.452427
C          2.548499       -1.773516       -0.316803
C          3.283416       -1.483000        0.828207
C          2.658177       -0.777730        1.846352
C          1.328313       -0.386384        1.740411
C          3.196107       -2.541072       -1.436067
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F          2.742315       -2.145947       -2.634982
C          3.431945       -0.333066        3.052347
F          2.787373       -0.613556        4.193187
C         -6.115822       -2.471036       -0.939097
F          4.528970       -2.389445       -1.436894
F          2.950885       -3.855679       -1.339830
F          4.643126       -0.895051        3.114374
F          3.615684        1.004111        3.039050
H         -2.715407        1.035912        0.194838
H         -0.889196        0.611949        1.100137
H         -4.223279        1.429202       -1.924157
H         -5.802071        0.684954       -1.619837
H         -5.723522        2.880054       -0.514626
H         -4.247028        2.470451        0.332700
H         -6.979411        1.137591        0.702231
H         -6.142094        2.161054        1.873932
H         -5.816540       -0.231077        2.488054
H         -4.291227        0.474302        2.013399
H         -4.044618       -0.984022       -1.375535
H         -4.490098       -1.720661        0.982259
H         -5.586182       -2.134819       -1.832802
H         -5.538035       -3.297396       -0.487604
H         -7.084276       -2.861420       -1.262540
H         -6.800855       -2.555198        1.717142
H         -8.130815       -2.258860        0.571796
H         -7.595497       -0.960138        1.636413
H          0.677506       -1.600709       -1.363279
H          4.325169       -1.769979        0.908478
H          0.856589        0.158347        2.554781
N         -0.956435        2.712600       -0.570169
O         -1.365590        2.738035        0.586719
O         -1.620952        2.411990       -1.530814
C          0.516171        3.011901       -0.769650
C          1.210959        1.884078       -1.423261
H          0.572404        1.051828       -1.724184
O          0.844488        3.100326       -2.103839
C          2.658531        1.565253       -1.255366
C          5.340591        0.822075       -1.036833
C          3.312962        0.959435       -2.333485
C          3.349343        1.776888       -0.063294
C          4.690778        1.411334        0.042364
C          4.648200        0.591450       -2.225599
H          2.765585        0.763578       -3.251736
H          2.841887        2.190301        0.802667
H          5.214010        1.566685        0.980782
H          5.144391        0.109459       -3.061745
H          6.381504        0.526321       -0.949831
C          1.032858        4.035372        0.199199
H          0.968001        3.678929        1.227460
H          0.445393        4.952731        0.105472
H          2.070089        4.253316       -0.055378

RS epoxide:Catalyst, binary complex 125; Energy = -2449.852781; 6-31G(d) basis set.
N         -2.422083       -0.878953       -0.612453
C         -1.306039       -1.579912       -0.326748
S         -1.275008       -3.087441        0.408140
C         -3.781704       -1.387491       -0.503989
C         -4.738033       -0.197219       -0.702910
C         -6.194312       -0.680134       -0.625530
C         -6.480157       -1.753083       -1.677949
C         -5.514764       -2.927679       -1.515555
C         -4.063562       -2.451431       -1.573163
N         -4.392160        0.920690        0.185746
C         -4.852794        0.726550        1.557355
N         -0.174488       -0.921940       -0.766102
C          1.168271       -1.112813       -0.416120
C          2.142330       -0.810990       -1.375125
C          3.486583       -0.858727       -1.038723
C          3.894898       -1.210555        0.244345
C          2.919140       -1.509760        1.185478
C          1.563482       -1.465714        0.875282
C          4.532342       -0.555376       -2.073700
F          5.563687        0.122817       -1.543372
C          3.313581       -1.754487        2.613705
F          2.541963       -2.676293        3.199376
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C	-4.852430	2.202850	-0.327144
F	5.042695	-1.674995	-2.608537
F	4.044317	0.177048	-3.084550
F	4.587307	-2.152389	2.724392
F	3.191468	-0.625779	3.340210
H	-2.349129	0.138318	-0.557699
H	-0.340596	-0.203910	-1.462267
H	-3.857873	-2.005437	-2.556264
H	-3.373639	-3.288423	-1.441486
H	-5.697279	-3.417730	-0.549543
H	-5.689193	-3.681296	-2.290415
H	-7.518701	-2.091398	-1.598008
H	-6.360436	-1.321429	-2.681203
H	-6.384939	-1.101922	0.369807
H	-6.872907	0.172434	-0.747340
H	-3.928223	-1.831448	0.491506
H	-4.559373	0.168581	-1.726349
H	-5.951401	2.284493	-0.390462
H	-4.499210	2.997259	0.338826
H	-4.434591	2.374526	-1.324383
H	-5.951391	0.751348	1.642685
H	-4.445419	1.518010	2.190455
H	-4.489324	-0.228913	1.944967
H	1.842604	-0.522689	-2.377986
H	4.946879	-1.232953	0.506616
H	0.817956	-1.687885	1.630459
N	-1.993816	2.318449	1.775441
O	-2.693057	3.187901	2.261728
O	-1.984633	1.152122	2.102268
C	-1.043963	2.739192	0.672050
C	0.114638	1.828179	0.535109
H	0.142430	1.008678	1.251475
O	-1.025213	1.775809	-0.333337
C	1.417246	2.199860	-0.073756
C	3.906561	2.711015	-1.215420
C	2.581402	1.988998	0.667508
C	1.500511	2.654236	-1.391307
C	2.745563	2.906723	-1.959779
C	3.822688	2.254060	0.098532
H	2.517511	1.582306	1.674203
H	0.591636	2.777942	-1.973906
H	2.810219	3.242954	-2.989805
H	4.727964	2.072344	0.669713
H	4.877563	2.887286	-1.666841
C	-1.117582	4.189214	0.319739
H	-2.102612	4.428348	-0.087712
H	-0.351653	4.404351	-0.426905
H	-0.941995	4.804223	1.203154

RS epoxide:Catalyst, binary complex 126; Energy = -2449.841048; 6-31G(d) basis set.

N	2.946659	1.332255	-0.569871
C	1.904093	2.198430	-0.619770
S	2.017181	3.688727	-1.384837
C	3.274282	0.425398	0.545982
C	4.661316	-0.206390	0.285499
C	5.038252	-1.112675	1.467444
C	4.997598	-0.381665	2.809088
C	3.621296	0.237859	3.043832
C	3.254007	1.167862	1.889469
N	4.815376	-0.938798	-0.969369
C	5.182550	-0.165894	-2.142187
N	0.740346	1.820360	-0.003098
C	0.247547	0.502314	0.124111
C	-0.505062	0.167812	1.246428
C	-1.101289	-1.089321	1.330692
C	-0.907299	-2.045916	0.342463
C	-0.111010	-1.713810	-0.753780
C	0.440642	-0.445481	-0.886490
C	-1.961965	-1.373828	2.530462
F	-1.308482	-1.098610	3.669369
C	0.176276	-2.759922	-1.797811
F	-0.865116	-3.570583	-1.993146
C	3.755501	-1.877015	-1.279039
F	-3.061075	-0.590128	2.528778
F	-2.366306	-2.640980	2.584533

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F          0.505663       -2.208619       -2.972291
F          1.211600       -3.534478       -1.422635
H          3.756220        1.715044       -1.045819
H          0.044639        2.561636        0.048126
H          3.973889        1.996439        1.834081
H          2.266646        1.613110        2.049695
H          2.868230       -0.558919        3.122870
H          3.599004        0.790863        3.988370
H          5.254046       -1.072641        3.618795
H          5.756146        0.413226        2.815773
H          4.345922       -1.964684        1.505057
H          6.032918       -1.521360        1.267527
H          2.540411       -0.389333        0.575337
H          5.391900        0.617286        0.258176
H          2.848914       -1.383383       -1.670223
H          4.101560       -2.578325       -2.045679
H          3.474682       -2.459581       -0.398086
H          4.331542        0.346025       -2.624613
H          5.620957       -0.836433       -2.889631
H          5.939834        0.578779       -1.877644
H         -0.641553        0.899398        2.037594
H         -1.384911       -3.017961        0.410991
H          1.006417       -0.178210       -1.773265
N         -3.815477       -1.591662       -0.677224
O         -3.267454       -2.056024       -1.653448
O         -4.086486       -2.202860        0.339967
C         -4.111505       -0.107786       -0.670176
C         -2.934137        0.676299       -1.081848
H         -2.067687        0.092510       -1.393429
O         -4.059679        0.442945       -1.939081
C         -2.647151        2.063070       -0.614799
C         -1.856638        4.600084        0.239359
C         -2.158312        2.992771       -1.535897
C         -2.740739        2.408276        0.735258
C         -2.345169        3.675160        1.161186
C         -1.767186        4.259382       -1.110150
H         -2.067775        2.715464       -2.582477
H         -3.095708        1.675160        1.454970
H         -2.413001        3.936538        2.212573
H         -1.368212        4.969786       -1.825878
H         -1.535573        5.581670        0.572442
C         -5.222519        0.281643        0.257048
H         -4.997050       -0.012117        1.281202
H         -6.147134       -0.209246       -0.058112
H         -5.356373        1.362680        0.196388

RS epoxide:Catalyst, binary complex 127; Energy = -2449.834998; 6-31G(d) basis set.
N         -1.848675        0.724327       -0.363338
C         -1.324656        0.303864       -1.531678
S         -2.217409       -0.558055       -2.664426
C         -1.526446        2.009603        0.283999
C         -2.208204        3.164393       -0.514359
C         -3.694896        3.323039       -0.138056
C         -4.055483        3.180549        1.346913
C         -3.448192        1.913440        1.948071
C         -1.930178        1.921937        1.759408
N         -1.460262        4.420794       -0.528851
C         -0.223208        4.323585       -1.283447
N         -0.004933        0.621173       -1.790015
C          1.101916        0.547334       -0.922000
C          2.367348        0.762215       -1.473551
C          3.503449        0.609586       -0.687939
C          3.413226        0.261572        0.653855
C          2.147069        0.067531        1.195383
C          0.999232        0.201298        0.429407
C          4.853982        0.873876       -1.294032
F          5.213980        2.157994       -1.152352
C          2.024551       -0.238390        2.662691
F          2.911878       -1.163738        3.052757
C         -1.231940        5.071385        0.749021
F          5.806358        0.131187       -0.714506
F          4.869140        0.604619       -2.607309
F          2.257218        0.856986        3.402553
F          0.800890       -0.679999        2.989200
H         -2.804605        0.396930       -0.232393
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H          0.228595        0.445253       -2.760706
H         -1.470758        1.031190        2.206734
H         -1.514113        2.788166        2.285487
H         -3.683702        1.843131        3.014632
H         -3.894465        1.024778        1.479878
H         -3.712630        4.045744        1.925313
H         -5.146166        3.159060        1.442682
H         -4.040320        4.282281       -0.536873
H         -4.245775        2.543301       -0.681647
H         -0.445724        2.150117        0.221348
H         -2.193192        2.840448       -1.563207
H         -2.172059        5.193277        1.289658
H         -0.516213        4.535389        1.398487
H         -0.821281        6.069739        0.566986
H          0.559212        3.715008       -0.791210
H          0.187626        5.327601       -1.427900
H         -0.422195        3.888064       -2.267386
H          2.465333        1.024800       -2.522943
H          4.304809        0.135979        1.258887
H          0.033975        0.001728        0.874974
N         -3.907787       -2.301949       -0.397021
O         -4.681403       -2.604537       -1.275312
O         -4.050934       -1.371354        0.379797
C         -2.666191       -3.158414       -0.241457
C         -1.565993       -2.499067        0.471275
H         -1.761585       -1.487007        0.823125
O         -2.426301       -3.458043        1.098735
C         -0.133494       -2.850720        0.251580
C          2.612167       -3.216364       -0.059685
C          0.454546       -2.685311       -1.003709
C          0.650542       -3.221458        1.345642
C          2.020031       -3.407435        1.188812
C          1.828553       -2.863082       -1.155309
H         -0.162956       -2.392874       -1.851255
H          0.186041       -3.347511        2.319484
H          2.628167       -3.686070        2.043099
H          2.286437       -2.721768       -2.129844
H          3.683871       -3.345776       -0.177559
C         -2.544981       -4.228534       -1.279277
H         -3.407304       -4.896673       -1.238269
H         -1.634178       -4.794320       -1.077826
H         -2.487280       -3.782080       -2.274570

RS epoxide:Catalyst, binary complex 128; Energy = -2449.840313; 6-31G(d) basis set.
N          3.518113       -1.201328        0.297833
C          3.212414       -2.496249        0.046099
S          4.326245       -3.731661        0.259746
C          3.080909       -0.013392       -0.462547
C          4.011143        1.162955       -0.074937
C          3.639712        2.410646       -0.887608
C          3.670492        2.156814       -2.393950
C          2.759597        0.989391       -2.764724
C          3.123385       -0.267224       -1.975914
N          4.079752        1.493459        1.345166
C          5.040865        0.773564        2.159056
N          1.949522       -2.795279       -0.411972
C          0.715887       -2.224150       -0.060272
C          0.562634       -1.350080        1.017994
C         -0.707379       -0.894417        1.357000
C         -1.844250       -1.314296        0.675229
C         -1.675693       -2.192946       -0.391411
C         -0.416497       -2.634793       -0.773735
C         -0.838670        0.120643        2.458314
F         -1.982918       -0.019026        3.137619
C         -2.877731       -2.621798       -1.187378
F         -3.962187       -2.752771       -0.416199
C          2.809642        1.626334        2.029365
F          0.166796        0.041022        3.339040
F         -0.820863        1.370646        1.955012
F         -3.180168       -1.721406       -2.142653
F         -2.671354       -3.789351       -1.809895
H          4.466390       -1.128977        0.649532
H          1.890277       -3.750895       -0.744367
H          4.140399       -0.592497       -2.236276
H          2.448306       -1.089834       -2.234493
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H	1.722009	1.270745	-2.547428
H	2.812282	0.778260	-3.837926
H	3.361992	3.061333	-2.927577
H	4.698954	1.928714	-2.706790
H	2.639512	2.759574	-0.600662
H	4.339474	3.203434	-0.607079
H	2.056090	0.255238	-0.165956
H	5.028838	0.868641	-0.375811
H	2.954205	2.198334	2.952465
H	2.082814	2.164069	1.414494
H	2.376695	0.652217	2.317057
H	4.678778	-0.205048	2.522951
H	5.281976	1.371930	3.044994
H	5.969103	0.621317	1.599315
H	1.425810	-1.060587	1.606364
H	-2.833762	-0.975453	0.970430
H	-0.310490	-3.322010	-1.607816
N	-0.028660	3.064558	-0.989049
O	0.547124	3.358561	-2.017568
O	0.334391	3.352366	0.134620
C	-1.288685	2.240202	-1.150773
C	-2.410632	2.631119	-0.288310
H	-2.215058	3.450413	0.401738
O	-2.319308	3.007657	-1.677675
C	-3.501399	1.698829	0.102892
C	-5.483365	-0.093090	0.908485
C	-3.826490	1.573913	1.454118
C	-4.196862	0.949161	-0.849026
C	-5.180557	0.052418	-0.444705
C	-4.810846	0.675356	1.856523
H	-3.293757	2.164671	2.193738
H	-3.975270	1.081788	-1.903755
H	-5.705136	-0.539843	-1.187549
H	-5.046737	0.573175	2.911112
H	-6.246217	-0.798921	1.221932
C	-0.965608	0.906510	-1.751475
H	-0.595562	1.054296	-2.769276
H	-0.198605	0.397752	-1.156636
H	-1.857814	0.281662	-1.777692

RS epoxide:Catalyst, binary complex 129; Energy = -2449.842082; 6-31G(d) basis set.

N	-3.773296	-0.246643	0.032503
C	-3.970041	-1.240877	0.932683
S	-5.498673	-1.859822	1.253390
C	-2.782846	0.845034	0.113940
C	-3.148765	1.888325	-0.967860
C	-2.251123	3.128112	-0.848426
C	-2.247690	3.722837	0.557618
C	-1.804024	2.668372	1.567307
C	-2.749255	1.469092	1.516093
N	-3.133019	1.407757	-2.349218
C	-4.342361	0.771986	-2.841707
N	-2.876271	-1.732118	1.593619
C	-1.554515	-1.831112	1.103987
C	-0.495691	-1.801665	2.007694
C	0.808565	-1.970779	1.548537
C	1.079533	-2.140426	0.197247
C	0.009051	-2.149891	-0.695593
C	-1.301683	-2.027491	-0.256129
C	1.924426	-1.939742	2.557292
F	3.065182	-2.429088	2.068742
C	0.293296	-2.268476	-2.167746
F	0.664603	-1.076889	-2.684214
C	-1.959346	0.646745	-2.729216
F	2.165149	-0.688495	2.986268
F	1.606075	-2.657210	3.647678
F	1.281114	-3.128947	-2.419024
F	-0.785653	-2.663944	-2.856645
H	-4.653828	0.029302	-0.387965
H	-3.120520	-2.364148	2.347247
H	-3.768639	1.785689	1.777448
H	-2.452606	0.709766	2.247032
H	-0.779837	2.344851	1.328358
H	-1.778252	3.079962	2.581824
H	-1.589359	4.596904	0.593910

H	-3.257445	4.071959	0.815356
H	-1.221028	2.856839	-1.113964
H	-2.593764	3.853411	-1.592512
H	-1.785577	0.450745	-0.120381
H	-4.180304	2.214021	-0.760971
H	-1.047175	1.115599	-2.348489
H	-1.987895	-0.395219	-2.367233
H	-1.885961	0.609979	-3.821322
H	-4.447248	-0.284616	-2.539146
H	-4.338170	0.796298	-3.937136
H	-5.221725	1.326972	-2.499912
H	-0.692600	-1.659884	3.066724
H	2.098910	-2.244656	-0.158989
H	-2.130301	-2.089193	-0.953680
N	4.267805	-0.481433	-1.737998
O	5.210704	-0.217469	-2.455636
O	3.516502	-1.426940	-1.873469
C	3.988774	0.478448	-0.606160
C	2.547921	0.778874	-0.432859
H	1.871614	0.283824	-1.131044
O	3.258747	-0.126223	0.408112
C	2.094759	2.063227	0.166329
C	1.281515	4.504755	1.237492
C	2.262727	2.316700	1.528201
C	1.509719	3.027614	-0.657099
C	1.110361	4.248400	-0.122360
C	1.852977	3.536892	2.060572
H	2.703559	1.551696	2.159252
H	1.376994	2.826234	-1.717943
H	0.660513	4.997199	-0.767837
H	1.979339	3.730213	3.121236
H	0.963437	5.455631	1.654214
C	5.136530	1.380444	-0.277409
H	5.400944	1.990908	-1.141111
H	6.006965	0.790786	0.019132
H	4.839437	2.026952	0.549444

RS epoxide:Catalyst, binary complex 130; Energy = -2449.848035; 6-31G(d) basis set.

N	-4.023758	-1.298106	-1.021393
C	-2.788229	-1.787258	-1.265069
S	-2.535101	-3.438910	-1.469208
C	-4.384790	-0.095417	-0.261530
C	-3.396646	0.280919	0.864710
C	-4.087293	1.338416	1.746447
C	-4.426950	2.581992	0.916399
C	-5.308748	2.234271	-0.284048
C	-4.670896	1.132477	-1.135655
N	-2.846688	-0.889484	1.541166
C	-3.823025	-1.736815	2.204896
N	-1.809680	-0.847512	-1.412889
C	-0.430555	-1.077322	-1.251077
C	0.475073	-0.449674	-2.105759
C	1.839075	-0.607411	-1.891590
C	2.322057	-1.390559	-0.847995
C	1.406282	-2.010841	-0.005316
C	0.036749	-1.856090	-0.190767
C	2.833451	0.080969	-2.782504
F	3.732803	0.771427	-2.061722
C	1.874811	-2.860489	1.142095
F	1.629190	-4.159532	0.931305
C	-1.754949	-0.544925	2.434060
F	3.530013	-0.802574	-3.514793
F	2.250021	0.934634	-3.630267
F	3.187690	-2.729106	1.366943
F	1.238309	-2.532985	2.285269
H	-4.723691	-2.028216	-1.035701
H	-2.085687	0.117302	-1.561547
H	-3.735832	1.507454	-1.575683
H	-5.327522	0.841826	-1.961783
H	-6.288990	1.885092	0.069113
H	-5.489903	3.124122	-0.895346
H	-4.920443	3.330952	1.544846
H	-3.492877	3.030529	0.555728
H	-5.002464	0.919366	2.187458
H	-3.427596	1.615554	2.576392

H	-5.335482	-0.364331	0.217343
H	-2.532810	0.782453	0.407850
H	-2.077130	-0.025848	3.353180
H	-1.220595	-1.453837	2.730015
H	-1.049247	0.107377	1.904144
H	-4.337863	-1.241892	3.046077
H	-3.310992	-2.621583	2.594367
H	-4.573048	-2.084513	1.488767
H	0.115953	0.179538	-2.912719
H	3.388941	-1.487961	-0.675261
H	-0.679262	-2.315519	0.483523
N	-0.577559	2.979178	-0.208171
O	-1.218102	3.859567	0.326217
O	-1.036176	2.111400	-0.930571
C	0.907156	2.942972	0.082480
C	1.416111	1.570494	0.322416
H	0.670120	0.776736	0.264254
O	1.598042	2.265313	-0.909125
C	2.612264	1.265842	1.148142
C	4.819888	0.541734	2.683425
C	3.872963	1.772847	0.832749
C	2.460713	0.386189	2.221104
C	3.562484	0.023201	2.987434
C	4.973050	1.413423	1.607134
H	3.989488	2.413632	-0.036212
H	1.481975	-0.035236	2.437379
H	3.440496	-0.678203	3.806716
H	5.955393	1.802866	1.358943
H	5.683004	0.255092	3.275851
C	1.437542	4.222595	0.648762
H	1.319130	5.033089	-0.074431
H	2.496916	4.088396	0.869921
H	0.907538	4.483526	1.564728

RS epoxide:Catalyst, binary complex 131; Energy = -2449.844329; 6-31G(d) basis set.

N	0.123250	-0.758844	-0.295448
C	0.511884	0.397431	-0.870208
S	2.032786	0.591926	-1.582289
C	-0.780986	-0.909280	0.861334
C	-0.809754	-2.392795	1.286828
C	-1.704470	-2.541582	2.527344
C	-1.307976	-1.611669	3.674252
C	-1.294211	-0.155280	3.212340
C	-0.352964	0.000553	2.020435
N	-1.244295	-3.340515	0.260204
C	-0.215930	-3.893545	-0.601919
N	-0.359132	1.451900	-0.853849
C	-1.773188	1.352456	-0.787821
C	-2.477557	2.110859	0.139120
C	-3.860447	1.962391	0.238985
C	-4.543294	1.065918	-0.568809
C	-3.824079	0.326440	-1.508066
C	-2.451996	0.475117	-1.637687
C	-4.578803	2.747938	1.300362
F	-4.212354	2.341584	2.526878
C	-4.565756	-0.672123	-2.353278
F	-3.791112	-1.198313	-3.307837
C	-2.408727	-2.946871	-0.506150
F	-4.285726	4.053219	1.221271
F	-5.906435	2.619017	1.212006
F	-5.024650	-1.687229	-1.602219
F	-5.631412	-0.117359	-2.945772
H	0.833507	-1.483832	-0.368694
H	0.034424	2.313036	-1.214582
H	0.669510	-0.270791	2.310207
H	-0.324386	1.041429	1.678965
H	-2.308615	0.156310	2.922666
H	-0.979239	0.506653	4.025685
H	-1.995339	-1.745652	4.516223
H	-0.305272	-1.881245	4.032806
H	-2.744489	-2.330058	2.242519
H	-1.670482	-3.590185	2.836732
H	-1.801432	-0.644114	0.564527
H	0.217499	-2.669716	1.565696
H	-2.175154	-2.201140	-1.288231

H	-2.828493	-3.825493	-1.007775
H	-3.186895	-2.532866	0.141222
H	0.095783	-3.218703	-1.419365
H	-0.598206	-4.810209	-1.065665
H	0.668356	-4.149516	-0.013943
H	-1.946162	2.791074	0.799109
H	-5.617116	0.943124	-0.472915
H	-1.897270	-0.098747	-2.373017
N	3.174484	-1.756893	0.570372
O	2.675058	-2.507240	-0.249900
O	2.647704	-1.418299	1.609805
C	4.534790	-1.189714	0.250287
C	4.718545	0.197706	0.725652
H	3.854711	0.643175	1.216329
O	5.253061	-0.934380	1.413069
C	5.681125	1.126622	0.073469
C	7.448048	2.893821	-1.160362
C	5.191290	2.248293	-0.598404
C	7.055942	0.896788	0.136974
C	7.936721	1.780951	-0.480070
C	6.074994	3.126025	-1.218134
H	4.119082	2.421658	-0.640731
H	7.425505	0.032173	0.680535
H	9.006109	1.602555	-0.424655
H	5.691110	3.994447	-1.744351
H	8.136440	3.582724	-1.640079
C	5.177872	-1.819036	-0.943682
H	5.309093	-2.892431	-0.789957
H	6.151250	-1.351702	-1.097147
H	4.553647	-1.655718	-1.823937

RS epoxide:Catalyst, binary complex 132; Energy = -2449.844385; 6-31G(d) basis set.

N	-2.259289	-1.004680	0.550082
C	-1.130844	-0.978577	-0.192166
S	-1.135363	-0.909393	-1.871448
C	-3.604947	-1.037604	-0.005843
C	-4.540745	-1.637757	1.055393
C	-5.939235	-1.803483	0.442024
C	-6.480340	-0.445264	-0.021238
C	-5.520235	0.235514	-1.000919
C	-4.111970	0.345800	-0.414682
N	-3.936390	-2.820498	1.674610
C	-3.721273	-3.935082	0.760808
N	-0.007304	-0.985321	0.601493
C	1.359565	-1.023766	0.286449
C	2.238158	-0.562606	1.278457
C	3.607128	-0.595196	1.071733
C	4.142403	-1.075435	-0.119717
C	3.265403	-1.540951	-1.087723
C	1.885036	-1.534071	-0.902515
C	4.545781	-0.144060	2.155668
F	5.543384	0.601268	1.667507
C	3.802297	-2.132286	-2.361504
F	3.827704	-3.474734	-2.303807
C	-4.647320	-3.256275	2.866054
F	3.924550	0.566508	3.105473
F	5.115592	-1.200178	2.765363
F	3.046324	-1.805222	-3.418044
F	5.053976	-1.726635	-2.613959
H	-2.206718	-1.454575	1.464105
H	-0.183801	-0.719217	1.564175
H	-4.119465	0.992443	0.472603
H	-3.421335	0.792023	-1.136261
H	-5.477012	-0.346723	-1.931525
H	-5.888270	1.232187	-1.267980
H	-7.468737	-0.570045	-0.475817
H	-6.614003	0.200449	0.857886
H	-5.887134	-2.489821	-0.413452
H	-6.619951	-2.250686	1.175117
H	-3.596007	-1.678905	-0.897983
H	-4.621894	-0.897083	1.867263
H	-4.799659	-2.404846	3.536463
H	-5.629901	-3.707180	2.648646
H	-4.045476	-4.004603	3.390835
H	-4.659078	-4.365162	0.372527

H	-3.184426	-4.725740	1.292994
H	-3.102736	-3.622609	-0.085787
H	1.845295	-0.153672	2.204085
H	5.213426	-1.075973	-0.288447
H	1.230349	-1.908080	-1.677028
N	2.558139	2.309522	0.161005
O	2.794933	1.751157	-0.889295
O	3.341846	2.458858	1.078903
C	1.163603	2.848050	0.402872
C	0.086955	2.114720	-0.273735
H	0.395312	1.292427	-0.919567
O	0.410345	1.915736	1.118711
C	-1.235402	2.723993	-0.580877
C	-3.704428	3.852052	-1.218982
C	-1.649830	2.793371	-1.913143
C	-2.064190	3.208481	0.431268
C	-3.295829	3.774032	0.110277
C	-2.879494	3.360879	-2.230451
H	-1.013071	2.387392	-2.694471
H	-1.746012	3.124158	1.466422
H	-3.940577	4.146376	0.900611
H	-3.198594	3.410558	-3.266736
H	-4.665955	4.291202	-1.467248
C	1.185831	4.280623	0.835096
H	1.690197	4.365981	1.799347
H	0.160847	4.644176	0.920144
H	1.716869	4.886990	0.096958

RS epoxide:Catalyst, binary complex 133; Energy = -2449.839215; 6-31G(d) basis set.

N	-3.352640	0.013113	0.965755
C	-3.033965	-0.351217	2.231395
S	-4.194584	-0.489119	3.434800
C	-2.555560	0.866439	0.064922
C	-3.454471	1.296942	-1.119568
C	-2.647898	2.206284	-2.057968
C	-2.093248	3.433226	-1.336256
C	-1.238330	3.022074	-0.140331
C	-2.008483	2.098687	0.800166
N	-4.096762	0.232619	-1.883695
C	-5.359115	-0.282610	-1.386356
N	-1.714860	-0.597446	2.528580
C	-0.712673	-1.171587	1.725926
C	0.606078	-1.118099	2.182252
C	1.614519	-1.759155	1.469230
C	1.346766	-2.435238	0.284455
C	0.030304	-2.468086	-0.165922
C	-0.998965	-1.871001	0.550726
C	3.010707	-1.713172	2.026208
F	3.034062	-2.100351	3.308579
C	-0.322964	-3.170539	-1.449941
F	-1.452036	-3.884256	-1.313502
C	-3.232523	-0.839085	-2.330992
F	3.857083	-2.484156	1.346516
F	3.505018	-0.454754	2.006288
F	-0.547553	-2.290924	-2.441593
F	0.640342	-3.999256	-1.854359
H	-4.353492	0.153121	0.881497
H	-1.564411	-0.689410	3.526695
H	-2.861560	2.634970	1.239265
H	-1.364790	1.784689	1.629038
H	-0.332512	2.506959	-0.489918
H	-0.895874	3.902122	0.410751
H	-1.506544	4.045914	-2.029772
H	-2.927751	4.057440	-0.988604
H	-1.812826	1.636813	-2.489165
H	-3.300601	2.491480	-2.887972
H	-1.718453	0.282667	-0.341803
H	-4.268188	1.906127	-0.695845
H	-2.283308	-0.448461	-2.704089
H	-3.015775	-1.580067	-1.541285
H	-3.717397	-1.377272	-3.152504
H	-5.969876	0.536729	-0.994033
H	-5.251594	-1.054259	-0.603801
H	-5.909948	-0.742184	-2.214718
H	0.837275	-0.600075	3.109498

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H          2.138039       -2.928078       -0.269706
H         -2.027480       -1.969306        0.219975
N          2.880223       -0.855938       -1.867829
O          3.888319       -1.225375       -1.300440
O          2.110670       -1.576500       -2.472704
C          2.529617        0.614881       -1.796072
C          3.130446        1.320307       -0.639987
H          3.726923        0.705187        0.028286
O          3.663842        1.399947       -1.961890
C          2.544375        2.556262       -0.054669
C          1.540091        4.870214        1.133901
C          2.150374        2.541118        1.285667
C          2.431556        3.730813       -0.799526
C          1.928290        4.884641       -0.204099
C          1.646281        3.695318        1.876734
H          2.264567        1.629557        1.865945
H          2.766856        3.740186       -1.832526
H          1.854145        5.800292       -0.782492
H          1.348514        3.681933        2.920683
H          1.156393        5.773682        1.597880
C          1.254651        0.949439       -2.503889
H          0.438647        0.337176       -2.111162
H          1.031579        2.006150       -2.345774
H          1.351020        0.752953       -3.573928

RS epoxide:Catalyst, binary complex 134; Energy = -2449.834952; 6-31G(d) basis set.
N         -1.370129       -1.274376       -1.143290
C         -0.588784       -1.059899       -2.211776
S         -1.191176       -0.568070       -3.701913
C         -1.150163       -2.276912       -0.091339
C         -2.385604       -2.260433        0.828883
C         -2.461887       -3.603525        1.570039
C         -2.819715       -4.726661        0.577614
C         -2.208436       -4.467084       -0.813614
C         -0.902172       -3.688056       -0.677336
N         -2.429378       -1.047685        1.655309
C         -1.445525       -1.037615        2.733547
N          0.765560       -1.281775       -2.053072
C          1.578461       -0.906686       -0.967235
C          1.121710       -0.113892        0.091538
C          2.016533        0.299492        1.069788
C          3.358323       -0.061559        1.035870
C          3.795729       -0.861742       -0.013122
C          2.923541       -1.286211       -1.006869
C          1.530853        1.162935        2.199806
F          0.337001        1.711445        1.932735
C          5.252385       -1.227227       -0.091917
F          5.752612       -1.500981        1.120428
C         -3.764418       -0.850058        2.213564
F          1.395103        0.457663        3.336095
F          2.387878        2.157487        2.459973
F          5.456872       -2.298027       -0.869485
F          5.983142       -0.223032       -0.598657
H         -2.326247       -0.952164       -1.266063
H          1.249599       -1.327887       -2.942502
H         -0.387068       -3.598974       -1.637829
H         -0.222879       -4.229629       -0.007974
H         -2.036440       -5.411306       -1.338116
H         -2.901744       -3.890002       -1.437882
H         -2.460494       -5.683225        0.970840
H         -3.908353       -4.809508        0.491590
H         -1.494658       -3.808254        2.046520
H         -3.202774       -3.558443        2.374165
H         -0.275526       -1.992232        0.500266
H         -3.272172       -2.196823        0.179700
H         -4.507606       -0.859476        1.410862
H         -4.038506       -1.616417        2.957365
H         -3.813059        0.124293        2.710471
H         -0.434633       -1.189020        2.346043
H         -1.641649       -1.804821        3.500917
H         -1.459495       -0.060302        3.226850
H          0.085793        0.208696        0.132869
H          4.046234        0.273935        1.805075
H          3.285077       -1.911862       -1.817246
N         -3.978156        1.213212       -0.220153
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O         -4.957757        1.442273        0.455463
O         -3.875703        0.283278       -1.001082
C         -2.838482        2.206638       -0.065349
C         -1.979343        2.419024       -1.244109
H         -2.175738        1.794047       -2.116122
O         -3.062912        3.302538       -0.892591
C         -0.598980        2.970045       -1.120665
C          2.024810        3.874570       -0.797376
C         -0.340598        4.131122       -0.386335
C          0.456349        2.305811       -1.746998
C          1.765280        2.749537       -1.574490
C          0.966388        4.575930       -0.220916
H         -1.168451        4.689506        0.040110
H          0.248481        1.442739       -2.375510
H          2.581768        2.212323       -2.048823
H          1.160352        5.474561        0.356321
H          3.045127        4.217827       -0.657692
C         -2.506981        2.399366        1.381670
H         -3.375849        2.804343        1.904171
H         -1.664430        3.081027        1.481213
H         -2.229279        1.433366        1.808116

RS epoxide:Catalyst, binary complex 135; Energy = -2449.835613; 6-31G(d) basis set.
N         -1.851432        0.606741       -0.014706
C         -1.413598        0.382273       -1.274172
S         -2.375696       -0.349543       -2.442023
C         -1.573391        1.848258        0.722271
C         -2.478003        2.963570        0.158674
C         -2.585875        4.092051        1.192601
C         -3.368980        3.597008        2.427498
C         -3.165303        2.088297        2.680056
C         -1.768006        1.651402        2.238659
N         -2.037595        3.315922       -1.186312
C         -0.863771        4.170621       -1.232163
N         -0.115673        0.731899       -1.570705
C          1.037041        0.662041       -0.774591
C          1.042419        0.170578        0.535731
C          2.242526        0.039978        1.217614
C          3.456356        0.392747        0.638693
C          3.438056        0.894641       -0.657038
C          2.249662        1.036924       -1.361821
C          2.232319       -0.455600        2.637264
F          1.049633       -0.984623        2.981853
C          4.731201        1.334557       -1.285018
F          5.740531        0.519407       -0.947937
C         -3.108198        3.853692       -2.008377
F          3.172580       -1.389840        2.842109
F          2.484733        0.542171        3.499351
F          4.656265        1.358396       -2.622785
F          5.075355        2.568575       -0.886352
H         -2.792101        0.240395        0.126024
H          0.059052        0.722762       -2.568205
H         -1.575441        0.605228        2.502771
H         -1.020029        2.250363        2.771237
H         -3.316590        1.857369        3.738267
H         -3.917546        1.506344        2.132423
H         -3.051810        4.165122        3.308022
H         -4.436592        3.798910        2.291685
H         -1.576607        4.411879        1.483226
H         -3.076682        4.967032        0.752322
H         -0.533659        2.116567        0.528753
H         -3.481308        2.530469        0.037599
H         -3.490773        4.825276       -1.648371
H         -2.739845        3.994551       -3.028894
H         -3.937062        3.140981       -2.043642
H         -1.054543        5.196145       -0.871506
H         -0.514790        4.236875       -2.267388
H         -0.049065        3.746101       -0.636531
H          0.122741       -0.145391        1.009048
H          4.390326        0.272035        1.177529
H          2.265204        1.418021       -2.378577
N         -3.812609       -2.481156       -0.285585
O         -3.932835       -1.686014        0.631819
O         -4.645399       -2.696864       -1.135830
C         -2.522893       -3.274954       -0.361437
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C	-1.400048	-2.663944	0.358058
H	-1.616399	-1.730536	0.875255
O	-2.154440	-3.759483	0.893206
C	0.024098	-2.880950	-0.027008
C	2.744700	-2.986934	-0.624479
C	0.937230	-3.299712	0.943197
C	0.471767	-2.538277	-1.303654
C	1.833269	-2.586317	-1.597766
C	2.294258	-3.356529	0.643069
H	0.581370	-3.565180	1.934797
H	-0.244300	-2.203185	-2.052117
H	2.181473	-2.305266	-2.587311
H	3.002115	-3.674636	1.401429
H	3.806137	-3.013712	-0.851870
C	-2.444034	-4.169671	-1.557512
H	-3.267891	-4.885935	-1.548631
H	-1.494059	-4.704820	-1.519860
H	-2.496328	-3.577305	-2.473770

RS epoxide:Catalyst, binary complex 136; Energy = -2449.844429; 6-31G(d) basis set.

N	1.922519	-1.216447	0.574602
C	0.738660	-1.069581	1.184337
S	0.566397	-0.516667	2.763069
C	3.227791	-0.982575	1.171047
C	4.277485	-1.669619	0.281968
C	5.654398	-1.542030	0.951004
C	6.023615	-0.066534	1.139249
C	4.946713	0.680101	1.930340
C	3.566983	0.508543	1.290175
N	3.848572	-3.014923	-0.101621
C	3.745601	-3.952105	1.007017
N	-0.321521	-1.422704	0.369645
C	-1.677734	-1.085852	0.487210
C	-2.613041	-1.936770	-0.108990
C	-3.960101	-1.601923	-0.107114
C	-4.411478	-0.428685	0.487993
C	-3.471532	0.410598	1.072239
C	-2.116180	0.101557	1.077423
C	-4.939520	-2.495181	-0.814841
F	-4.540864	-3.774909	-0.808061
C	-3.904583	1.687754	1.735488
F	-3.916065	1.578994	3.070263
C	4.642562	-3.569677	-1.184703
F	-6.154224	-2.444142	-0.251278
F	-5.088699	-2.138170	-2.099883
F	-3.068287	2.700250	1.437756
F	-5.133763	2.058288	1.354202
H	1.958191	-1.655770	-0.343344
H	-0.096985	-1.997592	-0.437645
H	3.558742	0.948800	0.282867
H	2.797342	1.011460	1.882046
H	4.913601	0.291300	2.957117
H	5.195276	1.743887	2.002917
H	6.994036	0.018479	1.639609
H	6.133169	0.401202	0.151242
H	5.635018	-2.042946	1.928236
H	6.413195	-2.048203	0.343623
H	3.229859	-1.420571	2.178543
H	4.306886	-1.097128	-0.659565
H	5.672762	-3.830034	-0.887452
H	4.161300	-4.481082	-1.552815
H	4.691814	-2.851050	-2.008459
H	4.717855	-4.187112	1.472058
H	3.316268	-4.888194	0.637539
H	3.075703	-3.558688	1.777204
H	-2.283166	-2.861029	-0.573911
H	-5.465102	-0.174811	0.489936
H	-1.405053	0.777339	1.535846
N	0.296074	-0.464392	-2.482709
O	-0.898286	-0.542125	-2.673347
O	1.031945	-1.407817	-2.245381
C	0.888348	0.922663	-2.508050
C	1.070686	1.501776	-1.161851
H	0.789684	0.871688	-0.318845
O	2.148353	0.965146	-1.941377

C	1.037306	2.968166	-0.920368
C	0.922962	5.707812	-0.438002
C	2.030567	3.805163	-1.428219
C	-0.009393	3.500202	-0.164917
C	-0.067628	4.869196	0.071048
C	1.971071	5.174959	-1.184515
H	2.849438	3.375878	-1.998338
H	-0.782116	2.846481	0.231353
H	-0.884571	5.278898	0.656685
H	2.747209	5.825938	-1.574395
H	0.879588	6.775669	-0.248360
C	0.581308	1.655584	-3.778332
H	1.090055	1.176623	-4.618899
H	0.934770	2.683379	-3.683057
H	-0.494801	1.657442	-3.956223

RS epoxide:Catalyst, binary complex 137; Energy = -2449.841756; 6-31G(d) basis set.

N	-3.011797	0.153922	0.316700
C	-2.003745	0.433729	1.155140
S	-2.007178	0.038930	2.789086
C	-4.329757	-0.324287	0.707254
C	-5.305251	-0.007131	-0.440481
C	-6.729868	-0.370156	0.003079
C	-6.815214	-1.858955	0.357404
C	-5.784032	-2.237115	1.423282
C	-4.369741	-1.826843	1.005031
N	-5.095528	1.346455	-0.958205
C	-5.391759	2.407091	-0.006928
N	-0.987891	1.140793	0.546448
C	0.371254	1.199399	0.880086
C	1.114822	2.256366	0.350063
C	2.501717	2.261799	0.470207
C	3.169720	1.240489	1.131243
C	2.413181	0.207542	1.680957
C	1.030318	0.176869	1.575436
C	3.298823	3.311576	-0.247088
F	2.611361	4.448743	-0.407726
C	3.135590	-0.919214	2.367819
F	3.483028	-0.594674	3.622905
C	-5.769840	1.574873	-2.225060
F	4.435834	3.604914	0.396227
F	3.648088	2.888625	-1.479326
F	2.389037	-2.028358	2.434109
F	4.269005	-1.230411	1.719795
H	-2.978014	0.499125	-0.641377
H	-1.210180	1.581339	-0.341249
H	-4.065786	-2.371070	0.100619
H	-3.647621	-2.057851	1.791810
H	-6.035311	-1.733104	2.366459
H	-5.817822	-3.313226	1.622051
H	-7.826147	-2.107643	0.697254
H	-6.630163	-2.451560	-0.549185
H	-7.007729	0.231258	0.878916
H	-7.442272	-0.129544	-0.794224
H	-4.627454	0.212229	1.619135
H	-5.036580	-0.677323	-1.273360
H	-5.413212	2.515108	-2.656952
H	-5.528712	0.764708	-2.919947
H	-6.867113	1.641330	-2.133797
H	-6.459825	2.468505	0.260096
H	-5.101467	3.365630	-0.447775
H	-4.810261	2.270397	0.909793
H	0.613326	3.050023	-0.195633
H	4.252483	1.231830	1.196502
H	0.469752	-0.665688	1.957987
N	-0.556651	-0.119501	-2.329112
O	-1.712275	-0.470752	-2.461624
O	-0.182923	1.038859	-2.284728
C	0.459965	-1.228937	-2.112854
C	1.655095	-0.816721	-1.360148
H	1.724237	0.246593	-1.143030
O	0.530343	-1.467974	-0.742376
C	2.950367	-1.544516	-1.346406
C	5.429590	-2.809353	-1.238085
C	3.031931	-2.883621	-0.964152

C	4.112487	-0.832030	-1.650199
C	5.348448	-1.466804	-1.604408
C	4.272541	-3.513158	-0.912744
H	2.128647	-3.415356	-0.679639
H	4.045531	0.224865	-1.898794
H	6.249935	-0.910734	-1.841523
H	4.335616	-4.552745	-0.606898
H	6.396059	-3.301459	-1.191932
C	0.297581	-2.359942	-3.076551
H	-0.674743	-2.835282	-2.935785
H	1.091806	-3.086598	-2.897801
H	0.377236	-1.994628	-4.103326

RS epoxide:Catalyst, binary complex 138; Energy = -2449.843865; 6-31G(d) basis set.

N	2.194746	0.287051	-0.590690
C	1.853734	-0.031236	-1.845586
S	2.894663	-0.475026	-3.089002
C	3.539465	0.445447	-0.016961
C	4.362486	-0.865252	0.023052
C	5.692921	-0.586179	0.738901
C	6.471338	0.555124	0.082828
C	5.636957	1.835692	0.061276
C	4.312572	1.600169	-0.665859
N	3.692558	-2.014248	0.630420
C	2.859310	-2.807670	-0.251676
N	0.493505	-0.049771	-2.103514
C	-0.536682	0.695882	-1.505978
C	-1.845805	0.207040	-1.615001
C	-2.900294	0.931842	-1.078103
C	-2.687112	2.130797	-0.402100
C	-1.386731	2.601977	-0.295802
C	-0.314850	1.912025	-0.854114
C	-4.309600	0.417854	-1.172827
F	-5.128662	1.319063	-1.723811
C	-1.107085	3.901933	0.410365
F	-2.106241	4.244330	1.230324
C	3.026841	-1.757287	1.892546
F	-4.396069	-0.709886	-1.889423
F	-4.803233	0.145218	0.052798
F	0.017724	3.831933	1.130957
F	-0.948666	4.905377	-0.467924
H	1.441778	0.431796	0.075657
H	0.276314	-0.474296	-2.997253
H	4.504996	1.358998	-1.716285
H	3.688053	2.501020	-0.643772
H	5.438600	2.157073	1.093465
H	6.185932	2.648334	-0.425576
H	7.414837	0.721156	0.613701
H	6.728066	0.275371	-0.947862
H	5.501015	-0.326726	1.789637
H	6.273768	-1.513289	0.740807
H	3.336331	0.731017	1.024045
H	4.592572	-1.143091	-1.010677
H	3.696074	-1.239069	2.585742
H	2.102187	-1.160494	1.799197
H	2.749725	-2.712800	2.352362
H	1.860578	-2.371874	-0.446896
H	2.703597	-3.795583	0.199663
H	3.356776	-2.944596	-1.214619
H	-2.027290	-0.741430	-2.111614
H	-3.512407	2.674428	0.045190
H	0.685426	2.324288	-0.775136
N	-0.684256	0.736022	2.168519
O	0.483573	0.869799	1.842110
O	-1.430573	1.644037	2.460508
C	-1.259443	-0.666880	2.193366
C	-0.705698	-1.559462	1.158589
H	0.060281	-1.137847	0.506230
O	-0.287027	-1.599040	2.527606
C	-1.445160	-2.737013	0.620310
C	-2.729545	-4.940431	-0.502246
C	-0.790189	-3.968399	0.556153
C	-2.743668	-2.614124	0.127728
C	-3.384336	-3.713418	-0.437643
C	-1.434619	-5.068505	-0.000349

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H          0.220233       -4.059088        0.946662
H         -3.258943       -1.662083        0.197955
H         -4.392547       -3.606061       -0.824989
H         -0.925340       -6.025825       -0.046614
H         -3.227225       -5.798994       -0.942037
C         -2.617831       -0.734885        2.821482
H         -2.580826       -0.338059        3.838328
H         -2.925855       -1.780716        2.851627
H         -3.340498       -0.157433        2.241756

RS epoxide:Catalyst, binary complex 139; Energy = -2449.838794; 6-31G(d) basis set.
N          2.699146       -0.536159        0.317442
C          1.745176       -0.722771        1.246811
S          1.766836       -0.036124        2.773199
C          3.899928        0.267850        0.484658
C          5.077805       -0.391465       -0.260362
C          6.329213        0.482508       -0.103071
C          6.091893        1.916261       -0.581533
C          4.916995        2.554942        0.160600
C          3.656406        1.704433        0.009026
N          5.365121       -1.776163        0.115407
C          4.599566       -2.794577       -0.580225
N          0.784871       -1.622630        0.805502
C         -0.605989       -1.528988        0.903719
C         -1.296071       -0.724822        1.816184
C         -2.684370       -0.642303        1.737228
C         -3.417655       -1.345511        0.790991
C         -2.719784       -2.164189       -0.094128
C         -1.340380       -2.268964       -0.038924
C         -3.391549        0.316433        2.655868
F         -3.349702        1.566838        2.167437
C         -3.484159       -2.867396       -1.180574
F         -4.573241       -3.479255       -0.693661
C          5.382125       -2.029923        1.545792
F         -4.684331       -0.003762        2.807972
F         -2.832811        0.348187        3.870872
F         -3.911439       -1.993681       -2.106224
F         -2.743824       -3.786747       -1.809016
H          2.434118       -0.742815       -0.643380
H          1.066894       -2.121153       -0.032744
H          3.352317        1.676282       -1.048474
H          2.816974        2.121807        0.575858
H          5.164609        2.643496        1.226978
H          4.732962        3.569668       -0.207799
H          7.001037        2.511500       -0.445404
H          5.876347        1.907756       -1.659255
H          6.626125        0.503116        0.954280
H          7.146866        0.009512       -0.655113
H          4.116265        0.285065        1.557958
H          4.825444       -0.407275       -1.332609
H          6.000987       -1.289484        2.060359
H          4.376623       -2.020253        2.004204
H          5.823523       -3.015502        1.725897
H          3.569687       -2.916351       -0.201351
H          5.104571       -3.760581       -0.467912
H          4.553038       -2.562121       -1.648677
H         -0.757024       -0.161942        2.566672
H         -4.498395       -1.266189        0.745521
H         -0.823654       -2.894757       -0.762017
N         -0.161833       -0.721889       -2.429075
O         -1.114771       -1.190922       -3.006635
O          0.843563       -1.338527       -2.105397
C         -0.202003        0.753083       -2.101317
C         -1.166310        1.115828       -1.052797
H         -1.759065        0.295326       -0.650920
O          0.253244        0.987773       -0.816099
C         -1.767324        2.467885       -0.922991
C         -2.960000        4.972805       -0.682029
C         -0.972967        3.605837       -0.778296
C         -3.158268        2.582241       -0.925890
C         -3.752913        3.834209       -0.812643
C         -1.572132        4.856617       -0.659080
H          0.107341        3.502185       -0.731953
H         -3.771422        1.687918       -1.008315
H         -4.834719        3.920259       -0.815310
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H          -0.953791        5.740595       -0.538640
H          -3.424455        5.949019       -0.584781
C           0.273491        1.574369       -3.260822
H           1.335509        1.384531       -3.438482
H           0.126141        2.631230       -3.033449
H          -0.297867        1.317874       -4.155806

RS epoxide:Catalyst, binary complex 140; Energy = -2449.844386; 6-31G(d) basis set.
N          -1.917204        0.916064       -0.603050
C          -0.742387        1.516971       -0.307650
S          -0.633449        2.885664        0.658728
C          -3.232511        1.489947       -0.347511
C          -4.232874        0.773741       -1.273587
C          -5.604390        1.450803       -1.147758
C          -6.100767        1.359965        0.299531
C          -5.086678        1.969811        1.270351
C          -3.705203        1.333245        1.100818
N          -3.687988        0.616086       -2.625343
C          -3.526759        1.868122       -3.352967
N           0.317801        0.879058       -0.905028
C           1.693939        0.868993       -0.630078
C           2.368955        1.739847        0.225293
C           3.736612        1.561951        0.435305
C           4.457211        0.553322       -0.180871
C           3.775201       -0.295794       -1.049963
C           2.422159       -0.140737       -1.283976
C           4.417680        2.523257        1.369496
F           5.719851        2.245161        1.517987
C           4.546915       -1.380709       -1.746613
F           3.749806       -2.221481       -2.418682
C          -4.426186       -0.356952       -3.414217
F           4.324972        3.785711        0.923268
F           3.860073        2.504529        2.588843
F           5.415534       -0.863502       -2.633643
F           5.268448       -2.102408       -0.880259
H          -1.941773        0.282181       -1.403735
H           0.048830        0.054610       -1.430896
H          -3.755355        0.263191        1.335302
H          -2.977998        1.791376        1.775590
H          -5.011916        3.050633        1.088117
H          -5.428366        1.845641        2.303305
H          -7.073911        1.852445        0.398027
H          -6.248987        0.301423        0.557328
H          -5.525388        2.505172       -1.445263
H          -6.321115        0.975775       -1.827672
H          -3.194940        2.563740       -0.584343
H          -4.333153       -0.251016       -0.884195
H          -4.509651       -1.294894       -2.855489
H          -5.441548       -0.022132       -3.684268
H          -3.882043       -0.556553       -4.342422
H          -4.486050        2.353595       -3.595278
H          -3.003634        1.666959       -4.292435
H          -2.918285        2.567505       -2.772201
H           1.840832        2.538383        0.727305
H           5.517325        0.425448        0.006111
H           1.915388       -0.827895       -1.955638
N           1.868678       -2.312070        0.813731
O           2.188917       -1.405238        1.552466
O           2.624796       -2.968265        0.124304
C           0.398493       -2.648791        0.670158
C          -0.536855       -1.575392        1.035956
H          -0.095298       -0.657053        1.423623
O          -0.175943       -1.855867       -0.330749
C          -1.944327       -1.857201        1.432807
C          -4.581049       -2.324060        2.211127
C          -2.333795       -1.629688        2.753741
C          -2.875369       -2.316345        0.501161
C          -4.192741       -2.547482        0.891711
C          -3.648641       -1.867583        3.141877
H          -1.610566       -1.254305        3.472866
H          -2.565597       -2.475522       -0.528421
H          -4.916840       -2.899412        0.162552
H          -3.947590       -1.687270        4.169554
H          -5.608206       -2.503176        2.513268
C           0.145116       -4.122900        0.676268
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H          0.648023       -4.587134       -0.173489
H         -0.929992       -4.296895        0.611165
H          0.523169       -4.564568        1.601565

RS epoxide:Catalyst, binary complex 141; Energy = -2449.836346; 6-31G(d) basis set.
N          1.105994        1.649623       -1.117993
C          0.705708        0.793038       -2.092483
S          1.761511        0.270401       -3.286903
C          0.319196        2.737828       -0.509363
C          1.284980        3.644055        0.288244
C          0.475118        4.761910        0.959351
C         -0.330066        5.575597       -0.053814
C         -1.252742        4.672012       -0.871632
C         -0.458565        3.553942       -1.549302
N          2.141206        2.981190        1.267306
C          3.461852        2.568777        0.832003
N         -0.594716        0.351779       -2.099515
C         -1.480175        0.089972       -1.041967
C         -1.087131        0.065809        0.295911
C         -2.016418       -0.252624        1.278916
C         -3.323603       -0.596069        0.961887
C         -3.692448       -0.605922       -0.379799
C         -2.795337       -0.252598       -1.376303
C         -1.606233       -0.197759        2.724115
F         -1.881848        1.001845        3.262245
C         -5.064815       -1.089918       -0.753394
F         -5.438518       -0.655137       -1.963801
C          1.520963        1.971028        2.095988
F         -2.251216       -1.116373        3.456042
F         -0.290462       -0.400883        2.888941
F         -5.107078       -2.432158       -0.783840
F         -5.988747       -0.690559        0.129827
H          2.085956        1.882121       -1.244760
H         -0.812865       -0.139925       -2.958413
H          0.257167        3.978864       -2.266315
H         -1.127431        2.895405       -2.113129
H         -2.008531        4.227464       -0.209417
H         -1.793844        5.251210       -1.626661
H         -0.907641        6.351435        0.459160
H          0.362563        6.090946       -0.733321
H         -0.205805        4.318546        1.699773
H          1.174637        5.396614        1.510683
H         -0.399144        2.312869        0.201619
H          1.957573        4.118433       -0.442144
H          2.089988        1.855093        3.025248
H          0.498642        2.252088        2.367071
H          1.494923        0.978950        1.606707
H          3.899310        3.331039        0.181124
H          3.484748        1.598344        0.302347
H          4.113563        2.461998        1.706609
H         -0.054960        0.257426        0.561259
H         -4.034310       -0.863351        1.736516
H         -3.107942       -0.256286       -2.416396
N          5.024869       -1.464238        0.256870
O          5.766975       -1.879555        1.126172
O          5.111764       -0.385154       -0.291599
C          3.880156       -2.363536       -0.142524
C          2.617278       -1.638473       -0.381326
H          2.648028       -0.553297       -0.265272
O          3.449113       -2.105776       -1.436944
C          1.297198       -2.305852       -0.187343
C         -1.229256       -3.424506        0.180693
C          0.823468       -2.553947        1.102443
C          0.516028       -2.638134       -1.294432
C         -0.748890       -3.191689       -1.106726
C         -0.437091       -3.116021        1.285676
H          1.437414       -2.296379        1.962092
H          0.904609       -2.442160       -2.290595
H         -1.362660       -3.440346       -1.967655
H         -0.808888       -3.292728        2.290875
H         -2.221982       -3.842171        0.321340
C          4.016575       -3.775429        0.337202
H          4.942032       -4.215363       -0.041100
H          3.164143       -4.343067       -0.038795
H          4.028547       -3.814340        1.427433
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RS epoxide:Catalyst, binary complex 142; Energy = -2449.859404; 6-31G(d) basis set.

N	2.207260	0.905802	-0.966658
C	1.004333	1.479823	-0.785050
S	0.789221	3.036109	-0.174545
C	3.485692	1.545479	-0.689602
C	4.445733	0.546009	-0.028061
C	5.758659	1.273867	0.308865
C	6.391747	1.876010	-0.949332
C	5.425589	2.835412	-1.645572
C	4.100350	2.140576	-1.960291
N	3.798821	-0.159493	1.083741
C	3.335838	0.701373	2.162780
N	-0.033464	0.672172	-1.181823
C	-1.403231	0.770269	-0.892192
C	-2.291202	0.197249	-1.803107
C	-3.651564	0.152427	-1.517495
C	-4.152925	0.682723	-0.337304
C	-3.255451	1.251188	0.563144
C	-1.892701	1.294968	0.309383
C	-4.595986	-0.434648	-2.527021
F	-5.671764	-0.979559	-1.939952
C	-3.790908	1.825139	1.844898
F	-4.286013	3.058665	1.666530
C	4.615148	-1.249534	1.598389
F	-5.045890	0.493163	-3.384596
F	-4.006147	-1.391543	-3.259910
F	-4.793343	1.073464	2.333100
F	-2.852416	1.910475	2.796504
H	2.251334	-0.076187	-1.238979
H	0.218759	-0.143069	-1.731258
H	4.262388	1.335174	-2.690091
H	3.382755	2.842754	-2.398012
H	5.231457	3.694756	-0.989505
H	5.869844	3.231186	-2.564701
H	7.322950	2.391107	-0.690975
H	6.658214	1.064770	-1.640935
H	5.561383	2.075822	1.033252
H	6.456852	0.575218	0.782603
H	3.279584	2.366813	0.003502
H	4.678378	-0.232389	-0.770257
H	5.478893	-0.909994	2.194018
H	3.997595	-1.888316	2.240305
H	4.980277	-1.858264	0.765527
H	4.146461	1.256767	2.662989
H	2.856462	0.074885	2.922840
H	2.592046	1.416902	1.796547
H	-1.916298	-0.226781	-2.730026
H	-5.212753	0.634770	-0.111532
H	-1.211498	1.701131	1.044887
N	2.813397	-3.019299	-0.432016
O	3.468689	-3.887889	0.105347
O	3.256598	-2.138940	-1.143603
C	1.324986	-3.026676	-0.164418
C	0.844342	-1.766426	0.454541
H	1.629080	-1.029327	0.659594
O	0.688084	-2.074351	-0.943215
C	-0.406320	-1.655618	1.249503
C	-2.740082	-1.314704	2.741593
C	-1.629353	-2.118835	0.755072
C	-0.362125	-1.003015	2.482098
C	-1.525439	-0.837156	3.227876
C	-2.790281	-1.951314	1.502286
H	-1.674767	-2.573344	-0.230526
H	0.582718	-0.610815	2.849381
H	-1.486578	-0.316942	4.179422
H	-3.739324	-2.299537	1.106065
H	-3.650502	-1.165008	3.312989
C	0.763354	-4.405725	-0.008227
H	1.309148	-4.942540	0.767237
H	0.845815	-4.953487	-0.950551
H	-0.286323	-4.333815	0.276376

RS epoxide:Catalyst, binary complex 143; Energy = -2449.838912; 6-31G(d) basis set.

N	2.046254	-0.073560	0.963036

C	1.778935	0.028165	2.271233
S	2.888621	0.507073	3.441258
C	3.361649	0.019347	0.325551
C	3.424220	-1.104430	-0.750407
C	2.535233	-0.743735	-1.955661
C	2.676466	0.694342	-2.480855
C	2.589704	1.735346	-1.361995
C	3.584708	1.421527	-0.245051
N	4.762372	-1.545899	-1.133556
C	5.607985	-1.883966	-0.005210
N	0.481173	-0.258497	2.633834
C	-0.471894	-0.967939	1.871744
C	-0.099291	-2.077834	1.109146
C	-1.046204	-2.731276	0.327830
C	-2.374740	-2.331308	0.324505
C	-2.742301	-1.244536	1.114561
C	-1.809892	-0.559214	1.880962
C	-0.577122	-3.826469	-0.588496
F	-0.022030	-3.302525	-1.696326
C	-4.172037	-0.780941	1.044245
F	-5.019300	-1.778738	1.333580
C	5.492862	-0.841116	-2.168411
F	0.356453	-4.590876	-0.009226
F	-1.579372	-4.618903	-0.979454
F	-4.423939	0.226579	1.880614
F	-4.470901	-0.372604	-0.201704
H	1.266985	-0.254310	0.340813
H	0.253032	-0.026159	3.592734
H	3.500114	2.148324	0.570097
H	4.610629	1.481218	-0.629182
H	2.778541	2.736693	-1.762786
H	1.572887	1.767820	-0.944682
H	3.632506	0.822141	-2.997877
H	1.896571	0.874270	-3.229829
H	2.715990	-1.475113	-2.751197
H	1.486283	-0.900587	-1.658665
H	4.087183	-0.179125	1.117221
H	2.973504	-1.987724	-0.270531
H	4.914058	-0.809202	-3.093523
H	5.798385	0.186742	-1.906441
H	6.405651	-1.407787	-2.379145
H	6.430821	-2.519272	-0.348919
H	5.028837	-2.446404	0.734710
H	6.050857	-1.008703	0.501856
H	0.926126	-2.433691	1.128849
H	-3.108673	-2.845141	-0.288168
H	-2.114289	0.304667	2.462936
N	-3.427575	1.338561	-2.208916
O	-3.219393	0.666074	-3.200369
O	-4.450435	1.936619	-1.955449
C	-2.287231	1.461946	-1.230158
C	-2.142601	2.815237	-0.643967
H	-2.863511	3.558205	-0.982777
O	-2.739919	1.725638	0.054995
C	-0.832683	3.315499	-0.143446
C	1.600016	4.303556	0.796344
C	-0.209326	4.378537	-0.799565
C	-0.234865	2.749885	0.984034
C	0.977499	3.245421	1.456090
C	1.007733	4.866578	-0.332657
H	-0.679473	4.827245	-1.670918
H	-0.730893	1.930449	1.496178
H	1.437234	2.805848	2.337611
H	1.489883	5.692199	-0.846647
H	2.545572	4.689683	1.164766
C	-1.168550	0.496698	-1.478529
H	-1.536336	-0.529356	-1.544442
H	-0.468306	0.586139	-0.645153
H	-0.653536	0.744595	-2.409613

RS epoxide:Catalyst, binary complex 144; Energy = -2449.838479; 6-31G(d) basis set.

N	1.178770	2.428835	0.282771
C	2.460964	2.797624	0.400093
S	2.986316	4.398338	0.495265
C	0.043165	3.354926	0.300689

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C         -1.112748        2.721604       -0.522559
C         -2.465397        3.117955        0.074848
C         -2.637718        2.591542        1.513030
C         -1.292281        2.527840        2.257860
C         -0.370513        3.638175        1.755801
N         -1.062056        2.978246       -1.966526
C          0.207787        2.592616       -2.569490
N          3.389610        1.787104        0.417519
C          3.137984        0.399935        0.459685
C          2.265765       -0.136689        1.408053
C          1.990698       -1.499343        1.393152
C          2.612182       -2.352068        0.491692
C          3.524772       -1.813427       -0.408836
C          3.777292       -0.447942       -0.446239
C          0.933662       -2.012151        2.326379
F          0.836690       -3.344375        2.308500
C          4.262849       -2.720525       -1.353523
F          4.515991       -2.115006       -2.522307
C         -1.398946        4.342413       -2.347612
F          1.152635       -1.630216        3.590654
F         -0.275834       -1.516964        1.984380
F          5.446553       -3.097097       -0.845053
F          3.571330       -3.837264       -1.611788
H          0.968351        1.454711        0.078714
H          4.345754        2.103328        0.319954
H          0.535015        3.736276        2.362914
H         -0.891912        4.602178        1.805521
H         -1.449298        2.603644        3.337958
H         -0.816585        1.551986        2.080192
H         -3.322716        3.257213        2.049736
H         -3.096416        1.599670        1.500467
H         -2.551002        4.210902        0.078125
H         -3.259333        2.742128       -0.581153
H          0.378623        4.282513       -0.174417
H         -1.025847        1.631348       -0.411211
H         -0.720111        5.099162       -1.916435
H         -1.333494        4.423102       -3.436463
H         -2.423031        4.586424       -2.057769
H          1.050027        3.240457       -2.269242
H          0.112158        2.647231       -3.658688
H          0.449834        1.560778       -2.296898
H          1.790262        0.513644        2.137481
H          2.376614       -3.409394        0.478245
H          4.452931       -0.034012       -1.188211
N         -0.428921       -1.357747       -0.859519
O          0.385454       -0.454776       -0.953874
O         -0.161880       -2.536885       -0.786653
C         -1.885004       -0.945255       -0.862501
C         -2.729441       -1.642861        0.117629
H         -2.238099       -2.399424        0.726844
O         -2.215362       -0.313197        0.330516
C         -4.200378       -1.779187       -0.062968
C         -6.947605       -2.080469       -0.430241
C         -4.756266       -3.055409       -0.168831
C         -5.023921       -0.654370       -0.128859
C         -6.395413       -0.807271       -0.311811
C         -6.126366       -3.204177       -0.357565
H         -4.114784       -3.930652       -0.105748
H         -4.585861        0.334532       -0.024538
H         -7.033228        0.069813       -0.356540
H         -6.554114       -4.197953       -0.443847
H         -8.017222       -2.198294       -0.572754
C         -2.284798       -0.338463       -2.173990
H         -1.851363        0.662063       -2.286678
H         -3.373074       -0.256696       -2.203748
H         -1.958887       -0.978146       -2.998473

RS epoxide:Catalyst, binary complex 145; Energy = -2449.840751; 6-31G(d) basis set.
N         -1.861405       -1.790270       -0.750542
C         -1.526592       -0.806767       -1.602227
S         -2.594439        0.228183       -2.394952
C         -3.204928       -2.254189       -0.371121
C         -4.042823       -1.207698        0.399788
C         -5.345715       -1.878834        0.861967
C         -6.129496       -2.477055       -0.307106
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C	-5.280471	-3.496227	-1.066833
C	-3.977697	-2.857906	-1.550755
N	-3.371637	-0.569262	1.529500
C	-2.659983	0.659190	1.237603
N	-0.182312	-0.661994	-1.844412
C	0.917887	-1.068303	-1.065890
C	2.138524	-1.271414	-1.712991
C	3.272908	-1.575178	-0.972407
C	3.218188	-1.718854	0.409488
C	1.995113	-1.533769	1.042673
C	0.853636	-1.191832	0.326329
C	4.600386	-1.689437	-1.670592
F	5.241780	-0.515285	-1.695559
C	1.907411	-1.731137	2.530934
F	0.838458	-1.106254	3.057313
C	-2.628893	-1.448518	2.406285
F	5.403450	-2.567889	-1.054411
F	4.456257	-2.090803	-2.941801
F	1.783892	-3.031358	2.840322
F	2.995473	-1.277870	3.157101
H	-1.114250	-2.429204	-0.502047
H	0.012606	0.061644	-2.526472
H	-4.194538	-2.068413	-2.277567
H	-3.341617	-3.597793	-2.050172
H	-5.051721	-4.342917	-0.404111
H	-5.833645	-3.901575	-1.920410
H	-7.052169	-2.941316	0.057034
H	-6.425288	-1.671699	-0.993000
H	-5.114680	-2.675135	1.584414
H	-5.938797	-1.128759	1.393615
H	-3.000305	-3.070781	0.334650
H	-4.308942	-0.410264	-0.301238
H	-3.246173	-2.299744	2.708616
H	-1.697021	-1.848617	1.964316
H	-2.348724	-0.901719	3.312694
H	-2.462424	1.183897	2.180573
H	-3.282834	1.303522	0.610541
H	-1.692091	0.529033	0.717349
H	2.198700	-1.174476	-2.792303
H	4.109417	-1.957496	0.979417
H	-0.074227	-0.989503	0.849955
N	2.637436	1.565598	0.655745
O	3.220365	1.423011	-0.399420
O	3.084832	1.293453	1.753840
C	1.238569	2.135162	0.608844
C	1.019453	3.139817	-0.458980
H	1.886846	3.382416	-1.071559
O	0.602138	1.781438	-0.575738
C	-0.057261	4.161750	-0.347359
C	-2.059763	6.083724	-0.124283
C	-1.396936	3.785738	-0.455666
C	0.281103	5.499904	-0.141382
C	-0.720752	6.458465	-0.026174
C	-2.395490	4.749504	-0.343072
H	-1.644734	2.744787	-0.650681
H	1.326520	5.789895	-0.071085
H	-0.456812	7.498420	0.138239
H	-3.436925	4.456386	-0.433864
H	-2.839895	6.833352	-0.035667
C	0.520652	2.079704	1.920037
H	0.414017	1.047321	2.260210
H	-0.465808	2.527890	1.792740
H	1.077275	2.638286	2.674212

RS epoxide:Catalyst, binary complex 146; Energy = -2449.843857; 6-31G(d) basis set.

N	0.217271	-0.430603	0.449052
H	0.351024	0.323465	1.114940
C	1.382564	-1.024673	-0.015874
S	1.444078	-2.617473	-0.546270
N	2.412267	-0.168846	0.019268
H	2.202673	0.798829	0.248828
C	-1.111313	-0.846846	0.302620
C	-3.853418	-1.396045	0.023456
C	-2.018356	-0.464101	1.294263
C	-1.583982	-1.504052	-0.837469

C	-2.941597	-1.777192	-0.953995
C	-3.371367	-0.730562	1.144034
H	-1.667879	0.068640	2.173030
H	-0.901299	-1.780755	-1.630027
H	-4.914226	-1.587482	-0.098000
C	-3.441530	-2.498639	-2.173936
C	-4.339207	-0.303128	2.209623
F	-2.651541	-2.290761	-3.236365
F	-3.504265	-3.823743	-1.981652
F	-4.678371	-2.093658	-2.507685
F	-4.728712	-1.333093	2.974840
F	-3.813032	0.620700	3.028212
F	-5.454618	0.222899	1.675610
C	3.839935	-0.452193	-0.126268
C	5.882151	-1.603667	0.734480
C	5.783218	-0.849644	-1.667990
C	6.326065	-1.903119	-0.699924
C	4.259357	-0.742542	-1.572653
C	4.348278	-1.547636	0.831308
H	6.311024	-0.641669	1.049792
H	6.230232	0.125296	-1.426989
H	5.950284	-2.892188	-0.994735
H	3.792009	-1.677236	-1.900026
H	3.955799	-2.500902	0.462649
H	4.318737	0.494256	0.157516
H	6.266329	-2.365542	1.423155
H	6.075629	-1.086588	-2.696379
H	7.419103	-1.946737	-0.757667
H	3.886135	0.061589	-2.215916
N	3.796631	-1.382625	2.175049
C	3.834110	-2.612088	2.945759
H	3.342729	-3.410118	2.381735
H	3.285038	-2.467402	3.882102
H	4.856705	-2.940825	3.206350
C	4.360514	-0.277841	2.929116
H	5.408766	-0.441259	3.235792
H	3.768591	-0.126104	3.837806
H	4.317787	0.647200	2.344959
O	1.044841	2.568833	0.510814
C	0.244920	2.410242	-0.671485
C	1.120423	3.584389	-0.438810
H	0.640602	1.658338	-1.356568
N	2.427828	3.510080	-1.197906
O	3.051791	2.468018	-1.136022
O	2.744082	4.488566	-1.839310
C	-1.230012	2.417065	-0.485378
C	-3.997222	2.306901	-0.149694
C	-2.037994	1.887613	-1.494012
C	-1.810014	2.866142	0.703574
C	-3.191841	2.816497	0.866077
C	-3.417647	1.833622	-1.325796
H	-1.584626	1.498935	-2.402409
H	-1.176564	3.222650	1.510895
H	-3.637455	3.157426	1.794961
H	-4.038771	1.404470	-2.106068
H	-5.072250	2.252385	-0.013699
C	0.707963	4.983217	-0.104229
H	-0.278121	4.965523	0.359245
H	0.667368	5.584734	-1.011890
H	1.426536	5.429833	0.587424

RS epoxide:Catalyst, binary complex 147; Energy = -2449.839089; 6-31G(d) basis set.

N	0.050708	-0.702898	-0.298054
H	0.273581	0.285847	-0.390978
C	1.131446	-1.556757	-0.186617
S	1.023999	-3.081855	0.509408
N	2.259464	-0.992689	-0.656533
H	2.158292	-0.076478	-1.082558
C	-1.300517	-0.985841	-0.042859
C	-4.050262	-1.382984	0.369360
C	-2.076756	0.004065	0.567194
C	-1.908671	-2.172206	-0.456221
C	-3.268046	-2.361888	-0.228914
C	-3.438191	-0.193019	0.749839
H	-1.618366	0.935361	0.885060

H	-1.327550	-2.936324	-0.957169
H	-5.112320	-1.537082	0.526256
C	-3.879593	-3.671819	-0.641817
C	-4.295478	0.899791	1.319758
F	-3.458187	-4.045278	-1.859701
F	-3.550642	-4.658184	0.203373
F	-5.218026	-3.608550	-0.678899
F	-3.572684	1.921552	1.794805
F	-5.123954	1.398920	0.381639
F	-5.073990	0.452731	2.314627
C	3.644311	-1.467985	-0.536727
C	5.627298	-1.909715	0.935976
C	5.402772	-3.113076	-1.262473
C	5.891055	-3.214190	0.182897
C	3.912408	-2.770719	-1.300742
C	4.139982	-1.528573	0.928371
H	6.217169	-1.108026	0.469408
H	5.976504	-2.334376	-1.784972
H	5.364678	-4.037384	0.684404
H	3.335630	-3.581743	-0.847845
H	3.588093	-2.327326	1.435398
H	4.226340	-0.681749	-1.036319
H	5.953437	-1.979751	1.978057
H	5.580323	-4.052202	-1.796749
H	6.959447	-3.453492	0.211751
H	3.560367	-2.653573	-2.331902
N	3.925893	-0.308878	1.709425
C	4.320373	0.920236	1.059060
H	5.324779	0.840703	0.634598
H	4.334330	1.735563	1.791892
H	3.632848	1.211571	0.240518
C	2.625551	-0.167215	2.336703
H	1.843047	0.215073	1.654152
H	2.704789	0.537937	3.174038
H	2.287427	-1.130361	2.726345
O	1.398890	1.956736	-0.900086
C	0.824739	3.195250	-1.361668
C	1.712438	3.113276	-0.184931
H	1.284687	3.534777	-2.288472
N	3.129062	3.560866	-0.466806
O	3.666429	4.228639	0.392552
O	3.613762	3.240160	-1.531418
C	-0.648796	3.351090	-1.201406
C	-3.402725	3.627126	-0.899267
C	-1.504051	2.351032	-1.664883
C	-1.173121	4.498016	-0.602830
C	-2.549636	4.635042	-0.454307
C	-2.880953	2.488261	-1.507892
H	-1.092224	1.460549	-2.135469
H	-0.502549	5.276052	-0.246620
H	-2.955593	5.522960	0.019358
H	-3.545465	1.699523	-1.846861
H	-4.474588	3.723110	-0.761940
C	1.311132	3.240211	1.251703
H	0.299733	2.847353	1.367707
H	1.330496	4.285866	1.562018
H	1.997217	2.673030	1.885343

RS epoxide:Catalyst, binary complex 148; Energy = -2449.848019; 6-31G(d) basis set.

N	3.003246	0.601847	-0.635640
C	1.872346	1.309752	-0.472449
S	1.841100	2.918399	0.024823
C	4.333925	1.073453	-0.275231
C	5.260236	-0.153581	-0.183913
C	6.581657	0.261176	0.496928
C	6.978824	1.706958	0.138526
C	6.468096	2.072135	-1.257718
C	4.926078	2.069436	-1.292489
N	4.559977	-1.297613	0.386486
C	4.114162	-1.148908	1.760119
N	0.743109	0.587984	-0.773885
C	-0.600812	0.990311	-0.641925
C	-1.496642	0.642416	-1.652209
C	-2.855989	0.889681	-1.491157
C	-3.346796	1.490228	-0.339839

C	-2.442671	1.836323	0.657866
C	-1.081291	1.591995	0.523591
C	-3.794915	0.481724	-2.589570
F	-3.761248	1.338331	-3.620958
C	-2.934581	2.428631	1.948670
F	-2.642169	3.731368	2.049030
C	5.223489	-2.569757	0.179990
F	-3.474799	-0.727026	-3.083884
F	-5.065098	0.417238	-2.166799
F	-4.262311	2.303878	2.084889
F	-2.367768	1.823766	3.009911
H	2.944929	-0.419976	-0.651102
H	0.873715	-0.341772	-1.166914
H	4.566251	1.793722	-2.290180
H	4.534118	3.065323	-1.073581
H	6.843812	3.053310	-1.562870
H	6.867193	1.349040	-1.980139
H	6.548070	2.405425	0.866287
H	8.064974	1.825090	0.200411
H	6.479728	0.161403	1.583853
H	7.369219	-0.435065	0.186625
H	4.266255	1.563279	0.706295
H	5.484004	-0.448395	-1.220253
H	6.115310	-2.706110	0.816192
H	4.514330	-3.374574	0.403051
H	5.530416	-2.659134	-0.866807
H	4.935447	-1.164149	2.495932
H	3.436529	-1.978025	1.989094
H	3.557677	-0.213717	1.880263
H	-1.132383	0.147637	-2.547833
H	-4.410186	1.648559	-0.205836
H	-0.395401	1.832766	1.327823
C	-0.958661	-1.861412	0.464285
C	-0.362561	-3.146209	0.023552
C	-1.027659	-4.483080	-0.063227
O	-0.634982	-2.145713	-0.899815
N	1.122678	-3.220232	0.297934
H	-0.261915	-1.166683	0.935585
C	-2.394055	-1.668103	0.796202
C	-2.728452	-1.084725	2.018752
C	-4.059684	-0.819511	2.324527
C	-5.060457	-1.136441	1.408203
C	-4.728064	-1.715146	0.184512
C	-3.397080	-1.979799	-0.123902
H	-1.943601	-0.804076	2.716510
H	-4.310026	-0.342084	3.266462
H	-6.097907	-0.917974	1.641481
H	-5.502466	-1.937972	-0.542531
H	-3.126086	-2.376809	-1.097662
H	-0.635330	-5.045500	-0.914178
H	-0.850095	-5.049548	0.850876
H	-2.100135	-4.334096	-0.192670
O	1.536378	-4.212268	0.859733
O	1.798950	-2.264701	-0.032153

RS epoxide:Catalyst, binary complex 149; Energy = -2449.838399; 6-31G(d) basis set.

N	-0.914252	-1.237917	-0.730947
H	-0.827539	-1.138683	-1.738424
C	0.054562	-2.021143	-0.133135
S	-0.026516	-2.561348	1.454183
N	1.055147	-2.300449	-0.991028
H	1.077077	-1.732552	-1.831190
C	-2.147535	-0.774168	-0.244108
C	-4.652703	0.252230	0.519826
C	-3.159646	-0.577763	-1.191802
C	-2.389912	-0.432676	1.089466
C	-3.638548	0.066542	1.449043
C	-4.390928	-0.069812	-0.807835
H	-2.981895	-0.827328	-2.233625
H	-1.619589	-0.558477	1.837230
H	-5.619589	0.641511	0.819034
C	-3.902682	0.372806	2.897439
C	-5.449965	0.179977	-1.844315
F	-4.360738	-0.701984	3.555270
F	-2.791883	0.776082	3.530029

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F         -4.822884        1.338876        3.036523
F         -6.674439       -0.078793       -1.364413
F         -5.452166        1.458553       -2.250015
F         -5.271944       -0.578788       -2.934700
C          2.306708       -3.011740       -0.726744
C          4.576232       -3.039871        0.313547
C          3.477369       -5.202075       -0.376272
C          4.418643       -4.530672        0.625731
C          2.118122       -4.498918       -0.404605
C          3.213532       -2.325916        0.316263
H          5.049640       -2.926656       -0.672365
H          3.930752       -5.165223       -1.377122
H          4.008634       -4.645932        1.637969
H          1.624235       -4.605082        0.565215
H          2.748980       -2.477861        1.297370
H          2.827473       -2.973940       -1.692485
H          5.242929       -2.566836        1.043678
H          3.342694       -6.259764       -0.127362
H          5.397194       -5.022709        0.619755
H          1.461435       -4.944728       -1.159336
N          3.256762       -0.877098        0.116827
C          3.782857       -0.165607        1.269627
H          3.214352       -0.446373        2.162098
H          3.667550        0.913866        1.110774
H          4.853046       -0.359060        1.456878
C          3.913106       -0.437900       -1.102017
H          5.007892       -0.579064       -1.089059
H          3.711045        0.629704       -1.240011
H          3.505206       -0.958617       -1.973021
C          0.923064        2.046555       -0.872607
N          0.324210        1.181502       -1.953337
O         -0.834635        1.363350       -2.248401
O          1.037632        0.296400       -2.402731
C          1.925628        3.019952       -1.332026
C          3.008676        3.509977       -0.436695
C          5.071706        4.324797        1.254128
C          4.340315        3.318285       -0.811919
C          2.712872        4.137634        0.774507
C          3.744375        4.541758        1.617198
C          5.368932        3.717362        0.035968
H          4.571152        2.857073       -1.769220
H          1.675874        4.318327        1.041483
H          3.510344        5.031492        2.557105
H          6.401780        3.559764       -0.257935
H          5.874110        4.638453        1.914314
C          0.831698        1.341146        0.446649
H          1.334224        0.368099        0.379401
H         -0.222296        1.212829        0.713005
H          1.321131        1.947836        1.210358
H          2.138404        3.036784       -2.401245
O          0.568574        3.375549       -1.007229

RS epoxide:Catalyst, binary complex 150; Energy = -2449.849579; 6-31G(d) basis set.
N         -2.266629        1.002138        0.741893
C         -2.141116        2.305278        1.008076
S         -3.358819        3.299804        1.613537
C         -3.445524        0.185312        1.032886
C         -3.711606       -0.778845       -0.159637
C         -3.976074       -2.196954        0.351531
C         -2.790145       -2.722068        1.174688
C         -2.282273       -1.708370        2.226653
C         -3.257121       -0.542135        2.370492
N         -4.791599       -0.256700       -0.997474
C         -5.096647       -1.148799       -2.107581
N         -0.909085        2.851251        0.716204
C          0.338606        2.205128        0.684889
C          0.646450        1.144232        1.543298
C          1.919519        0.585852        1.522150
C          2.910775        1.070077        0.676100
C          2.590856        2.120863       -0.177181
C          1.320676        2.684981       -0.186717
C          2.233075       -0.536226        2.473549
F          3.309238       -1.229623        2.085105
C          3.591130        2.553278       -1.209926
F          4.850282        2.402982       -0.783947
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C	-4.446844	1.055766	-1.541161
F	2.475102	-0.081061	3.711220
F	1.203924	-1.393693	2.571025
F	3.465366	1.807923	-2.327249
F	3.425604	3.829515	-1.571724
H	-1.514328	0.551233	0.223751
H	-0.902151	3.863385	0.720220
H	-2.908842	0.187061	3.110228
H	-4.231297	-0.904335	2.717803
H	-2.132589	-2.196739	3.194124
H	-1.301816	-1.322037	1.923395
H	-3.087892	-3.659293	1.655085
H	-1.972126	-2.971555	0.486711
H	-4.900623	-2.195850	0.941134
H	-4.139204	-2.880359	-0.485942
H	-4.293983	0.866933	1.120716
H	-2.779898	-0.836828	-0.764647
H	-4.278668	1.784853	-0.744967
H	-3.544146	1.020440	-2.178829
H	-5.281133	1.414919	-2.149650
H	-4.197711	-1.390213	-2.709254
H	-5.817756	-0.659140	-2.766872
H	-5.547395	-2.078871	-1.757266
H	-0.104460	0.764654	2.229904
H	3.897338	0.620210	0.663122
H	1.080929	3.489465	-0.875145
N	-1.025193	-0.137265	-2.522560
O	-0.972612	0.954071	-1.985731
O	-1.549524	-0.376778	-3.589121
C	-0.373078	-1.295063	-1.797477
C	0.901794	-0.917802	-1.139137
H	1.208683	0.117170	-1.292633
O	-0.332712	-1.043396	-0.427739
C	1.976552	-1.888513	-0.808850
C	4.049757	-3.631021	-0.159759
C	3.265611	-1.650766	-1.291671
C	1.729546	-2.990419	0.010865
C	2.767431	-3.860117	0.331992
C	4.298596	-2.524683	-0.970477
H	3.459852	-0.771838	-1.902188
H	0.736041	-3.141786	0.423273
H	2.575139	-4.710926	0.977887
H	5.299487	-2.338000	-1.346456
H	4.858866	-4.307576	0.096623
C	-0.781909	-2.637814	-2.311962
H	-0.548952	-2.723394	-3.373732
H	-1.857973	-2.781041	-2.173361
H	-0.239842	-3.405975	-1.759007

RS epoxide:Catalyst, binary complex 151; Energy = -2449.837775; 6-31G(d) basis set.

N	-2.948837	-0.429975	1.153926
C	-1.934679	-1.215650	0.743132
S	-2.082000	-2.614680	-0.174171
C	-4.380107	-0.547584	0.845346
C	-4.691971	-0.312952	-0.652473
C	-6.212559	-0.356822	-0.861015
C	-6.829763	-1.651025	-0.328514
C	-6.523848	-1.823208	1.159569
C	-5.013029	-1.830983	1.394965
N	-4.134054	0.916460	-1.218226
C	-2.758277	0.845306	-1.673343
N	-0.716018	-0.741168	1.181727
C	0.580291	-1.131942	0.800597
C	1.590828	-1.055995	1.758584
C	2.913411	-1.287336	1.395311
C	3.255103	-1.614284	0.091612
C	2.238485	-1.683914	-0.856064
C	0.912360	-1.442107	-0.522592
C	3.974756	-1.099520	2.440021
F	3.973107	0.165660	2.906690
C	2.567970	-2.031300	-2.281486
F	1.831623	-1.316109	-3.146289
C	-4.360610	2.124524	-0.450434
F	3.779152	-1.893775	3.501301
F	5.201548	-1.344966	1.967329

F	3.858274	-1.804607	-2.566960
F	2.327816	-3.324046	-2.542490
H	-2.680440	0.470325	1.541357
H	-0.741790	-0.014212	1.888569
H	-4.570932	-2.698954	0.898743
H	-4.779242	-1.909122	2.462763
H	-6.985459	-0.998701	1.721508
H	-6.961107	-2.752162	1.540004
H	-7.911288	-1.648492	-0.501421
H	-6.418244	-2.506152	-0.881718
H	-6.682222	0.493597	-0.346687
H	-6.411702	-0.231146	-1.929601
H	-4.830497	0.287730	1.398394
H	-4.253012	-1.143909	-1.215690
H	-5.410450	2.209909	-0.157045
H	-3.739652	2.193873	0.463398
H	-4.112869	2.994444	-1.067669
H	-2.017918	0.946102	-0.857550
H	-2.565590	1.658754	-2.382124
H	-2.579597	-0.109268	-2.175871
H	1.344679	-0.801652	2.786419
H	4.289464	-1.773940	-0.187620
H	0.140589	-1.464258	-1.283342
N	-1.144760	3.168766	0.814999
O	-1.926609	4.078604	0.673698
O	-1.326519	2.187650	1.523116
C	0.159275	3.275259	0.046031
C	0.689209	2.011060	-0.459330
H	0.099430	1.121135	-0.247200
O	-0.029219	2.949463	-1.291753
C	2.141740	1.804505	-0.724539
C	4.833158	1.268794	-1.202835
C	3.054345	1.817800	0.330026
C	2.576128	1.520997	-2.020685
C	3.920467	1.252451	-2.257197
C	4.401085	1.551900	0.090319
H	2.710289	2.018155	1.342250
H	1.857903	1.500865	-2.835355
H	4.254054	1.018820	-3.263149
H	5.104047	1.550488	0.917562
H	5.880866	1.054919	-1.390455
C	0.913040	4.518917	0.403571
H	0.315027	5.395729	0.146799
H	1.843650	4.531088	-0.165638
H	1.143930	4.535855	1.471948

RS epoxide:Catalyst, binary complex 152; Energy = -2449.836784; 6-31G(d) basis set.

N	-2.912057	-0.427730	0.334170
C	-1.801349	-1.178156	0.317036
S	-1.754007	-2.802540	-0.090263
C	-4.277890	-0.904922	0.101489
C	-5.224994	0.105909	0.811005
C	-5.326318	1.415347	0.003936
C	-5.528335	1.255337	-1.510853
C	-4.516788	0.282707	-2.118239
C	-4.559964	-1.062050	-1.396525
N	-6.527237	-0.414457	1.223141
C	-6.443608	-1.621488	2.021909
N	-0.689076	-0.449029	0.722327
C	0.655770	-0.845479	0.668436
C	1.491288	-0.529501	1.739540
C	2.853541	-0.801444	1.662416
C	3.408030	-1.392152	0.536583
C	2.564956	-1.696286	-0.528002
C	1.202981	-1.432009	-0.477472
C	3.722611	-0.374910	2.809643
F	5.003952	-0.712407	2.630028
C	3.127647	-2.315106	-1.777868
F	4.454733	-2.148972	-1.864223
C	-7.612813	-0.479444	0.264140
F	3.683730	0.963359	2.977291
F	3.316146	-0.910845	3.968428
F	2.887541	-3.632021	-1.832324
F	2.580449	-1.774894	-2.880053
H	-2.790573	0.576637	0.442639

H	-0.887157	0.286718	1.393573
H	-3.829996	-1.760204	-1.816812
H	-5.549215	-1.521493	-1.514745
H	-4.721741	0.142745	-3.184759
H	-3.506332	0.702342	-2.042327
H	-6.537239	0.894101	-1.735980
H	-5.437703	2.240391	-1.981992
H	-6.118208	2.030141	0.446737
H	-4.392091	1.975028	0.153929
H	-4.344112	-1.882452	0.588484
H	-4.721978	0.349733	1.759239
H	-7.801739	0.504382	-0.168864
H	-7.465517	-1.204447	-0.554927
H	-8.518982	-0.776368	0.802523
H	-6.266209	-2.538407	1.433036
H	-7.382476	-1.756973	2.569177
H	-5.633412	-1.525451	2.752313
H	1.077891	-0.067652	2.632960
H	4.473093	-1.578803	0.473682
H	0.568427	-1.656047	-1.327678
N	-1.107426	2.470260	-0.057055
O	-1.792281	2.125482	-0.991880
O	-1.449826	2.413025	1.116370
C	0.310655	2.929141	-0.331720
C	1.050962	1.928080	-1.128032
H	0.465132	1.067771	-1.454836
O	0.525759	3.154325	-1.673253
C	2.527746	1.723095	-1.089994
C	5.267989	1.185040	-1.120616
C	3.132997	1.206216	-2.240517
C	3.299934	1.949372	0.048368
C	4.668791	1.686376	0.030490
C	4.496531	0.939043	-2.256492
H	2.526682	0.996864	-3.117690
H	2.838400	2.289568	0.968971
H	5.256335	1.852890	0.928157
H	4.953716	0.524586	-3.149196
H	6.332075	0.970340	-1.130534
C	0.801904	3.917598	0.685405
H	0.114072	4.766152	0.728510
H	1.782279	4.273722	0.368955
H	0.869416	3.468995	1.676944

RS epoxide:Catalyst, binary complex 153; Energy = -2449.833819; 6-31G(d) basis set.

N	-2.147226	-1.192767	0.510888
C	-1.001967	-1.071149	-0.201532
S	-0.977179	-0.776084	-1.849618
C	-3.479097	-1.147560	-0.077822
C	-4.448891	-1.912516	0.832122
C	-5.785635	-2.116627	0.079632
C	-6.056756	-0.992950	-0.939647
C	-5.518295	0.345018	-0.426311
C	-3.985576	0.293638	-0.247730
N	-3.823849	-3.117847	1.386404
C	-3.403239	-4.096168	0.390532
N	0.106209	-1.164158	0.608414
C	1.476446	-1.122014	0.316022
C	2.035397	-1.446739	-0.923668
C	3.415417	-1.377954	-1.083580
C	4.264186	-1.018016	-0.045317
C	3.694950	-0.721251	1.187273
C	2.322835	-0.769004	1.372583
C	3.992009	-1.609280	-2.451552
F	3.282050	-2.500983	-3.153539
C	4.584442	-0.327434	2.331245
F	5.109748	-1.395720	2.949025
C	-4.655662	-3.741110	2.404233
F	4.009502	-0.469906	-3.166824
F	5.256595	-2.050442	-2.391402
F	5.614194	0.425144	1.912311
F	3.922174	0.379358	3.259698
H	-2.121345	-1.741525	1.371226
H	-0.094771	-1.112690	1.600829
H	-3.706742	0.854499	0.654259
H	-3.470003	0.753563	-1.097135

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H         -5.784995        1.161269       -1.102707
H         -5.997730        0.568935        0.534711
H         -5.576937       -1.229869       -1.896806
H         -7.130389       -0.925532       -1.140052
H         -5.775914       -3.084614       -0.434635
H         -6.598942       -2.157774        0.812712
H         -3.429795       -1.631647       -1.060821
H         -4.639165       -1.266714        1.703234
H         -4.947248       -2.993726        3.148732
H         -5.571802       -4.195498        1.991252
H         -4.086237       -4.528172        2.907860
H         -2.840720       -4.886967        0.895867
H         -2.742608       -3.631611       -0.347691
H         -4.242215       -4.571256       -0.142554
H          1.404102       -1.735197       -1.752062
H          5.336740       -0.958008       -0.194654
H          1.902206       -0.497061        2.336300
N         -3.170409        3.486781        0.028383
O         -4.042152        3.313672       -0.794880
O         -3.337578        3.703490        1.215125
C         -1.738605        3.476058       -0.441444
C         -0.997133        2.246477       -0.141750
H         -1.548059        1.450900        0.362447
O         -1.510452        2.554088       -1.446897
C          0.482872        2.268235        0.042254
C          3.244348        2.345130        0.403055
C          1.015155        2.579691        1.295890
C          1.331840        1.988916       -1.027470
C          2.712901        2.018294       -0.842062
C          2.394829        2.623472        1.473845
H          0.346709        2.804988        2.124121
H          0.902241        1.740657       -1.993051
H          3.370221        1.772700       -1.670976
H          2.808796        2.869764        2.446744
H          4.320640        2.362525        0.547855
C         -1.181243        4.865178       -0.534998
H         -1.263226        5.366426        0.431816
H         -1.730001        5.434761       -1.289818
H         -0.131100        4.801088       -0.824742

RS epoxide:Catalyst, binary complex 154; Energy = -2449.838551; 6-31G(d) basis set.
N         -3.005455       -0.290588        0.095021
C         -1.905811       -0.928439       -0.334808
S         -1.892326       -2.058330       -1.576029
C         -4.334155       -0.388873       -0.506409
C         -5.401306       -0.362638        0.627974
C         -6.648658        0.382707        0.150820
C         -6.326184        1.860640       -0.125879
C         -4.944833        2.032540       -0.796726
C         -4.534416        0.750612       -1.521497
N         -5.724681       -1.667979        1.202495
C         -4.561604       -2.344788        1.755407
N         -0.787231       -0.578028        0.404158
C          0.547231       -0.981753        0.239959
C          1.331149       -1.121260        1.386692
C          2.691607       -1.385451        1.275791
C          3.299306       -1.531692        0.037355
C          2.507897       -1.393343       -1.097816
C          1.148163       -1.120788       -1.016004
C          3.500439       -1.449854        2.539161
F          3.148412       -2.489239        3.308508
C          3.123098       -1.513464       -2.464869
F          4.459429       -1.423260       -2.423191
C         -6.444414       -2.560117        0.308029
F          4.812146       -1.549069        2.296564
F          3.314581       -0.343199        3.286666
F          2.819393       -2.681543       -3.045907
F          2.678902       -0.545778       -3.284858
H         -2.865832        0.503954        0.716950
H         -0.983926       -0.157859        1.306753
H         -3.606364        0.883155       -2.085933
H         -5.310372        0.463586       -2.240891
H         -4.954898        2.880253       -1.488273
H         -4.181236        2.269608       -0.044222
H         -7.109675        2.280780       -0.765028
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H	-6.353084	2.424187	0.813269
H	-7.032385	-0.083868	-0.763981
H	-7.431730	0.286565	0.909439
H	-4.365307	-1.351346	-1.022370
H	-4.979640	0.227941	1.458440
H	-5.864447	-2.857453	-0.584309
H	-6.693429	-3.473765	0.856230
H	-7.381363	-2.104909	-0.020471
H	-3.855288	-2.705180	0.986239
H	-4.895301	-3.209629	2.338123
H	-4.022923	-1.665245	2.424071
H	0.881015	-1.004137	2.369611
H	4.365322	-1.705320	-0.043982
H	0.560807	-0.989314	-1.916738
N	-1.129031	2.442995	0.296029
O	-1.670423	2.137158	1.353670
O	-1.630101	2.339851	-0.796275
C	0.307094	2.922116	0.388882
C	1.185994	2.188169	-0.544158
H	0.681854	1.477337	-1.199249
O	0.720436	3.530049	-0.777781
C	2.643566	1.951929	-0.334200
C	5.365959	1.384555	-0.084931
C	3.449592	1.847976	-1.472786
C	3.206555	1.755351	0.926144
C	4.567356	1.479513	1.050382
C	4.804532	1.563825	-1.349309
H	3.005663	1.974061	-2.456203
H	2.584456	1.774180	1.815482
H	4.993990	1.317588	2.034991
H	5.419764	1.474213	-2.238850
H	6.423733	1.160567	0.012745
C	0.623540	3.556094	1.711779
H	-0.070414	4.380421	1.895323
H	1.638842	3.950494	1.666132
H	0.538920	2.838524	2.528392

RS epoxide:Catalyst, binary complex 155; Energy = -2449.835060; 6-31G(d) basis set.

N	2.126511	-0.993387	-0.426552
C	0.820765	-0.733709	-0.569943
S	0.294562	0.626379	-1.428303
C	2.760421	-1.976672	0.448914
C	4.288897	-1.977758	0.160025
C	5.048467	-2.582330	1.367164
C	4.196983	-3.548013	2.194930
C	2.998791	-2.812432	2.823246
C	2.526148	-1.652785	1.931065
N	4.712569	-2.601951	-1.090041
C	4.313403	-1.902151	-2.300539
N	-0.024659	-1.648526	0.000978
C	-1.433225	-1.577234	0.022065
C	-2.183355	-2.694718	-0.326036
C	-3.575485	-2.639821	-0.265718
C	-4.232022	-1.478867	0.111307
C	-3.465717	-0.367897	0.461531
C	-2.081232	-0.413565	0.444841
C	-4.345163	-3.879127	-0.625675
F	-4.027544	-4.311397	-1.854950
C	-4.148512	0.922004	0.819115
F	-3.410926	1.660612	1.660471
C	4.454652	-4.024793	-1.194332
F	-4.066322	-4.885282	0.218982
F	-5.667377	-3.679755	-0.593090
F	-4.365389	1.677407	-0.271379
F	-5.339531	0.711756	1.393628
H	2.735707	-0.319991	-0.882136
H	0.376100	-2.539486	0.270965
H	3.086606	-0.737070	2.150815
H	1.472450	-1.422049	2.116294
H	2.178679	-3.519639	2.991086
H	3.274552	-2.414808	3.805241
H	3.835381	-4.362247	1.555625
H	4.806241	-4.017232	2.973334
H	5.953355	-3.065979	0.987801
H	5.382710	-1.767799	2.019908

H	2.359199	-2.976074	0.214524
H	4.570867	-0.917739	0.078373
H	4.909046	-4.561230	-0.357188
H	3.380594	-4.285119	-1.235013
H	4.913642	-4.397974	-2.115024
H	3.248075	-2.023581	-2.559587
H	4.906548	-2.281161	-3.139575
H	4.523684	-0.832567	-2.194578
H	-1.688661	-3.603932	-0.656823
H	-5.314696	-1.438882	0.142351
H	-1.495742	0.441102	0.758936
N	3.156155	2.001568	-0.174532
O	3.216851	1.513922	0.934126
O	3.658800	1.516729	-1.175452
C	2.383797	3.289357	-0.340291
C	1.228553	3.407497	0.573801
H	1.056441	2.551166	1.224156
O	2.474522	4.066289	0.809347
C	0.049951	4.260410	0.256181
C	-2.189713	5.829491	-0.289428
C	-1.196515	3.660762	0.063520
C	0.171078	5.648648	0.182107
C	-0.948121	6.429912	-0.092614
C	-2.313081	4.443662	-0.209873
H	-1.285420	2.579155	0.109642
H	1.139930	6.108003	0.354439
H	-0.850449	7.509804	-0.146526
H	-3.277008	3.967425	-0.354454
H	-3.061535	6.440689	-0.501482
C	2.511057	3.889090	-1.703374
H	3.554337	4.122291	-1.926994
H	1.917863	4.803844	-1.732532
H	2.131965	3.185732	-2.446787

RS epoxide:Catalyst, binary complex 156; Energy = -2449.850872; 6-31G(d) basis set.

N	-2.273957	-0.755026	-1.071079
C	-1.105280	-1.416502	-1.023674
S	-0.960829	-3.054338	-0.652806
C	-3.590408	-1.339802	-0.869403
C	-4.450427	-0.440893	0.030552
C	-5.755922	-1.191027	0.399974
C	-6.179975	-2.209846	-0.672370
C	-5.824384	-1.690713	-2.065476
C	-4.296785	-1.564756	-2.221029
N	-3.690982	0.082684	1.171091
C	-3.137758	-0.937018	2.050053
N	-0.037210	-0.613010	-1.347289
C	1.325773	-0.769565	-1.059214
C	1.799141	-1.482170	0.049129
C	3.157450	-1.482584	0.327280
C	4.068870	-0.775446	-0.453235
C	3.582073	-0.054554	-1.532698
C	2.227764	-0.056524	-1.848986
C	3.670682	-2.250431	1.513004
F	4.220309	-3.418007	1.148287
C	4.501225	0.851352	-2.296396
F	4.144221	0.968173	-3.582193
C	-4.460300	1.064950	1.920833
F	4.626303	-1.562618	2.163189
F	2.702463	-2.523711	2.396255
F	4.483383	2.094720	-1.774945
F	5.771432	0.431455	-2.259051
H	-2.263224	0.257381	-1.197742
H	-0.268585	0.280245	-1.770327
H	-4.054061	-0.725047	-2.882641
H	-3.872273	-2.464979	-2.678004
H	-6.228488	-2.345477	-2.843182
H	-6.296169	-0.709952	-2.205096
H	-5.672271	-3.168002	-0.505438
H	-7.253099	-2.409100	-0.592334
H	-5.630020	-1.701979	1.361149
H	-6.553024	-0.452350	0.540088
H	-3.425532	-2.302955	-0.379736
H	-4.717697	0.443955	-0.564260
H	-5.300439	0.624624	2.484410

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H         -3.802255        1.569019        2.637891
H         -4.856611        1.818411        1.232675
H         -3.899826       -1.552672        2.556637
H         -2.556374       -0.439336        2.833933
H         -2.465776       -1.600756        1.495723
H          1.109088       -2.005981        0.696724
H          5.125036       -0.765145       -0.206330
H          1.868453        0.516231       -2.699524
N         -2.692120        3.029758       -0.036692
O         -3.185094        2.257421       -0.835400
O         -3.304236        3.829196        0.640499
C         -1.193201        2.987079        0.154866
C         -0.702190        1.665646        0.618011
H         -1.486040        0.918635        0.782996
O         -0.608440        2.112564       -0.747272
C          0.580968        1.473804        1.344192
C          2.973165        0.999689        2.701338
C          1.789281        1.947073        0.823417
C          0.580285        0.743199        2.532989
C          1.773471        0.508880        3.211058
C          2.979252        1.713502        1.503511
H          1.801510        2.464393       -0.131799
H         -0.354262        0.345843        2.919932
H          1.767423       -0.069734        4.129055
H          3.914150        2.068417        1.080322
H          3.904257        0.805356        3.222991
C         -0.597333        4.334202        0.422662
H         -1.089935        4.794832        1.278671
H         -0.718909        4.979056       -0.451705
H          0.464653        4.216827        0.638792

RS epoxide:Catalyst, binary complex 157; Energy = -2449.835623; 6-31G(d) basis set.
N         -2.845297       -0.373156        0.350934
C         -1.733256       -1.109255        0.206094
S         -1.697278       -2.640734       -0.479328
C         -4.165785       -0.729381       -0.160215
C         -5.239325        0.019028        0.682919
C         -5.699513        1.257249       -0.094872
C         -6.388936        0.895512       -1.421553
C         -5.746456       -0.344766       -2.068282
C         -4.275786       -0.439311       -1.668297
N         -6.338984       -0.892558        1.020210
C         -7.494695       -0.194764        1.569953
N         -0.622315       -0.470085        0.734099
C          0.724914       -0.854387        0.673403
C          1.298943       -1.417122       -0.471880
C          2.664879       -1.667935       -0.500041
C          3.488579       -1.367616        0.579587
C          2.908372       -0.795741        1.702813
C          1.542668       -0.543858        1.761434
C          3.252709       -2.275885       -1.743836
F          3.037288       -3.597313       -1.798828
C          3.753506       -0.354810        2.861984
F          5.040700       -0.680911        2.706395
C         -5.902747       -1.878617        2.003602
F          2.709436       -1.747221       -2.852933
F          4.577902       -2.086888       -1.814175
F          3.698369        0.984619        3.017463
F          3.332398       -0.885084        4.018249
H         -2.728464        0.603599        0.614759
H         -0.823970        0.239565        1.431448
H         -3.760462        0.501687       -1.898027
H         -3.755105       -1.232484       -2.211761
H         -6.262998       -1.247270       -1.723291
H         -5.848000       -0.306566       -3.157031
H         -7.457325        0.717077       -1.262500
H         -6.312648        1.754105       -2.098194
H         -6.336233        1.896614        0.522932
H         -4.796646        1.847833       -0.300896
H         -4.277562       -1.805783       -0.021795
H         -4.757747        0.365352        1.621000
H         -5.032479       -2.437002        1.652860
H         -5.636620       -1.405900        2.967585
H         -6.709387       -2.594580        2.183060
H         -7.239291        0.407134        2.462389
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H         -8.242175       -0.935569        1.866810
H         -7.952046        0.460793        0.827570
H          0.684559       -1.638881       -1.336043
H          4.556516       -1.541700        0.531079
H          1.111623       -0.096478        2.653922
N         -1.145280        2.428221       -0.181876
O         -1.803971        2.087939       -1.134744
O         -1.518871        2.372508        0.984470
C          0.277166        2.897753       -0.414216
C          1.056833        1.904216       -1.180478
H          0.496073        1.032259       -1.520616
O          0.530026        3.118706       -1.749870
C          2.535988        1.729494       -1.098395
C          5.288140        1.257459       -1.053649
C          3.269267        1.964366        0.063877
C          3.186556        1.237669       -2.235035
C          4.555864        1.002428       -2.213157
C          4.644390        1.735039        0.083211
H          2.773098        2.285030        0.973774
H          2.611020        1.022561       -3.131228
H          5.048593        0.605959       -3.095105
H          5.201970        1.907964        0.998550
H          6.356945        1.068363       -1.034519
C          0.726776        3.898652        0.610179
H          0.770357        3.457704        1.606527
H          0.028982        4.739980        0.626954
H          1.712382        4.262873        0.320168

RS epoxide:Catalyst, binary complex 158; Energy = -2449.838232; 6-31G(d) basis set.
N         -0.912819       -1.267081       -0.711353
H         -0.831277       -1.183411       -1.720597
C          0.066020       -2.032284       -0.106523
S         -0.004608       -2.554649        1.487154
N          1.067439       -2.310646       -0.963973
H          1.083482       -1.749072       -1.808536
C         -2.146667       -0.802319       -0.226952
C         -4.661498        0.204352        0.531729
C         -3.160938       -0.620261       -1.175965
C         -2.392217       -0.456012        1.104483
C         -3.645267        0.035103        1.461221
C         -4.396734       -0.122701       -0.794511
H         -2.982591       -0.878625       -2.215521
H         -1.625659       -0.586519        1.855571
H         -5.636367        0.572899        0.830850
C         -3.872064        0.454307        2.887464
C         -5.464323        0.099944       -1.828547
F         -3.464768        1.717587        3.094793
F         -5.169495        0.401335        3.219483
F         -3.198745       -0.317928        3.749426
F         -5.269261       -0.651485       -2.920959
F         -6.679964       -0.192770       -1.345283
F         -5.503016        1.378854       -2.231228
C          2.325478       -3.009145       -0.696165
C          4.598411       -3.008049        0.337370
C          3.515987       -5.185841       -0.328985
C          4.455141       -4.497339        0.663373
C          2.150527       -4.494756       -0.359443
C          3.229533       -2.306433        0.337997
H          5.067585       -2.899401       -0.651102
H          3.965531       -5.154573       -1.331766
H          4.050053       -4.607228        1.678191
H          1.660606       -4.596090        0.612939
H          2.769180       -2.453891        1.321688
H          2.843323       -2.976190       -1.663678
H          5.263116       -2.522307        1.060993
H          3.391275       -6.242296       -0.069763
H          5.437887       -4.980963        0.657874
H          1.495492       -4.953373       -1.107921
N          3.259737       -0.859164        0.125547
C          3.775205       -0.132168        1.273469
H          3.203383       -0.406320        2.165880
H          3.654938        0.944803        1.101979
H          4.845467       -0.317711        1.468318
C          3.917671       -0.425289       -1.094426
H          5.015045       -0.542895       -1.068703
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H          3.694708        0.635404       -1.251985
H          3.530824       -0.969740       -1.960459
C          0.897144        2.031398       -0.896581
N          0.298319        1.153894       -1.967236
O         -0.862420        1.327497       -2.259504
O          1.014463        0.268390       -2.411671
C          1.892501        3.006117       -1.368784
C          2.977798        3.508409       -0.483081
C          5.046654        4.343982        1.190495
C          4.308202        3.321562       -0.865129
C          2.685935        4.142080        0.725955
C          3.720385        4.556476        1.560049
C          5.339816        3.731002       -0.025883
H          4.535671        2.855615       -1.820954
H          1.649670        4.319384        0.998036
H          3.489411        5.050668        2.498370
H          6.371679        3.577016       -0.325127
H          5.851315        4.665456        1.844148
C          0.815548        1.336345        0.428768
H          1.327934        0.367922        0.368863
H         -0.236648        1.199626        0.698142
H          1.299985        1.954720        1.186259
H          2.099898        3.015299       -2.439146
O          0.535186        3.357356       -1.040411

RS epoxide:Catalyst, binary complex 159; Energy = -2449.837878; 6-31G(d) basis set.
N         -1.464344       -1.143148       -2.107915
C         -0.966947        0.084144       -2.314910
S         -1.823376        1.466190       -2.734325
C         -2.841055       -1.559889       -1.788166
C         -3.155845       -1.258884       -0.312617
C         -4.645546       -1.521983       -0.054044
C         -5.542316       -0.527102       -0.814414
C         -4.859799        0.004163       -2.085210
C         -3.954595       -1.046250       -2.734036
N         -2.229395       -1.990065        0.568517
C         -2.595884       -3.388682        0.774108
N          0.407908        0.190934       -2.213205
C          1.313787       -0.469172       -1.369214
C          0.946569       -1.279573       -0.290452
C          1.946134       -1.805438        0.528396
C          3.290194       -1.541537        0.321025
C          3.635161       -0.722010       -0.751994
C          2.672418       -0.202627       -1.596414
C          1.521496       -2.594259        1.733753
F          1.075276       -1.783811        2.712233
C          5.082013       -0.363217       -0.937706
F          5.271835        0.466618       -1.969987
C         -2.061910       -1.320799        1.853584
F          0.518223       -3.437817        1.447401
F          2.524464       -3.315833        2.246241
F          5.568508        0.246044        0.158909
F          5.840283       -1.449024       -1.140699
H         -0.778006       -1.872837       -1.959045
H          0.742168        1.076921       -2.575185
H         -3.506458       -0.657475       -3.651062
H         -4.566226       -1.911460       -3.017831
H         -5.611130        0.332458       -2.811035
H         -4.260235        0.883657       -1.838989
H         -6.487650       -1.021152       -1.064625
H         -5.788744        0.317256       -0.163163
H         -4.876285       -2.547641       -0.372269
H         -4.850600       -1.476271        1.021134
H         -2.794519       -2.647933       -1.900942
H         -2.962132       -0.189771       -0.156504
H         -1.506858       -0.385175        1.717429
H         -3.014411       -1.083017        2.355305
H         -1.468866       -1.956982        2.514870
H         -3.511110       -3.512162        1.374536
H         -1.777385       -3.894584        1.289805
H         -2.749790       -3.891145       -0.185361
H         -0.097637       -1.493473       -0.052549
H          4.049021       -1.947411        0.981195
H          2.962557        0.440252       -2.421063
N         -2.759641        1.846719        2.147553
```

O	-3.538981	1.525381	1.274366
O	-2.845932	1.539755	3.321427
C	-1.539651	2.642790	1.752648
C	-0.796109	2.058158	0.618684
H	-1.213253	1.156648	0.166027
O	-1.653421	3.187542	0.483903
C	0.670950	2.278952	0.469054
C	3.413758	2.641265	0.137889
C	1.568786	1.621134	1.312767
C	1.144002	3.117743	-0.540130
C	2.517080	3.291428	-0.707972
C	2.938462	1.809897	1.151372
H	1.194732	0.954330	2.087122
H	0.431760	3.624804	-1.185794
H	2.885871	3.942742	-1.494546
H	3.636887	1.298300	1.806467
H	4.483191	2.772772	0.004013
C	-0.955649	3.449152	2.872329
H	-1.701958	4.141529	3.269305
H	-0.112619	4.016405	2.475429
H	-0.611626	2.798854	3.677437

RS epoxide:Catalyst, binary complex 160; Energy = -2449.839856; 6-31G(d) basis set.

N	1.499080	0.448658	-0.653705
H	0.708804	-0.186363	-0.739376
C	1.145297	1.764999	-0.436467
S	2.094469	2.842839	0.438322
N	-0.041644	2.049223	-1.010887
H	-0.478485	1.265567	-1.486481
C	2.713605	-0.177674	-0.345700
C	5.088820	-1.576746	0.187965
C	2.671015	-1.472594	0.172604
C	3.952222	0.414464	-0.612704
C	5.117650	-0.285961	-0.332891
C	3.852538	-2.160866	0.427421
H	1.711728	-1.937189	0.384329
H	3.997940	1.408424	-1.039327
H	6.007431	-2.113599	0.395058
C	6.443343	0.382146	-0.569255
C	3.773737	-3.577145	0.920000
F	6.846124	1.080047	0.502824
F	7.406421	-0.513140	-0.836377
F	6.390955	1.238858	-1.598605
F	3.595245	-4.441827	-0.093038
F	4.890130	-3.947409	1.560343
F	2.743467	-3.752955	1.761399
C	-1.014578	3.057090	-0.577061
C	-2.423013	3.915641	1.337098
C	-1.699748	5.479105	-0.490367
C	-1.981064	5.342604	1.007035
C	-0.616054	4.493388	-0.930905
C	-1.357541	2.893465	0.916726
H	-3.364989	3.713096	0.808298
H	-2.627331	5.289047	-1.049570
H	-1.070293	5.584915	1.570566
H	0.326305	4.733251	-0.430608
H	-0.441426	3.123262	1.471520
H	-1.917303	2.812959	-1.155749
H	-2.629044	3.807657	2.409217
H	-1.388956	6.500972	-0.731222
H	-2.751264	6.055652	1.320433
H	-0.439034	4.556747	-2.009958
N	-1.676265	1.487687	1.206609
C	-1.205623	1.055571	2.511751
H	-0.135315	1.262956	2.599737
H	-1.352771	-0.026043	2.606812
H	-1.730812	1.545546	3.351398
C	-3.067317	1.132077	1.014636
H	-3.750153	1.569244	1.765012
H	-3.171934	0.041345	1.084300
H	-3.407257	1.448217	0.021165
C	-3.161952	-1.850520	-0.889686
N	-1.917267	-1.009102	-1.061404
O	-0.990342	-1.228333	-0.304195
O	-1.922078	-0.160301	-1.931826

C	-4.415445	-1.127975	-1.214111
C	-5.707766	-1.495059	-0.577559
C	-8.112935	-2.127114	0.676181
C	-6.305483	-0.579058	0.290153
C	-6.321520	-2.722257	-0.829437
C	-7.524108	-3.034795	-0.201572
C	-7.503344	-0.897708	0.920384
H	-5.834147	0.384931	0.467855
H	-5.859817	-3.416951	-1.525124
H	-8.003877	-3.987673	-0.401214
H	-7.962637	-0.185438	1.598235
H	-9.049698	-2.374285	1.165478
C	-2.992008	-2.971400	0.086888
H	-2.707538	-2.586556	1.067759
H	-2.220628	-3.662873	-0.259254
H	-3.941587	-3.501143	0.169636
H	-4.299492	-0.092224	-1.530108
O	-3.802417	-2.057409	-2.102971

RS epoxide:Catalyst, binary complex 161; Energy = -2449.837856; 6-31G(d) basis set.

N	1.270738	0.306106	0.605573
H	0.766071	-0.229323	1.307597
C	0.487447	1.135166	-0.164225
S	0.964713	1.733055	-1.652984
N	-0.722608	1.335861	0.427780
H	-0.679225	1.251139	1.440231
C	2.523825	-0.242254	0.273300
C	5.008263	-1.428935	-0.256339
C	2.709975	-1.609514	0.475873
C	3.586275	0.538611	-0.185000
C	4.808466	-0.066245	-0.453015
C	3.947490	-2.188859	0.217992
H	1.879367	-2.221546	0.818471
H	3.453207	1.603615	-0.331613
H	5.966903	-1.885652	-0.470879
C	5.943541	0.805058	-0.913880
C	4.117345	-3.656699	0.487776
F	5.562514	1.632795	-1.895964
F	6.404026	1.575724	0.084841
F	6.977093	0.083582	-1.367759
F	3.081505	-4.365646	0.013241
F	5.232790	-4.146448	-0.067314
F	4.183805	-3.908538	1.804964
C	-1.768047	2.291338	0.038765
C	-2.527475	4.678487	-0.012027
C	-3.576348	2.978220	-1.546655
C	-3.162345	4.442514	-1.384669
C	-2.372863	2.054303	-1.347880
C	-1.319932	3.753889	0.216463
H	-3.282793	4.486869	0.762892
H	-4.354071	2.732510	-0.809433
H	-2.438846	4.699810	-2.170124
H	-1.626390	2.253945	-2.119567
H	-0.577200	3.951614	-0.566859
H	-2.570149	2.082756	0.760563
H	-2.217660	5.724827	0.095764
H	-4.011191	2.811554	-2.537856
H	-4.025856	5.103372	-1.517230
H	-2.673879	1.005587	-1.438443
N	-0.619963	3.928568	1.491883
C	0.253238	5.089153	1.495291
H	0.933238	5.039021	0.639937
H	0.854070	5.086244	2.410465
H	-0.290757	6.049832	1.455002
C	-1.480687	3.927851	2.664021
H	-2.115769	4.826747	2.745454
H	-0.856809	3.878248	3.562059
H	-2.134343	3.048919	2.664543
C	-2.811289	-1.199747	0.459374
N	-1.883328	-0.963190	1.621329
O	-0.817557	-1.558174	1.603303
O	-2.245343	-0.209663	2.499678
C	-4.211391	-1.465663	0.875745
C	-5.141173	-2.258450	0.027514
C	-6.877362	-3.783374	-1.529455

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C         -5.608375       -3.486327        0.499913
C         -5.552320       -1.789119       -1.220600
C         -6.420748       -2.552531       -1.995705
C         -6.471157       -4.248868       -0.280289
H         -5.296014       -3.843939        1.477728
H         -5.199976       -0.822708       -1.570078
H         -6.744604       -2.183087       -2.963466
H         -6.830146       -5.204194        0.088757
H         -7.553308       -4.377354       -2.136337
C         -2.114384       -1.710137       -0.763558
H         -1.657770       -2.680371       -0.564432
H         -1.338037       -1.004315       -1.073738
H         -2.849765       -1.814401       -1.562497
H         -4.397191       -1.466801        1.949771
O         -3.771579       -0.203868        0.378849

RS epoxide:Catalyst, binary complex 1, AA-RS1; Energy = -2450.622356; TZVP basis set.
N         -2.623517        3.099868       -0.127892
O         -3.073705        2.310103       -0.926741
O         -3.262087        3.941145        0.458204
N         -2.255322       -0.796468       -1.056841
C         -1.067692       -1.411628       -0.963502
S         -0.887663       -3.032033       -0.535686
C         -3.545910       -1.421326       -0.806092
C         -4.453062       -0.441769       -0.054446
C         -5.794509       -1.130812        0.235941
C         -6.460494       -1.604038       -1.056660
C         -5.545085       -2.551332       -1.828581
C         -4.196677       -1.892337       -2.107054
N         -3.766291        0.130457        1.109726
C         -3.321746       -0.847544        2.092558
N         -0.020314       -0.586271       -1.290940
C          1.347372       -0.707876       -1.023825
C          2.210608        0.058530       -1.802055
C          3.570574        0.067991       -1.531565
C          4.102913       -0.687599       -0.503107
C          3.228618       -1.441806        0.269651
C          1.866118       -1.456442        0.035983
C          4.456150        0.983342       -2.328797
F          4.101723        1.032150       -3.618906
C          3.801007       -2.271238        1.387060
F          2.879334       -2.629552        2.285062
C         -4.540665        1.189072        1.741264
F          4.391198        2.246322       -1.866657
F          5.740780        0.619289       -2.278916
F          4.362020       -3.400289        0.927389
F          4.765661       -1.610787        2.048217
H         -2.279291        0.208114       -1.213688
H         -0.273847        0.289832       -1.731534
H         -4.331671       -1.028983       -2.767568
H         -3.514783       -2.585722       -2.603301
H         -5.384648       -3.460466       -1.239800
H         -6.011937       -2.857634       -2.766274
H         -7.410571       -2.091379       -0.830024
H         -6.689672       -0.734410       -1.681799
H         -5.630903       -1.991977        0.891683
H         -6.454208       -0.440534        0.764938
H         -3.358979       -2.296840       -0.182721
H         -4.651456        0.405430       -0.723027
H         -5.391935        0.814327        2.327424
H         -3.895015        1.754713        2.417393
H         -4.917608        1.873201        0.979567
H         -2.845905       -0.314681        2.917862
H         -2.584531       -1.526548        1.658954
H         -4.141886       -1.441755        2.519930
H          1.814391        0.655960       -2.614907
H          5.164923       -0.680987       -0.297585
H          1.207506       -2.027255        0.671279
C         -1.135838        3.020339        0.188007
C         -0.720869        1.672812        0.641698
H         -1.531685        0.945493        0.719838
O         -0.504097        2.164575       -0.692245
C         -0.543709        4.341092        0.553511
H          0.496893        4.197125        0.832045
H         -1.083552        4.769852        1.393838
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H         -0.600817        5.024161       -0.293987
C          0.489708        1.405574        1.456289
C          2.732673        0.769234        2.975577
C          1.745997        1.878237        1.079218
C          0.366829        0.593291        2.579840
C          1.485323        0.280644        3.340960
C          2.861626        1.563012        1.840853
H          1.854120        2.461922        0.173118
H         -0.603591        0.192248        2.847499
H          1.385053       -0.357534        4.209218
H          3.836699        1.923220        1.537329
H          3.606735        0.515216        3.561095

RS epoxide:Catalyst, binary complex 2, AS-RS2; Energy = -2450.620550; TZVP basis set.
N         -1.763990       -1.532907       -0.786035
C         -1.160192       -2.641386       -1.197951
S         -1.959730       -4.048351       -1.676441
C         -3.182477       -1.422006       -0.479104
C         -3.368168       -0.496023        0.726381
C         -4.857631       -0.474482        1.097895
C         -5.696790        0.017404       -0.083352
C         -5.471044       -0.846307       -1.322768
C         -3.987188       -0.917966       -1.676635
N         -2.430590       -0.825035        1.807234
C         -2.542059       -2.183287        2.319868
N          0.216906       -2.609405       -1.257088
C          1.129372       -1.877541       -0.487290
C          2.463963       -1.900210       -0.905167
C          3.438157       -1.255918       -0.168714
C          3.126019       -0.559075        0.989753
C          1.803195       -0.545239        1.392814
C          0.798736       -1.196910        0.686448
C          4.865791       -1.342303       -0.636220
F          5.643234       -0.418456       -0.063367
C          1.413161        0.161772        2.662246
F          2.451631        0.755336        3.256781
C         -2.489876        0.146490        2.890089
F          5.405485       -2.538234       -0.358847
F          4.966231       -1.178079       -1.964715
F          0.490968        1.115387        2.443702
F          0.874903       -0.684860        3.552700
H         -1.223504       -0.684773       -0.661251
H          0.597676       -3.405659       -1.748618
H         -3.617607        0.076010       -1.954062
H         -3.814871       -1.587962       -2.520771
H         -5.838867       -1.859800       -1.131236
H         -6.039321       -0.457057       -2.169471
H         -6.754603        0.025847        0.186174
H         -5.416894        1.052458       -0.307383
H         -5.183337       -1.479692        1.385819
H         -5.014595        0.178660        1.957927
H         -3.529453       -2.428255       -0.235644
H         -3.094088        0.514003        0.405964
H         -3.411120        0.071355        3.485358
H         -1.644326       -0.008171        3.560433
H         -2.425150        1.154730        2.477162
H         -3.513465       -2.390771        2.791369
H         -1.765689       -2.335022        3.072099
H         -2.378570       -2.911449        1.523237
H          2.729026       -2.426513       -1.814756
H          3.889115       -0.041642        1.552664
H         -0.218918       -1.175692        1.071794
N         -2.458647        3.387312       -0.645532
O         -2.929354        2.850778        0.329965
O         -2.899500        4.373567       -1.186293
C         -1.185370        2.791832       -1.233954
C         -0.217181        2.359294       -0.201293
H         -0.527543        2.508678        0.827436
O         -1.060260        1.448567       -0.912653
C          1.243558        2.301211       -0.455224
C          3.988520        2.293769       -0.910016
C          2.093804        3.016519        0.385272
C          1.774245        1.554925       -1.503458
C          3.142960        1.561048       -1.734045
C          3.462784        3.013304        0.156631
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H          1.682683        3.571072        1.220967
H          1.116820        0.961263       -2.127781
H          3.551605        0.980741       -2.551382
H          4.118526        3.571780        0.812045
H          5.055955        2.290015       -1.089518
C         -0.892979        3.279803       -2.613781
H         -0.796503        4.362701       -2.616434
H         -1.699894        2.995748       -3.288715
H          0.037819        2.835767       -2.955420

RS epoxide:Catalyst, binary complex 3; Energy = -2450.617120; TZVP basis set.
N          2.219175       -0.820494       -0.691771
C          1.711788       -1.269729       -1.843893
S          2.603493       -1.866215       -3.138655
C          3.635832       -0.906373       -0.351945
C          3.874729       -0.058233        0.903062
C          5.363272       -0.097850        1.269708
C          5.824523       -1.530933        1.531410
C          5.536321       -2.415487        0.320863
C          4.061332       -2.349872       -0.067266
N          3.290213        1.279883        0.773754
C          4.042557        2.175627       -0.092655
N          0.336462       -1.201356       -1.983125
C         -0.691949       -1.304228       -1.044751
C         -1.998529       -1.288017       -1.547186
C         -3.084501       -1.373344       -0.695493
C         -2.920872       -1.470004        0.677521
C         -1.624440       -1.489259        1.164663
C         -0.515141       -1.421338        0.335210
C         -4.463487       -1.387411       -1.298508
F         -5.417589       -1.162929       -0.391422
C         -1.379013       -1.592055        2.646136
F         -2.478092       -1.334081        3.361723
C          3.035487        1.888144        2.069294
F         -4.598338       -0.459982       -2.259613
F         -4.736136       -2.569548       -1.872172
F         -0.955900       -2.814664        2.999040
F         -0.431744       -0.730035        3.051942
H          1.731178       -0.039222       -0.247881
H          0.060343       -1.403553       -2.934424
H          3.442768       -2.730418        0.753128
H          3.866593       -2.966764       -0.942675
H          6.145178       -2.082381       -0.526125
H          5.818179       -3.449613        0.526239
H          6.889231       -1.544327        1.772081
H          5.294527       -1.928015        2.403648
H          5.949614        0.320208        0.445498
H          5.544154        0.529730        2.145321
H          4.225589       -0.520325       -1.191495
H          3.314538       -0.544466        1.711943
H          2.398873        1.232389        2.665011
H          3.952662        2.101822        2.638174
H          2.507453        2.831737        1.929858
H          5.025364        2.447085        0.317639
H          3.479551        3.101338       -0.229705
H          4.181830        1.723731       -1.075345
H         -2.158036       -1.197187       -2.615950
H         -3.771866       -1.503253        1.342278
H          0.473809       -1.448831        0.766452
N          1.212027        2.827039       -1.611527
O          1.547608        3.942466       -1.943081
O          1.529848        1.802151       -2.162509
C          0.289305        2.725382       -0.409223
C         -0.841488        1.796529       -0.628251
H         -0.867003        1.322352       -1.605911
O          0.314351        1.452652        0.134262
C         -2.130595        1.877205        0.101929
C         -4.581419        1.877227        1.415430
C         -3.313119        1.968461       -0.626782
C         -2.177294        1.781302        1.490003
C         -3.401663        1.783014        2.144076
C         -4.535746        1.971823        0.029446
H         -3.278173        2.009897       -1.709553
H         -1.256272        1.666982        2.048797
H         -3.434136        1.693440        3.222377
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H         -5.452783        2.028702       -0.542721
H         -5.536068        1.867598        1.925570
C          0.282345        3.950850        0.443790
H          1.296585        4.233133        0.721080
H         -0.299495        3.748601        1.339817
H         -0.168893        4.777964       -0.100340

RS epoxide:Catalyst, binary complex 4; Energy = -2450.617248; TZVP basis set.
N          3.019478       -0.480398        1.500049
C          1.685441       -0.388212        1.688575
S          0.945131       -1.362498        2.866091
C          3.759851       -0.081360        0.293770
C          3.965888        1.457526        0.216388
C          5.370506        1.805161       -0.278227
C          6.433769        1.287017        0.699374
C          6.088568       -0.119706        1.233420
C          5.099405       -0.823076        0.306189
N          2.868267        2.070333       -0.561658
C          3.021896        1.939436       -2.007571
N          1.065577        0.497614        0.876958
C         -0.286190        0.825300        0.730052
C         -0.616416        1.451941       -0.479286
C         -1.913219        1.846537       -0.731493
C         -2.929985        1.605450        0.186245
C         -2.591546        0.991052        1.376891
C         -1.285451        0.616418        1.675443
C         -2.254423        2.502498       -2.040081
F         -3.109197        3.520576       -1.876088
C         -3.645647        0.776259        2.429814
F         -3.472617       -0.374876        3.090239
C          2.619090        3.458373       -0.187256
F         -1.170832        2.989063       -2.659854
F         -2.839226        1.649492       -2.898061
F         -3.624096        1.753618        3.352068
F         -4.881269        0.760159        1.914829
H          3.433008       -1.218332        2.052460
H          1.672867        1.033000        0.216849
H          4.929614       -1.860638        0.599171
H          5.496349       -0.853582       -0.710337
H          6.993212       -0.716899        1.346898
H          5.643278       -0.040895        2.228942
H          7.399830        1.270140        0.192563
H          6.530476        1.983707        1.534233
H          5.529004        1.364707       -1.265315
H          5.466183        2.886131       -0.399034
H          3.173756       -0.408713       -0.570173
H          3.863155        1.840761        1.236252
H          2.395357        3.515141        0.878673
H          3.470234        4.115824       -0.407302
H          1.753601        3.827584       -0.739788
H          3.826093        2.572739       -2.401874
H          2.090870        2.233934       -2.494736
H          3.230757        0.903688       -2.275933
H          0.158911        1.611236       -1.218161
H         -3.951283        1.893007       -0.024838
H         -1.050541        0.150997        2.619904
N          1.564575       -3.359721       -1.076028
O          1.807778       -4.520498       -1.313260
O          2.267134       -2.613536       -0.434920
C          0.249925       -2.808948       -1.607532
C         -0.496019       -2.025511       -0.599652
H         -0.028822       -1.946924        0.379751
O          0.263938       -1.426350       -1.652825
C         -1.972399       -1.877781       -0.631559
C         -4.737526       -1.586417       -0.592883
C         -2.626235       -1.295497       -1.711925
C         -2.703905       -2.298518        0.477812
C         -4.083787       -2.159775        0.492439
C         -4.007711       -1.151432       -1.691556
H         -2.048801       -0.929863       -2.552202
H         -2.185350       -2.710149        1.336880
H         -4.646830       -2.477236        1.360612
H         -4.509835       -0.684416       -2.529178
H         -5.813305       -1.466580       -0.574086
C         -0.315552       -3.609339       -2.733909
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H          0.374402       -3.612509       -3.577488
H         -1.257349       -3.159922       -3.039047
H         -0.491867       -4.634385       -2.417440

RS epoxide:Catalyst, binary complex 5; Energy = -2450.616035; TZVP basis set.
N         -3.202313        0.219998        2.188069
C         -1.946747       -0.266085        2.327662
S         -1.274408       -0.455980        3.862350
C         -3.777190        0.821712        0.979804
C         -4.548633       -0.171047        0.084829
C         -5.068963        0.591850       -1.136127
C         -5.978248        1.745783       -0.716526
C         -5.243902        2.716648        0.201736
C         -4.671402        1.983331        1.409920
N         -3.683840       -1.331272       -0.245401
C         -3.939311       -2.457494        0.655616
N         -1.374768       -0.604752        1.141095
C         -0.089087       -1.040907        0.840497
C          0.063778       -1.673477       -0.401655
C          1.305029       -2.117060       -0.811081
C          2.427368       -1.958617       -0.007236
C          2.269822       -1.308125        1.204104
C          1.037674       -0.835030        1.636589
C          1.477479       -2.758547       -2.160947
F          2.184993       -1.969939       -2.987304
C          3.457861       -1.139351        2.113899
F          4.615989       -1.190252        1.436350
C         -3.720054       -1.802746       -1.628284
F          2.148923       -3.915823       -2.074250
F          0.312726       -3.017382       -2.758434
F          3.430579        0.026716        2.766333
F          3.512122       -2.104714        3.041808
H         -3.642923        0.449095        3.067972
H         -2.074877       -0.776424        0.387172
H         -5.491021        1.588065        2.021681
H         -4.092330        2.662381        2.039016
H         -4.426700        3.190240       -0.352119
H         -5.910544        3.514559        0.532529
H         -6.344265        2.264530       -1.604003
H         -6.854758        1.346005       -0.196116
H         -4.219290        0.985673       -1.702893
H         -5.613948       -0.085177       -1.793849
H         -2.947733        1.213498        0.381354
H         -5.421285       -0.531407        0.650260
H         -3.431826       -1.012027       -2.315489
H         -2.995316       -2.612676       -1.729069
H         -4.702879       -2.200433       -1.914085
H         -3.896475       -2.131154        1.692832
H         -3.176287       -3.222746        0.503818
H         -4.925129       -2.905084        0.468265
H         -0.802043       -1.809557       -1.039826
H          3.395104       -2.324349       -0.325332
H          0.947515       -0.329212        2.585357
N         -0.507840        0.789320       -2.118958
O         -0.138661        0.161536       -3.078428
O         -1.582039        0.652095       -1.568210
C          0.431491        1.844955       -1.546274
C          1.861673        1.625037       -1.860873
H          2.094536        0.720530       -2.415559
O          1.037011        2.542416       -2.578431
C          2.951448        2.201541       -1.030730
C          5.017752        3.225698        0.525748
C          3.897567        1.346669       -0.472700
C          3.059422        3.575334       -0.831225
C          4.090266        4.083518       -0.053146
C          4.922853        1.856450        0.311634
H          3.835819        0.281741       -0.662373
H          2.346182        4.241079       -1.300991
H          4.172616        5.152382        0.096838
H          5.647530        1.183426        0.750692
H          5.819060        3.624513        1.134363
C         -0.135423        2.548961       -0.358640
H         -1.028697        3.106794       -0.638505
H          0.613543        3.232639        0.033009
H         -0.395330        1.825873        0.414254
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RS epoxide:Catalyst, binary complex 6; Energy = -2450.617556; TZVP basis set.

N	-1.732106	0.908367	1.028923
C	-1.119375	0.204996	1.989280
S	-1.939127	-0.780968	3.079642
C	-1.348002	2.247211	0.557827
C	-2.453514	2.738805	-0.385904
C	-2.135103	4.155608	-0.877726
C	-1.961499	5.124249	0.290016
C	-0.866154	4.630489	1.231605
C	-1.171472	3.219479	1.728996
N	-2.710452	1.754314	-1.434812
C	-1.732959	1.748431	-2.511433
N	0.247899	0.340662	2.092732
C	1.195068	0.401820	1.058925
C	2.512409	0.672243	1.419212
C	3.513880	0.644211	0.462409
C	3.232264	0.370759	-0.864168
C	1.912951	0.111187	-1.211760
C	0.893593	0.116423	-0.275574
C	4.939809	0.847963	0.897665
F	5.035208	1.725200	1.903853
C	1.608184	-0.155424	-2.661472
F	1.572852	0.985563	-3.370832
C	-4.064779	1.809382	-1.959104
F	5.483704	-0.300551	1.332304
F	5.711511	1.292810	-0.098282
F	2.538487	-0.931140	-3.230199
F	0.425890	-0.755453	-2.837784
H	-2.708929	0.663574	0.893751
H	0.601333	-0.024276	2.966989
H	-2.098412	3.221549	2.311718
H	-0.376963	2.863050	2.386158
H	0.093015	4.630449	0.702688
H	-0.758269	5.303745	2.083474
H	-1.724149	6.122126	-0.082727
H	-2.903970	5.204032	0.841469
H	-1.211152	4.135933	-1.464461
H	-2.932206	4.490807	-1.545416
H	-0.409549	2.191532	-0.001012
H	-3.369721	2.789163	0.215729
H	-4.272536	2.730934	-2.523580
H	-4.220078	0.962867	-2.630517
H	-4.781479	1.724516	-1.142214
H	-1.836896	2.605061	-3.192316
H	-1.849316	0.834375	-3.097413
H	-0.719061	1.757138	-2.108634
H	2.751157	0.891466	2.452978
H	4.017301	0.352489	-1.608187
H	-0.120965	-0.127642	-0.566327
N	-3.888087	-2.039931	0.537489
O	-4.413529	-2.878385	1.220960
O	-4.249664	-0.883293	0.441107
C	-2.647745	-2.434750	-0.252345
C	-1.665228	-3.180559	0.567566
H	-1.957578	-3.356768	1.597583
O	-2.528333	-3.805612	-0.381498
C	-0.203649	-3.156839	0.302141
C	2.551352	-3.071726	-0.109165
C	0.326462	-3.451996	-0.952378
C	0.654994	-2.853730	1.357614
C	2.027478	-2.807446	1.150251
C	1.698530	-3.403370	-1.156500
H	-0.334879	-3.741935	-1.759357
H	0.236298	-2.650266	2.337228
H	2.690653	-2.571764	1.973739
H	2.103598	-3.630060	-2.134534
H	3.621439	-3.032822	-0.271108
C	-2.405214	-1.554237	-1.432579
H	-3.192858	-1.720954	-2.170098
H	-1.448858	-1.813954	-1.877407
H	-2.412076	-0.501382	-1.149267

RS epoxide:Catalyst, binary complex 7; Energy = -2450.619226; TZVP basis set.

N	-2.460037	-0.602415	0.251552

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C         -1.254773       -1.138232        0.005792
S         -0.984454       -2.276576       -1.205504
C         -3.702201       -0.981838       -0.407645
C         -4.852857       -0.464936        0.470265
C         -6.184062       -0.942535       -0.118110
C         -6.352809       -0.411640       -1.543082
C         -5.174818       -0.821384       -2.426438
C         -3.841659       -0.393804       -1.812620
N         -4.610962       -0.765507        1.882616
C         -4.715734       -2.177104        2.219609
N         -0.279910       -0.627466        0.835187
C          1.111268       -0.807131        0.794805
C          1.727978       -2.006344        0.454503
C          3.115204       -2.060945        0.398272
C          3.907758       -0.968344        0.702315
C          3.277575        0.207171        1.088904
C          1.900441        0.292823        1.138275
C          3.763249       -3.336817       -0.067865
F          3.088958       -4.419571        0.333074
C          4.120159        1.389169        1.480270
F          3.432104        2.538915        1.439006
C         -5.415675        0.051756        2.775522
F          3.825633       -3.391846       -1.408658
F          5.017988       -3.457174        0.382313
F          4.592016        1.267250        2.731217
F          5.184181        1.531544        0.681936
H         -2.626218       -0.186533        1.168373
H         -0.579905        0.152244        1.411493
H         -3.794378        0.697805       -1.736023
H         -3.009232       -0.726928       -2.431744
H         -5.175833       -1.909405       -2.551164
H         -5.279161       -0.388793       -3.422856
H         -7.290863       -0.771691       -1.969767
H         -6.414819        0.681098       -1.511294
H         -6.207973       -2.036937       -0.132012
H         -7.010347       -0.607308        0.512807
H         -3.737583       -2.074422       -0.482873
H         -4.824179        0.629035        0.398964
H         -6.488364       -0.187872        2.731227
H         -5.080717       -0.102507        3.802151
H         -5.281836        1.105249        2.526921
H         -5.743954       -2.559162        2.146030
H         -4.374103       -2.323185        3.244987
H         -4.076641       -2.771645        1.565619
H          1.135742       -2.876642        0.221237
H          4.986492       -1.028244        0.646264
H          1.425773        1.228135        1.407242
N         -2.014321        2.441145        0.600665
O         -1.928029        1.915306        1.698957
O         -3.031188        2.573567       -0.023184
C         -0.702670        2.889216       -0.027553
C         -0.375560        2.098799       -1.245234
H         -1.112048        1.349043       -1.533328
O         -0.884144        3.434689       -1.274117
C          1.015812        1.847910       -1.691497
C          3.640215        1.245724       -2.390483
C          1.368117        0.544711       -2.036263
C          1.971205        2.860559       -1.748653
C          3.281655        2.555050       -2.090167
C          2.678484        0.242795       -2.377065
H          0.620205       -0.240803       -2.023236
H          1.687130        3.885280       -1.544080
H          4.024411        3.341647       -2.124146
H          2.944736       -0.776681       -2.627824
H          4.665833        1.012062       -2.646684
C          0.210831        3.552807        0.957214
H         -0.083419        4.597970        1.060117
H          1.236398        3.506791        0.599879
H          0.148910        3.072124        1.929965

RS epoxide:Catalyst, binary complex 8; Energy = -2450.613445; TZVP basis set.
N         -1.158235       -2.013426       -0.005544
C         -0.462704       -3.152473       -0.132453
S         -1.148855       -4.688310       -0.275522
C         -2.606919       -1.954519       -0.214324
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C         -3.243463       -0.765284        0.525836
C         -4.750051       -0.747772        0.237696
C         -5.063207       -0.710683       -1.255409
C         -4.419604       -1.893625       -1.971785
C         -2.917311       -1.915472       -1.713830
N         -3.013920       -0.718167        1.971055
C         -1.918188        0.138531        2.377034
N          0.904598       -3.046964       -0.153751
C          1.693156       -1.939205        0.199752
C          2.763813       -1.571598       -0.614361
C          3.569269       -0.507811       -0.244508
C          3.312176        0.221518        0.909885
C          2.239678       -0.150765        1.704447
C          1.445343       -1.237936        1.374948
C          4.755663       -0.116497       -1.086420
F          4.774773       -0.740585       -2.263002
C          1.914010        0.670342        2.922915
F          3.017569        1.122293        3.529339
C         -2.992209       -2.008234        2.637281
F          4.770133        1.203529       -1.325966
F          5.908906       -0.403239       -0.463616
F          1.183150        1.752524        2.600026
F          1.211581       -0.019613        3.824874
H         -0.658063       -1.139232       -0.153560
H          1.375672       -3.899453       -0.419873
H         -2.453512       -1.022639       -2.148074
H         -2.448587       -2.781413       -2.184303
H         -4.859891       -2.826142       -1.603722
H         -4.613806       -1.851389       -3.045125
H         -6.143655       -0.705050       -1.411588
H         -4.676024        0.223054       -1.680896
H         -5.202605       -1.640226        0.683838
H         -5.175461        0.115290        0.750960
H         -3.014061       -2.880359        0.194454
H         -2.821280        0.159459        0.110315
H         -2.099252       -2.609329        2.404961
H         -3.025697       -1.849492        3.716046
H         -3.872921       -2.589828        2.362078
H         -1.893313        0.202489        3.466365
H         -2.073513        1.144530        1.983720
H         -0.932942       -0.204807        2.035227
H          2.944792       -2.107647       -1.537193
H          3.942007        1.058056        1.187215
H          0.645072       -1.558237        2.028326
N          1.041914        0.455969       -2.259747
O          2.030472        0.708237       -2.905585
O          0.409480       -0.574771       -2.313499
C          0.556496        1.521961       -1.289718
C         -0.916969        1.614255       -1.208303
H         -1.465570        0.939091       -1.859421
O         -0.123461        0.934673       -0.229516
C         -1.625373        2.847548       -0.785213
C         -2.996053        5.149350       -0.046875
C         -1.402310        3.418655        0.464877
C         -2.545056        3.422112       -1.658986
C         -3.224332        4.574961       -1.291410
C         -2.088741        4.568216        0.830731
H         -0.703729        2.952345        1.149030
H         -2.730605        2.965693       -2.624658
H         -3.936767        5.020460       -1.973441
H         -1.918681        5.007165        1.805285
H         -3.530893        6.044870        0.242051
C          1.533665        2.627450       -1.072136
H          1.118544        3.320724       -0.344902
H          1.714810        3.151244       -2.008535
H          2.479489        2.234395       -0.704444

RS epoxide:Catalyst, binary complex 9; Energy = -2450.618784; TZVP basis set.
N         -2.130756       -1.049192       -0.818715
C         -0.910737       -1.583605       -0.642833
S         -0.652712       -3.008324        0.225258
C         -3.385751       -1.689799       -0.443843
C         -4.364067       -0.664942        0.139968
C         -5.644322       -1.397228        0.568423
C         -6.280559       -2.130621       -0.612684
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C         -5.298110       -3.120063       -1.234413
C         -4.004185       -2.417993       -1.638895
N         -3.729713        0.153665        1.177424
C         -3.218501       -0.588486        2.321516
N          0.088423       -0.842978       -1.226974
C          1.466479       -0.812858       -0.955972
C          2.093683        0.429856       -1.109435
C          3.435156        0.572472       -0.825816
C          4.199398       -0.505479       -0.392356
C          3.576554       -1.733314       -0.281542
C          2.226807       -1.910634       -0.569800
C          4.106322        1.906486       -0.995774
F          4.870635        2.217627        0.061366
C          4.349379       -2.924230        0.216560
F          5.672488       -2.738044        0.138669
C         -4.572567        1.257266        1.613798
F          4.916249        1.920620       -2.066424
F          3.229815        2.905977       -1.159565
F          4.068760       -3.187961        1.503538
F          4.061790       -4.033692       -0.474544
H         -2.211563       -0.125025       -1.235816
H         -0.233026        0.002422       -1.683137
H         -4.205345       -1.690238       -2.432653
H         -3.274492       -3.133491       -2.023599
H         -5.065951       -3.905370       -0.507623
H         -5.743620       -3.610378       -2.101737
H         -7.187140       -2.645433       -0.289246
H         -6.582708       -1.398004       -1.368699
H         -5.405430       -2.119110        1.356355
H         -6.351788       -0.679998        0.989044
H         -3.144369       -2.432109        0.316358
H         -4.631302        0.033843       -0.661894
H         -5.388097        0.941328        2.279624
H         -3.963467        1.982937        2.159402
H         -5.006616        1.757220        0.746842
H         -4.010505       -1.061331        2.919651
H         -2.680719        0.104029        2.973363
H         -2.514860       -1.358555        2.001161
H          1.508995        1.288397       -1.414764
H          5.248549       -0.385964       -0.157199
H          1.772630       -2.884094       -0.481311
N         -2.945006        2.980794       -0.677830
O         -3.440563        2.048537       -1.265329
O         -3.543808        3.926853       -0.222730
C         -1.434120        2.971408       -0.460019
C         -1.032169        1.844754        0.402837
H         -1.853532        1.180850        0.686895
O         -0.866282        1.866556       -1.052387
C          0.200392        1.709319        1.220062
C          2.585019        1.140305        2.549036
C          0.420634        0.447239        1.773147
C          1.168492        2.699601        1.378392
C          2.352722        2.414097        2.042881
C          1.611990        0.157250        2.422376
H         -0.331214       -0.327410        1.662418
H          1.013645        3.695257        0.990540
H          3.103663        3.185814        2.152229
H          1.780076       -0.837858        2.814762
H          3.521377        0.917814        3.045038
C         -0.844058        4.335990       -0.661107
H          0.220204        4.229660       -0.853909
H         -1.008622        4.964342        0.211127
H         -1.307708        4.810556       -1.525527

RS epoxide:Catalyst, binary complex 10; Energy = -2450.618185; TZVP basis set.
N         -1.632806       -1.695752       -0.296712
C         -0.364774       -1.867992        0.094891
S          0.089962       -2.972847        1.285050
C         -2.774073       -2.450666        0.195318
C         -4.039269       -1.598439        0.055323
C         -5.235609       -2.382200        0.612131
C         -5.407919       -3.715976       -0.115225
C         -4.134921       -4.554396       -0.024010
C         -2.934671       -3.775063       -0.554686
N         -3.847876       -0.257433        0.619184
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C	-3.571257	-0.234932	2.048545
N	0.504177	-1.024807	-0.555680
C	1.884979	-0.871957	-0.379071
C	2.406642	0.411053	-0.509545
C	3.771708	0.627119	-0.392868
C	4.642816	-0.417777	-0.144869
C	4.110858	-1.697315	-0.036084
C	2.754797	-1.942605	-0.158681
C	4.287503	2.026942	-0.574075
F	5.538542	2.171217	-0.130646
C	5.051011	-2.837546	0.249558
F	4.512719	-4.026086	-0.035978
C	-4.929489	0.650877	0.274498
F	4.281855	2.396032	-1.865332
F	3.527585	2.924326	0.076994
F	6.184240	-2.732020	-0.460860
F	5.412576	-2.868287	1.541426
H	-1.844885	-0.969383	-0.974018
H	0.069171	-0.264435	-1.068854
H	-3.069257	-3.558906	-1.619913
H	-2.013532	-4.349149	-0.444688
H	-3.952342	-4.825823	1.021049
H	-4.249568	-5.487062	-0.579020
H	-6.256786	-4.261181	0.301552
H	-5.638308	-3.523555	-1.168464
H	-5.080174	-2.572612	1.678912
H	-6.143137	-1.782182	0.518427
H	-2.591380	-2.676929	1.248024
H	-4.207273	-1.442258	-1.018273
H	-5.853919	0.465975	0.839485
H	-4.621654	1.681097	0.479253
H	-5.152922	0.569857	-0.790951
H	-4.413058	-0.588897	2.659456
H	-3.353700	0.791455	2.351077
H	-2.690194	-0.835597	2.276303
H	1.734537	1.239795	-0.697204
H	5.706348	-0.246999	-0.046793
H	2.369258	-2.947011	-0.086363
N	-2.854579	1.543129	-2.242869
O	-3.813271	2.124469	-2.688704
O	-2.686529	0.343830	-2.278335
C	-1.805565	2.396270	-1.555784
C	-1.602153	2.031826	-0.136647
H	-2.197372	1.190716	0.227679
O	-0.695995	1.655961	-1.189654
C	-1.128487	3.035329	0.850975
C	-0.305447	4.915382	2.728838
C	0.162400	3.550861	0.801948
C	-2.008218	3.466572	1.840891
C	-1.598533	4.407454	2.774237
C	0.573451	4.485054	1.743456
H	0.847126	3.220227	0.032057
H	-3.015966	3.069349	1.878736
H	-2.286752	4.740392	3.540276
H	1.583674	4.871907	1.706551
H	0.016584	5.642851	3.462634
C	-1.648177	3.748503	-2.169660
H	-1.334139	3.654054	-3.209034
H	-0.890071	4.293343	-1.611822
H	-2.589032	4.291569	-2.127652

SR epoxide:Catalyst, binary complex 1; Energy = -2449.847037; 6-31G(d) basis set.

N	-2.148195	-0.160592	-0.828991
C	-1.567738	-1.163495	-1.508506
S	-2.314105	-2.627050	-1.886736
C	-3.527149	-0.160094	-0.354586
C	-3.698592	1.058053	0.570751
C	-5.109715	1.025920	1.176610
C	-6.170042	1.076352	0.071692
C	-5.968982	-0.058419	-0.933482
C	-4.546364	-0.059258	-1.495603
N	-2.582442	1.187474	1.518857
C	-2.511397	2.530792	2.082941
N	-0.253540	-0.993923	-1.877179
C	0.637289	0.054353	-1.611888

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C          1.986542       -0.284220       -1.458048
C          2.907652        0.676764       -1.073669
C          2.526786        1.999109       -0.867392
C          1.202425        2.341353       -1.105977
C          0.258487        1.395917       -1.494740
C          4.344170        0.275147       -0.885321
F          5.036992        0.366208       -2.028621
C          0.746012        3.749744       -0.848173
F          1.726754        4.637509       -1.046266
C         -2.596595        0.186041        2.579679
F          4.961178        1.048003        0.016068
F          4.447809       -0.998888       -0.467456
F         -0.285359        4.091638       -1.631715
F          0.333054        3.902009        0.425147
H         -1.560830        0.494326       -0.312557
H          0.163577       -1.859454       -2.207792
H         -4.355077        0.871672       -2.046478
H         -4.404959       -0.890642       -2.188680
H         -6.158212       -1.020962       -0.439527
H         -6.691362        0.023568       -1.751714
H         -7.171532        1.026864        0.511529
H         -6.098128        2.040313       -0.450049
H         -5.235273        0.103055        1.758607
H         -5.242157        1.864360        1.869027
H         -3.715519       -1.092957        0.198176
H         -3.629142        1.948052       -0.074224
H         -2.693630       -0.816106        2.150800
H         -1.648235        0.230969        3.125224
H         -3.415610        0.334136        3.301535
H         -1.659992        2.590316        2.766803
H         -3.411612        2.808608        2.653825
H         -2.360725        3.261396        1.282750
H          2.292190       -1.318124       -1.594229
H          3.244015        2.739881       -0.532366
H         -0.755300        1.711427       -1.711388
C          1.822436       -2.381432        1.035529
O          1.670117       -3.608211        1.785663
C          0.625525       -3.218112        0.950199
N          0.546534       -4.084287       -0.295606
O          1.108602       -3.695226       -1.307920
O         -0.066809       -5.120148       -0.189490
C         -0.724155       -3.020017        1.573092
H         -0.608443       -2.396223        2.460912
H         -1.120400       -3.995821        1.862951
H         -1.420797       -2.555369        0.868474
C          1.865622       -1.058665        1.720242
C          2.108098        1.557799        2.662869
C          0.802060       -0.163988        1.596485
C          3.050778       -0.638754        2.327114
C          3.167451        0.663345        2.805885
C          0.924122        1.142300        2.057180
H         -0.113871       -0.476997        1.099176
H          3.889184       -1.326226        2.398350
H          4.094352        0.986092        3.269414
H          0.105655        1.836995        1.901349
H          2.209143        2.581470        3.010587
H          2.554378       -2.501350        0.239991

SR epoxide:Catalyst, binary complex 2; Energy = -2449.852746; 6-31G(d) basis set.
N         -2.401990       -1.047609       -0.722185
C         -1.485512       -1.939701       -0.336877
S         -1.850678       -3.408226        0.408127
C         -3.823987       -1.108740       -0.412532
C         -4.389697        0.318588       -0.451254
C         -5.864416        0.280304       -0.018571
C         -6.673442       -0.635328       -0.943206
C         -6.081643       -2.045254       -0.983826
C         -4.602247       -2.013017       -1.373535
N         -3.517140        1.260730        0.258358
C         -3.908971        2.645703        0.036117
N         -0.170709       -1.617025       -0.585014
C          0.397453       -0.360673       -0.833439
C         -0.134853        0.827040       -0.308622
C          0.523188        2.028394       -0.530615
C          1.722962        2.087143       -1.232334
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C	2.251110	0.901388	-1.726107
C	1.594588	-0.312443	-1.554478
C	-0.093075	3.303669	-0.026851
F	-0.852616	3.105058	1.062824
C	3.604895	0.907165	-2.375669
F	3.710618	-0.024870	-3.328369
C	-3.367169	0.986360	1.681486
F	0.837239	4.214097	0.290790
F	-0.888756	3.861476	-0.953740
F	3.897311	2.092457	-2.920815
F	4.566444	0.647191	-1.464787
H	-2.096850	-0.196277	-1.181376
H	0.464959	-2.412638	-0.585151
H	-4.487636	-1.624086	-2.394481
H	-4.167095	-3.015835	-1.347795
H	-6.180191	-2.509869	0.006629
H	-6.639341	-2.674631	-1.684751
H	-7.718616	-0.667241	-0.618443
H	-6.668642	-0.212911	-1.957519
H	-5.936734	-0.087359	1.013781
H	-6.283229	1.292193	-0.031378
H	-3.917392	-1.526189	0.598153
H	-4.367101	0.642199	-1.505195
H	-2.968075	-0.021802	1.837378
H	-2.646841	1.698209	2.095558
H	-4.307242	1.084229	2.249048
H	-4.856054	2.915299	0.531882
H	-4.017310	2.826918	-1.037853
H	-3.127050	3.305551	0.417070
H	-1.044955	0.822317	0.283511
H	2.239372	3.029728	-1.375101
H	2.011557	-1.227095	-1.969293
C	3.105475	-1.088276	1.202907
O	3.866712	-2.069476	1.937524
C	2.766089	-2.525417	1.247876
N	3.126139	-3.180525	-0.069493
O	2.174147	-3.525195	-0.760587
O	4.287014	-3.276813	-0.379283
C	1.698226	-3.295184	1.977508
H	1.675829	-2.948647	3.010779
H	1.964383	-4.356004	1.977361
H	0.709906	-3.188704	1.523996
C	2.396392	0.022117	1.895895
C	1.163057	2.244571	3.059451
C	2.965220	1.292941	1.776830
C	1.188211	-0.124275	2.584744
C	0.579694	0.983125	3.166720
C	2.354767	2.400536	2.357628
H	3.884818	1.411740	1.208257
H	0.696770	-1.088669	2.643126
H	-0.361769	0.861218	3.693533
H	2.801648	3.383595	2.250001
H	0.677354	3.107340	3.504479
H	3.649259	-0.771198	0.312269

SR epoxide:Catalyst, binary complex 3; Energy = -2449.852071; 6-31G(d) basis set.

N	-2.812080	-0.865047	0.603072
C	-2.665865	-1.626716	1.697223
S	-3.858821	-1.930197	2.843160
C	-4.022279	-0.145713	0.220631
C	-3.635376	0.751597	-0.972296
C	-4.839617	1.606679	-1.387194
C	-6.015115	0.713090	-1.790341
C	-6.376155	-0.251331	-0.658705
C	-5.164188	-1.072350	-0.210570
N	-2.381450	1.472233	-0.719441
C	-2.536119	2.629807	0.153766
N	-1.416701	-2.177664	1.889938
C	-0.263829	-2.079235	1.098148
C	-0.302699	-2.090641	-0.302156
C	0.877424	-1.956789	-1.024773
C	2.112358	-1.839151	-0.395636
C	2.142244	-1.888897	0.992954
C	0.977186	-2.011809	1.738881
C	0.789995	-1.896880	-2.524615

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F          0.480774       -0.656184       -2.949225
C          3.436051       -1.689711        1.731462
F          3.523101       -0.434535        2.210394
C         -1.696498        1.840058       -1.952548
F          1.944674       -2.236057       -3.108221
F         -0.163256       -2.711362       -2.996158
F          3.533822       -2.511065        2.785206
F          4.502627       -1.893116        0.951684
H         -1.978999       -0.423680        0.207667
H         -1.308653       -2.593684        2.806706
H         -4.805154       -1.698253       -1.039305
H         -5.431957       -1.736088        0.613624
H         -6.757174        0.320880        0.198169
H         -7.181636       -0.923348       -0.971818
H         -6.880003        1.327057       -2.062041
H         -5.739666        0.136585       -2.683923
H         -5.142718        2.246363       -0.547921
H         -4.556869        2.270049       -2.212818
H         -4.361649        0.465232        1.071077
H         -3.410576        0.065542       -1.803576
H         -2.270920        2.547330       -2.573867
H         -0.742716        2.312015       -1.698670
H         -1.492450        0.940788       -2.540586
H         -3.161284        3.421845       -0.287440
H         -1.549876        3.064703        0.346052
H         -2.974763        2.329247        1.110769
H         -1.244943       -2.219093       -0.823511
H          3.024071       -1.712580       -0.968990
H          1.024358       -2.018822        2.824663
C          2.341420        2.899881        0.042971
O          1.016950        3.230993       -0.372890
C          1.141219        2.550828        0.832018
N          0.899697        3.461519        2.010560
O          1.078306        4.650086        1.846180
O          0.565845        2.926817        3.049811
C          0.589318        1.172719        1.006111
H          0.736616        0.625169        0.070864
H         -0.477243        1.201968        1.243848
H          1.123346        0.667726        1.811420
C          3.077781        1.872389       -0.747250
C          4.541070        0.028454       -2.242677
C          4.283928        1.370148       -0.253110
C          2.593873        1.432845       -1.979384
C          3.330939        0.519064       -2.729141
C          5.010202        0.445626       -0.997304
H          4.654367        1.704342        0.712308
H          1.650504        1.819643       -2.352800
H          2.955173        0.186216       -3.690825
H          5.942814        0.052835       -0.605548
H          5.114897       -0.682402       -2.829588
H          2.909886        3.762236        0.389874

SR epoxide:Catalyst, binary complex 4; Energy = -2449.855160; 6-31G(d) basis set.
N         -1.596297        0.410394       -0.920661
C         -0.926291        0.771838       -2.020970
S         -1.599267        1.636353       -3.301151
C         -3.039444        0.514982       -0.755501
C         -3.511704       -0.595737        0.192805
C         -5.045463       -0.544331        0.287401
C         -5.501888        0.822141        0.809894
C         -4.986852        1.953866       -0.081441
C         -3.465640        1.888708       -0.229366
N         -2.910939       -1.887556       -0.156596
C         -3.292928       -2.390453       -1.469981
N          0.406447        0.439803       -2.059477
C          1.079559       -0.584462       -1.377343
C          0.437445       -1.753767       -0.951414
C          1.173738       -2.737338       -0.300234
C          2.536932       -2.598797       -0.064513
C          3.163771       -1.442507       -0.516871
C          2.455212       -0.444894       -1.172693
C          0.465345       -3.976339        0.171832
F         -0.552182       -4.306997       -0.637952
C          4.613058       -1.197265       -0.203018
F          5.254340       -0.629269       -1.231989
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C	-3.136000	-2.894124	0.869956
F	1.290820	-5.026703	0.236919
F	-0.058813	-3.817500	1.402981
F	4.736343	-0.366822	0.844671
F	5.256707	-2.329606	0.107233
H	-1.099254	-0.057420	-0.166487
H	0.921780	0.920583	-2.786100
H	-2.981405	2.056093	0.743694
H	-3.104699	2.657056	-0.920978
H	-5.446528	1.870162	-1.075434
H	-5.283297	2.926952	0.323415
H	-6.594215	0.854556	0.878161
H	-5.114049	0.961238	1.829255
H	-5.485064	-0.720669	-0.703461
H	-5.407315	-1.339725	0.947831
H	-3.485576	0.378525	-1.747650
H	-3.114085	-0.351176	1.189954
H	-4.190842	-3.203185	0.957171
H	-2.542263	-3.781053	0.638717
H	-2.806355	-2.506005	1.839638
H	-3.032139	-1.665719	-2.248393
H	-4.367103	-2.624525	-1.554126
H	-2.731584	-3.308732	-1.667428
H	-0.626896	-1.903182	-1.112195
H	3.098187	-3.375484	0.441807
H	2.957780	0.462513	-1.491799
C	1.611013	2.509097	1.353877
O	2.024054	2.246105	0.009786
C	1.303168	3.413516	0.229316
N	2.197460	4.632404	0.173983
O	1.662415	5.689264	-0.096701
O	3.373484	4.475209	0.425771
C	-0.028923	3.603871	-0.425380
H	-0.558705	4.448904	0.016695
H	-0.613151	2.693506	-0.281698
H	0.092944	3.782472	-1.497073
C	0.568343	1.610348	1.931527
C	-1.326164	-0.082833	3.080280
C	-0.557307	2.144410	2.560053
C	0.743217	0.226106	1.876993
C	-0.209223	-0.620702	2.441404
C	-1.501326	1.298746	3.137767
H	-0.693209	3.222517	2.598119
H	1.633191	-0.183399	1.405567
H	-0.074666	-1.696131	2.385513
H	-2.374231	1.718809	3.628370
H	-2.060807	-0.741310	3.535117
H	2.440699	2.799802	1.997582

SR epoxide:Catalyst, binary complex 5; Energy = -2449.847593; 6-31G(d) basis set.

N	-0.781553	-1.401120	-1.206686
C	-0.208569	-0.957986	-2.334843
S	-0.957297	-0.885550	-3.839590
C	-2.121791	-1.963904	-1.108664
C	-2.198378	-2.674082	0.256063
C	-3.537525	-3.413180	0.358620
C	-4.692071	-2.411662	0.253100
C	-4.600384	-1.575196	-1.026624
C	-3.229471	-0.909731	-1.181771
N	-0.984534	-3.453473	0.511637
C	-0.873165	-4.661913	-0.294107
N	1.096026	-0.535126	-2.219567
C	1.906967	-0.421847	-1.077620
C	1.406494	-0.070042	0.178757
C	2.273906	0.015231	1.264804
C	3.637816	-0.191942	1.126521
C	4.131076	-0.497018	-0.140315
C	3.285099	-0.625946	-1.229698
C	1.690202	0.358055	2.607545
F	2.547607	0.113431	3.604090
C	5.602688	-0.764850	-0.298737
F	5.995173	-0.659756	-1.574554
C	-0.783801	-3.739483	1.923623
F	1.331214	1.645260	2.692316
F	0.576627	-0.364612	2.846268

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F          6.334481        0.091197        0.426757
F          5.920946       -2.000191        0.116360
H         -0.169115       -1.783430       -0.481286
H          1.538837       -0.369651       -3.115156
H         -3.070575       -0.180298       -0.374711
H         -3.166620       -0.376590       -2.134634
H         -4.784687       -2.220868       -1.896132
H         -5.382163       -0.807602       -1.030506
H         -5.652902       -2.935575        0.296626
H         -4.652085       -1.741793        1.121310
H         -3.613376       -4.152434       -0.449917
H         -3.593730       -3.962442        1.305774
H         -2.267311       -2.685056       -1.926637
H         -2.194215       -1.874435        1.014533
H         -1.546306       -4.415926        2.344665
H          0.193848       -4.212133        2.056827
H         -0.790520       -2.804705        2.491787
H         -0.999591       -4.422810       -1.354244
H         -1.611606       -5.432457       -0.018624
H          0.125656       -5.087163       -0.160901
H          0.354210        0.155352        0.315318
H          4.304059       -0.117495        1.978481
H          3.688050       -0.888559       -2.202903
C         -1.278794        3.336638        0.587695
O          0.012956        2.743823        0.458525
C         -0.606525        3.163567       -0.714189
N          0.018007        4.432260       -1.243914
O          0.564156        5.164387       -0.445530
O         -0.096938        4.639172       -2.436074
C         -0.970487        2.171572       -1.771788
H         -1.373589        1.281721       -1.282008
H         -0.091013        1.893393       -2.357683
H         -1.722686        2.579260       -2.448923
C         -2.398933        2.444507        1.004853
C         -4.516041        0.864844        1.890617
C         -3.691992        2.684624        0.537736
C         -2.160947        1.400803        1.899765
C         -3.222221        0.615417        2.345403
C         -4.748538        1.892594        0.978079
H         -3.870018        3.492310       -0.167648
H         -1.152025        1.226860        2.260605
H         -3.038591       -0.185785        3.055990
H         -5.753579        2.080831        0.613717
H         -5.344505        0.259555        2.246087
H         -1.246225        4.337487        1.017900

SR epoxide:Catalyst, binary complex 6; Energy = -2449.856977; 6-31G(d) basis set.
N          1.343617       -0.414149        1.430264
C          0.714078       -0.590873        2.597974
S          1.486794       -0.645608        4.097667
C          2.786773       -0.487614        1.259144
C          3.121659       -1.181152       -0.068057
C          4.645696       -1.384597       -0.129590
C          5.375922       -0.039571       -0.030480
C          4.974279        0.733164        1.227888
C          3.454717        0.888197        1.320554
N          2.287434       -2.365922       -0.290479
C          2.436698       -3.411577        0.712332
N         -0.653768       -0.703341        2.552967
C         -1.475029       -0.917718        1.430742
C         -2.737262       -0.317118        1.402395
C         -3.559375       -0.490602        0.296720
C         -3.140351       -1.232844       -0.803077
C         -1.892704       -1.837398       -0.749163
C         -1.066816       -1.717856        0.361713
C         -4.935002        0.118249        0.303524
F         -4.976044        1.237148        1.037034
C         -1.345771       -2.576910       -1.935153
F         -0.755973       -3.727588       -1.571575
C          2.450452       -2.907712       -1.630875
F         -5.353779        0.414159       -0.931450
F         -5.834630       -0.729550        0.831690
F         -2.290944       -2.871978       -2.834024
F         -0.408167       -1.846497       -2.566920
H          0.795819       -0.294890        0.580862
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H         -1.096470       -0.664539        3.462699
H          3.087363        1.503900        0.484653
H          3.165958        1.378392        2.256759
H          5.329756        0.194977        2.117040
H          5.454169        1.717597        1.238534
H          6.459295       -0.198840       -0.050179
H          5.125153        0.565118       -0.912072
H          4.962155       -2.037643        0.695141
H          4.919157       -1.888873       -1.062978
H          3.167408       -1.084624        2.095098
H          2.852481       -0.482266       -0.873902
H          3.426770       -3.395750       -1.788650
H          1.666561       -3.645555       -1.818463
H          2.341087       -2.104470       -2.366780
H          2.236589       -3.016368        1.713717
H          3.435389       -3.880084        0.712786
H          1.699253       -4.195049        0.508535
H         -3.060264        0.306473        2.231736
H         -3.769964       -1.327508       -1.680196
H         -0.093868       -2.205677        0.361568
C         -0.385203        2.274013       -1.336066
O         -0.724182        1.052521       -0.664164
C         -0.937933        2.242297        0.030304
N         -2.418554        2.559871        0.098325
O         -3.102390        2.247189       -0.854801
O         -2.815212        3.102689        1.109312
C         -0.205690        2.525466        1.305412
H          0.844578        2.258684        1.174099
H         -0.626638        1.938818        2.126473
H         -0.284278        3.583662        1.560669
C          1.066085        2.489390       -1.601863
C          3.763646        2.842486       -2.201328
C          1.767457        1.489135       -2.277484
C          1.713165        3.667927       -1.230886
C          3.063653        3.840225       -1.525898
C          3.113860        1.668512       -2.580388
H          1.251609        0.571830       -2.554223
H          1.163177        4.446779       -0.709096
H          3.568791        4.753723       -1.228854
H          3.657629        0.888195       -3.105721
H          4.815814        2.979032       -2.431820
H         -1.086192        2.515906       -2.133581

SR epoxide:Catalyst, binary complex 7; Energy = -2449.852899; 6-31G(d) basis set.
N          1.551274       -1.671463       -0.182293
C          0.849483       -2.747279       -0.574930
S          1.510789       -4.245126       -0.953059
C          2.985096       -1.720008        0.085064
C          3.592452       -0.316258       -0.008150
C          5.115764       -0.443158        0.182849
C          5.454569       -1.092681        1.528533
C          4.777349       -2.454141        1.681568
C          3.270356       -2.333834        1.459267
N          3.148600        0.388442       -1.218498
C          3.756509        1.706791       -1.321496
N         -0.516299       -2.573496       -0.695071
C         -1.386408       -1.771086        0.048417
C         -2.732055       -1.751674       -0.336913
C         -3.661520       -1.027204        0.398572
C         -3.284740       -0.280629        1.507714
C         -1.943248       -0.299148        1.875842
C         -1.000522       -1.045515        1.183862
C         -5.083837       -0.963600       -0.083646
F         -5.941598       -0.774451        0.926229
C         -1.511902        0.571470        3.022536
F         -0.227052        0.374722        3.358616
C          3.323329       -0.349902       -2.464136
F         -5.254254        0.057698       -0.941633
F         -5.443545       -2.080766       -0.726747
F         -1.638110        1.871675        2.702134
F         -2.255471        0.367020        4.114900
H          1.157768       -0.753861       -0.394609
H         -0.953662       -3.342216       -1.189123
H          2.823164       -1.691200        2.231120
H          2.786784       -3.313358        1.518725
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H	5.191541	-3.156167	0.945565
H	4.979597	-2.875513	2.671570
H	6.540418	-1.188162	1.633717
H	5.114816	-0.430439	2.336993
H	5.537123	-1.042890	-0.635887
H	5.580775	0.546181	0.128793
H	3.447260	-2.363829	-0.674549
H	3.200579	0.279287	0.834723
H	4.378682	-0.565633	-2.701138
H	2.767684	-1.291030	-2.440623
H	2.911619	0.250938	-3.281735
H	3.235959	2.290972	-2.088067
H	4.822363	1.670878	-1.599541
H	3.657900	2.236092	-0.367564
H	-3.051909	-2.315151	-1.208570
H	-4.011819	0.300247	2.065334
H	0.022550	-1.075136	1.535514
C	0.431138	1.856194	-1.679014
O	-0.044387	0.539350	-1.428824
C	-0.984508	1.463839	-1.875179
N	-1.345274	1.216757	-3.319930
O	-0.522384	0.657674	-4.014571
O	-2.429150	1.624759	-3.687795
C	-2.141369	1.867145	-1.017289
H	-2.944303	1.130393	-1.082630
H	-2.528953	2.833288	-1.344716
H	-1.799010	1.946487	0.016396
C	0.854121	2.671402	-0.508763
C	1.739449	4.199567	1.649417
C	0.870619	2.127487	0.774054
C	1.278483	3.985483	-0.710070
C	1.719431	4.747318	0.367233
C	1.311293	2.889844	1.852387
H	0.543477	1.102514	0.923523
H	1.276551	4.405988	-1.712963
H	2.051361	5.768045	0.205694
H	1.311262	2.458280	2.848209
H	2.084726	4.794694	2.488893
H	1.036601	1.930749	-2.581881

SR epoxide:Catalyst, binary complex 8; Energy = -2449.852206; 6-31G(d) basis set.

N	-2.836268	-1.877248	0.646317
C	-2.795457	-2.320191	-0.633129
S	-3.943039	-3.357104	-1.273876
C	-2.488821	-0.507215	1.043908
C	-3.640932	0.447029	0.667540
C	-3.344049	1.869113	1.168248
C	-3.072036	1.888639	2.672703
C	-1.910235	0.956242	3.018223
C	-2.188984	-0.470373	2.543115
N	-3.938539	0.334904	-0.755918
C	-5.322516	0.627726	-1.080707
N	-1.715974	-1.923729	-1.395499
C	-0.377865	-1.767391	-1.000971
C	0.094929	-2.139418	0.262017
C	1.442520	-1.993754	0.566860
C	2.357963	-1.515593	-0.362148
C	1.880192	-1.164677	-1.619808
C	0.531346	-1.269830	-1.941432
C	1.879691	-2.371783	1.954476
F	1.502792	-3.619857	2.265276
C	2.822316	-0.653314	-2.674087
F	2.784126	-1.412977	-3.776598
C	-3.028296	1.065861	-1.620497
F	3.205299	-2.294850	2.113131
F	1.319486	-1.566446	2.881009
F	2.497510	0.597299	-3.066095
F	4.089127	-0.614398	-2.248518
H	-3.644925	-2.248350	1.136700
H	-1.850549	-2.124721	-2.379053
H	-3.053920	-0.875807	3.089036
H	-1.334882	-1.120646	2.761160
H	-0.997897	1.319289	2.524357
H	-1.717210	0.958651	4.095844
H	-2.857988	2.910174	3.007564

H	-3.972053	1.562713	3.211966
H	-2.462126	2.256136	0.639775
H	-4.180166	2.529978	0.910145
H	-1.590337	-0.201503	0.502034
H	-4.532396	0.082859	1.202342
H	-1.989144	0.854118	-1.351894
H	-3.180006	0.738302	-2.654608
H	-3.177551	2.160374	-1.590195
H	-5.598635	1.684317	-0.912269
H	-5.984956	-0.006386	-0.484491
H	-5.497589	0.400196	-2.136575
H	-0.586979	-2.555247	0.995620
H	3.405939	-1.396305	-0.109261
H	0.180633	-0.971899	-2.926522
C	1.246120	1.925969	-0.446577
O	-0.011266	1.468878	0.065332
C	0.182850	2.849308	0.005223
N	-0.644684	3.440875	-1.122551
O	-1.286497	4.439993	-0.867020
O	-0.626187	2.868200	-2.192719
C	0.164464	3.676261	1.251785
H	-0.847728	3.732127	1.660094
H	0.509675	4.689036	1.036780
H	0.829951	3.220635	1.986184
C	2.458835	1.611850	0.353412
C	4.761350	0.856007	1.731419
C	2.360398	1.083001	1.642101
C	3.710289	1.752358	-0.247289
C	4.860100	1.379998	0.444223
C	3.509727	0.705044	2.327529
H	1.380804	0.915625	2.080977
H	3.781762	2.125847	-1.265391
H	5.831067	1.485557	-0.029136
H	3.424314	0.266765	3.316693
H	5.656668	0.552817	2.264977
H	1.336240	1.804701	-1.522705

SR epoxide:Catalyst, binary complex 9; Energy = -2449.843263; 6-31G(d) basis set.

N	-0.470197	0.159319	-0.725670
C	-0.607089	1.474632	-0.935986
S	0.617831	2.519455	-1.431644
C	0.764045	-0.604508	-0.851760
C	0.477380	-1.985634	-0.226622
C	1.755465	-2.833090	-0.234122
C	2.278347	-3.002159	-1.663583
C	2.488852	-1.644337	-2.338360
C	1.215575	-0.795760	-2.301614
N	-0.199231	-1.838681	1.065069
C	0.687580	-1.426093	2.148167
N	-1.861524	1.987414	-0.690777
C	-3.059211	1.306539	-0.420436
C	-3.354910	0.059777	-0.979857
C	-4.558157	-0.567137	-0.676201
C	-5.505783	0.033318	0.140346
C	-5.218989	1.292719	0.659699
C	-4.011744	1.925251	0.398066
C	-4.823435	-1.908774	-1.301350
F	-5.066449	-1.800533	-2.615304
C	-6.205845	1.945618	1.588317
F	-6.125230	3.281859	1.538657
C	-0.967450	-3.016815	1.437704
F	-3.761142	-2.722177	-1.172271
F	-5.874547	-2.522479	-0.746816
F	-7.464319	1.599540	1.287951
F	-5.992394	1.584612	2.862475
H	-1.101818	-0.278489	-0.049839
H	-1.891282	2.999115	-0.686888
H	0.409427	-1.293867	-2.858027
H	1.386338	0.178349	-2.766291
H	3.285293	-1.098494	-1.814466
H	2.820617	-1.778673	-3.373180
H	3.209790	-3.579979	-1.660600
H	1.551090	-3.583994	-2.246464
H	2.515841	-2.336806	0.383105
H	1.557111	-3.810857	0.220332

H	1.563645	-0.094008	-0.297778
H	-0.256861	-2.473525	-0.887922
H	-0.341085	-3.907293	1.614932
H	-1.516661	-2.806142	2.360323
H	-1.694033	-3.247316	0.652936
H	0.081979	-1.134174	3.011198
H	1.291575	-0.567995	1.842361
H	1.376049	-2.225487	2.465665
H	-2.652827	-0.418973	-1.653022
H	-6.443812	-0.461345	0.363680
H	-3.802786	2.899147	0.830759
C	4.710408	0.568415	1.265723
O	3.656332	-0.260479	0.781386
C	4.902948	-0.857012	0.905950
N	4.945025	-1.785800	2.094776
O	4.116188	-1.618499	2.965695
O	5.827679	-2.621384	2.103275
C	5.622752	-1.380027	-0.297308
H	5.167340	-2.316098	-0.633715
H	6.671602	-1.563084	-0.062378
H	5.551267	-0.635264	-1.091755
C	5.166545	1.663723	0.366263
C	6.022465	3.729691	-1.293639
C	4.437457	1.982172	-0.779999
C	6.319511	2.383156	0.686081
C	6.748544	3.411317	-0.146598
C	4.866302	3.018483	-1.605276
H	3.521906	1.442173	-1.008578
H	6.878982	2.138206	1.585358
H	7.647046	3.967225	0.101782
H	4.287899	3.273020	-2.487926
H	6.354756	4.537032	-1.938736
H	4.633561	0.785249	2.330969

SR epoxide:Catalyst, binary complex 10; Energy = -2449.844912; 6-31G(d) basis set.

N	-0.530395	2.475264	0.231377
C	-1.620413	3.073972	0.743140
S	-1.692428	4.695121	1.203923
C	0.636478	3.216957	-0.259812
C	1.899620	2.340229	-0.175485
C	3.087261	3.045492	-0.846469
C	2.785476	3.455404	-2.287326
C	1.561897	4.369319	-2.330033
C	0.361271	3.666701	-1.701781
N	2.288645	1.872279	1.158623
C	2.462947	2.919901	2.153673
N	-2.743663	2.301522	0.893029
C	-2.917842	0.921473	0.669154
C	-2.012021	-0.017716	1.167440
C	-2.246862	-1.372998	0.972856
C	-3.379464	-1.823345	0.306113
C	-4.282788	-0.880154	-0.169598
C	-4.059465	0.481880	-0.003422
C	-1.286356	-2.352176	1.586314
F	-1.476467	-2.464808	2.906675
C	-5.548139	-1.327085	-0.849681
F	-6.587150	-1.311464	-0.000705
C	1.486841	0.795734	1.714063
F	-1.391970	-3.575725	1.059386
F	-0.005392	-1.951620	1.421053
F	-5.867603	-0.521259	-1.871549
F	-5.443116	-2.573042	-1.326121
H	-0.653110	1.554617	-0.189683
H	-3.564507	2.836258	1.147820
H	0.113068	2.774401	-2.295611
H	-0.522940	4.313184	-1.696665
H	1.776485	5.294353	-1.778106
H	1.326800	4.658519	-3.359475
H	3.657981	3.952795	-2.723565
H	2.591085	2.559295	-2.892875
H	3.351883	3.946960	-0.278945
H	3.948904	2.370686	-0.794350
H	0.747718	4.095834	0.382008
H	1.682576	1.441563	-0.766927
H	1.158218	0.119806	0.918686

H	2.087334	0.215896	2.426473
H	0.597674	1.164176	2.251485
H	2.932442	2.486102	3.042600
H	1.506994	3.375371	2.466357
H	3.119825	3.708541	1.781249
H	-1.146976	0.310822	1.732848
H	-3.548568	-2.882482	0.151496
H	-4.763956	1.206120	-0.401037
C	2.822046	-1.281976	-1.007445
O	2.500581	-1.848621	-2.279500
C	1.691399	-2.218120	-1.207604
N	0.322836	-1.561185	-1.334766
O	-0.639914	-2.295900	-1.347356
O	0.273207	-0.346535	-1.440042
C	1.600396	-3.655952	-0.802660
H	2.603139	-4.026217	-0.589213
H	1.159294	-4.242622	-1.611076
H	0.981931	-3.761490	0.088548
C	4.103294	-1.658167	-0.354079
C	6.493495	-2.264817	0.941708
C	4.556248	-0.848098	0.690383
C	4.865670	-2.749049	-0.774724
C	6.057433	-3.052004	-0.122413
C	5.746164	-1.158808	1.341230
H	3.987969	0.039963	0.967956
H	4.538105	-3.337585	-1.626979
H	6.651057	-3.899187	-0.451316
H	6.095796	-0.529232	2.153447
H	7.423509	-2.503888	1.447988
H	2.563906	-0.229552	-0.928462

SR epoxide:Catalyst, binary complex 11; Energy = -2449.842261; 6-31G(d) basis set.

N	0.219596	0.349786	-0.501659
C	0.201053	-0.907730	-0.971095
S	-1.175863	-1.736484	-1.466340
C	-0.955040	1.188572	-0.305337
C	-0.504225	2.370750	0.572780
C	-1.714337	3.253318	0.902218
C	-2.350372	3.784582	-0.386515
C	-2.738294	2.635304	-1.319006
C	-1.546766	1.720043	-1.613678
N	0.290891	1.889834	1.705793
C	1.112763	2.930660	2.302585
N	1.417271	-1.550190	-1.010443
C	2.705945	-1.059480	-0.754218
C	3.088900	0.259038	-1.017277
C	4.390116	0.667916	-0.740895
C	5.342749	-0.210870	-0.247691
C	4.961902	-1.532672	-0.028071
C	3.663983	-1.957505	-0.264633
C	4.739902	2.102461	-1.024999
F	3.908838	2.940274	-0.381267
C	5.960052	-2.501766	0.544457
F	5.948014	-2.483066	1.886047
C	-0.486048	1.177678	2.711766
F	5.987169	2.401787	-0.647160
F	4.631468	2.383610	-2.331184
F	5.700899	-3.760501	0.166301
F	7.207914	-2.206371	0.158383
H	0.960971	0.595296	0.159128
H	1.338124	-2.536667	-1.223414
H	-0.766974	2.279824	-2.147659
H	-1.845812	0.883504	-2.251688
H	-3.536478	2.048170	-0.841799
H	-3.152143	3.021264	-2.255742
H	-3.226649	4.397465	-0.150241
H	-1.632857	4.439715	-0.899054
H	-2.454245	2.660943	1.457984
H	-1.408457	4.082803	1.550339
H	-1.728035	0.607590	0.219574
H	0.191016	2.967106	-0.039601
H	0.199982	0.720779	3.431531
H	-1.178024	1.832006	3.267713
H	-1.072779	0.376890	2.249066
H	1.747136	3.382418	1.534123

H	1.762268	2.482677	3.060546
H	0.525094	3.727041	2.788815
H	2.385390	0.961917	-1.448993
H	6.355881	0.118238	-0.049105
H	3.386263	-2.989219	-0.070775
C	-4.238867	-0.860985	-0.331852
O	-4.381431	-2.166319	-0.874403
C	-5.537516	-1.400864	-0.787696
N	-5.965730	-0.874812	-2.135571
O	-5.106192	-0.713998	-2.975445
O	-7.148139	-0.620308	-2.270251
C	-6.670405	-1.845809	0.084128
H	-7.244732	-2.631912	-0.411174
H	-7.335822	-1.010472	0.306387
H	-6.250696	-2.234524	1.013243
C	-3.932564	-0.744471	1.122078
C	-3.370122	-0.502433	3.842884
C	-3.328908	-1.799994	1.804702
C	-4.247416	0.435950	1.800342
C	-3.967067	0.555906	3.158476
C	-3.049556	-1.676580	3.164557
H	-3.082965	-2.706565	1.260497
H	-4.725755	1.254983	1.266963
H	-4.219049	1.472351	3.683668
H	-2.579175	-2.499467	3.693824
H	-3.153460	-0.409767	4.902732
H	-3.730203	-0.175661	-1.009632

SR epoxide:Catalyst, binary complex 12; Energy = -2449.852133; 6-31G(d) basis set.

N	-3.913932	0.438295	0.122042
C	-2.947206	1.355252	0.298934
S	-3.319455	2.967095	0.628512
C	-3.758058	-0.975350	-0.188610
C	-5.137355	-1.646680	-0.062536
C	-4.971173	-3.162445	-0.253104
C	-4.368995	-3.470916	-1.628706
C	-3.047434	-2.728212	-1.838012
C	-3.210557	-1.226593	-1.599850
N	-5.837050	-1.203739	1.142485
C	-5.221966	-1.628197	2.390866
N	-1.671849	0.864015	0.219782
C	-0.477883	1.608121	0.265347
C	0.562703	1.165250	1.087182
C	1.771355	1.854253	1.095822
C	1.959428	2.986857	0.310045
C	0.918182	3.408790	-0.508019
C	-0.292786	2.727100	-0.546815
C	2.923069	1.384027	1.938961
F	2.566743	0.464709	2.837094
C	1.075191	4.636345	-1.362357
F	0.407672	5.680120	-0.854537
C	-7.253930	-1.527681	1.120913
F	3.896104	0.846380	1.172007
F	3.489459	2.404382	2.599798
F	2.360281	5.001013	-1.477975
F	0.600121	4.433243	-2.600169
H	-4.844651	0.719082	0.415733
H	-1.551237	-0.143842	0.275637
H	-3.919549	-0.798966	-2.320430
H	-2.255077	-0.717683	-1.745720
H	-2.291680	-3.114564	-1.140799
H	-2.665411	-2.903360	-2.849151
H	-4.224984	-4.550543	-1.742720
H	-5.081101	-3.161851	-2.405993
H	-4.315615	-3.561285	0.532919
H	-5.942463	-3.657844	-0.144673
H	-3.076054	-1.447969	0.539904
H	-5.740475	-1.268038	-0.902427
H	-7.459661	-2.606683	1.225493
H	-7.752157	-1.010373	1.946173
H	-7.696035	-1.180631	0.182272
H	-4.174771	-1.314504	2.425452
H	-5.270070	-2.718177	2.552340
H	-5.740842	-1.140932	3.221197
H	0.427188	0.289709	1.715336

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H          2.899979        3.526604        0.331696
H         -1.091891        3.055637       -1.201142
C          2.387305       -2.604398        0.048770
O          2.162771       -1.407465        0.788751
C          1.957722       -1.328507       -0.578581
N          0.483059       -1.288315       -0.899413
O         -0.289757       -1.721646       -0.056419
O          0.160760       -0.835987       -1.975510
C          2.775275       -0.416511       -1.439088
H          2.415372        0.611697       -1.343709
H          2.710169       -0.722213       -2.483873
H          3.812110       -0.465876       -1.106764
C          3.786387       -3.097678       -0.056621
C          6.390240       -4.062690       -0.270354
C          4.843160       -2.376469        0.501347
C          4.031973       -4.305730       -0.711421
C          5.333327       -4.784356       -0.821874
C          6.142973       -2.862419        0.392369
H          4.637517       -1.446690        1.023721
H          3.204386       -4.870746       -1.133080
H          5.521425       -5.723179       -1.332885
H          6.963824       -2.304632        0.831967
H          7.404842       -4.439565       -0.352179
H          1.607318       -3.352704        0.187082

SR epoxide:Catalyst, binary complex 13; Energy = -2449.847479; 6-31G(d) basis set.
N          3.104477       -1.599987       -0.671706
C          2.625740       -2.830608       -0.893100
S          3.590203       -4.200482       -0.943656
C          2.543738       -0.319577       -1.111818
C          3.550551        0.775107       -0.717690
C          3.029080        2.146871       -1.168335
C          2.770339        2.174481       -2.675821
C          1.787689        1.071669       -3.071496
C          2.298148       -0.299381       -2.626177
N          3.904707        0.658547        0.696171
C          2.876281        1.152363        1.604968
N          1.256159       -2.923485       -1.096471
C          0.277039       -2.353003       -0.257941
C          0.588592       -1.773422        0.976717
C         -0.433402       -1.288369        1.781745
C         -1.767955       -1.376091        1.400293
C         -2.064630       -1.970476        0.179626
C         -1.059815       -2.445915       -0.653427
C         -0.097804       -0.655600        3.103873
F         -0.983243       -1.001022        4.049366
C         -3.504207       -2.182749       -0.198013
F         -3.979209       -3.321986        0.331734
C          5.188778        1.263834        1.010989
F          1.119436       -1.008652        3.535124
F         -0.116705        0.684676        3.025804
F         -4.284893       -1.191282        0.247258
F         -3.665306       -2.276359       -1.525765
H          4.059040       -1.561320       -0.331472
H          0.993400       -3.821693       -1.486746
H          3.243836       -0.532525       -3.133880
H          1.582951       -1.083004       -2.894355
H          0.816506        1.260474       -2.592007
H          1.618351        1.073640       -4.153128
H          2.395153        3.158172       -2.980332
H          3.718195        2.023761       -3.210174
H          2.092094        2.357400       -0.636353
H          3.741136        2.928135       -0.879376
H          1.593243       -0.124200       -0.598861
H          4.473345        0.564513       -1.281788
H          5.189846        2.363092        0.909170
H          5.449856        1.026375        2.046718
H          5.965729        0.852811        0.359504
H          3.066310        0.767855        2.611773
H          1.881663        0.815561        1.296454
H          2.850833        2.253716        1.661034
H          1.618703       -1.719058        1.313567
H         -2.559468       -1.009718        2.046079
H         -1.309993       -2.901429       -1.606915
C         -1.529764        1.892075        0.424685
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O         -0.271657        1.429363       -0.069768
C         -0.514009        2.802487       -0.154690
N          0.308919        3.566669        0.861240
O          0.806892        4.611674        0.489144
O          0.418900        3.087639        1.969300
C         -0.585887        3.487627       -1.483766
H         -1.205091        2.893066       -2.155847
H          0.413048        3.601890       -1.910287
H         -1.028562        4.478623       -1.368738
C         -2.756319        1.542044       -0.342459
C         -5.084135        1.037868       -1.791255
C         -2.689229        0.849911       -1.552788
C         -3.992924        1.957996        0.152644
C         -5.153671        1.709667       -0.572954
C         -3.852626        0.603498       -2.276042
H         -1.725887        0.500304       -1.915770
H         -4.044458        2.484160        1.102686
H         -6.112362        2.040253       -0.186093
H         -3.798289        0.059128       -3.213437
H         -5.989824        0.842103       -2.356509
H         -1.593752        1.871797        1.511226

SR epoxide:Catalyst, binary complex 14; Energy = -2449.844290; 6-31G(d) basis set.
N          0.278542        0.179076        1.367505
C          0.243165        1.374139        0.773691
S         -1.167353        2.265657        0.513440
C         -0.892701       -0.629946        1.675629
C         -0.534089       -2.117487        1.544520
C         -1.819925       -2.940638        1.736439
C         -2.447731       -2.655263        3.104721
C         -2.732522       -1.162812        3.285731
C         -1.467821       -0.331538        3.062075
N          0.232724       -2.376856        0.321059
C          0.795472       -3.719681        0.297340
N          1.450506        1.900672        0.377360
C          2.666101        1.247965        0.118656
C          3.840789        2.006604        0.185500
C          5.062471        1.428313       -0.126340
C          5.155278        0.089841       -0.495057
C          3.983394       -0.651625       -0.557693
C          2.741548       -0.094507       -0.269520
C          6.310634        2.257386        0.001024
F          6.745392        2.294705        1.269788
C          4.025735       -2.107164       -0.931443
F          3.858191       -2.893541        0.143450
C         -0.498175       -2.108847       -0.911561
F          7.309180        1.769347       -0.745408
F          6.100397        3.526133       -0.376583
F          3.046319       -2.420593       -1.795549
F          5.189243       -2.447652       -1.497401
H          1.176903       -0.262747        1.526294
H          1.392227        2.875873        0.112530
H         -0.714584       -0.570482        3.826122
H         -1.684226        0.739308        3.128802
H         -3.491282       -0.850004        2.556144
H         -3.140894       -0.968419        4.283085
H         -3.368529       -3.236609        3.221872
H         -1.758761       -2.990289        3.892817
H         -2.536064       -2.683937        0.944024
H         -1.597847       -4.009109        1.641143
H         -1.657590       -0.372091        0.937585
H          0.148323       -2.366496        2.374776
H         -0.900576       -1.089956       -0.905016
H          0.196003       -2.187434       -1.754697
H         -1.324955       -2.816254       -1.090617
H          0.031602       -4.508582        0.201554
H          1.366444       -3.895979        1.214356
H          1.478772       -3.805795       -0.550496
H          3.792018        3.051746        0.477401
H          6.112273       -0.355802       -0.738905
H          1.850157       -0.714045       -0.354105
C         -3.717841        0.529149       -1.058359
O         -3.674816       -0.512035       -0.065829
C         -4.366674       -0.777057       -1.249038
N         -3.585107       -1.783661       -2.067001
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O	-2.767945	-1.379458	-2.868379
O	-3.815970	-2.952253	-1.821651
C	-5.827486	-1.097296	-1.197458
H	-5.978062	-2.056164	-0.698521
H	-6.239103	-1.150215	-2.208502
H	-6.340769	-0.308553	-0.645512
C	-4.496391	1.752316	-0.719972
C	-5.952968	4.055650	-0.134226
C	-4.559362	2.794132	-1.646556
C	-5.149267	1.871651	0.506647
C	-5.876719	3.022690	0.796645
C	-5.290887	3.941054	-1.355263
H	-4.032621	2.706963	-2.593389
H	-5.066457	1.068685	1.233152
H	-6.377430	3.115855	1.755319
H	-5.339642	4.748144	-2.079484
H	-6.519283	4.952918	0.094862
H	-2.767885	0.686552	-1.564674

SR epoxide:Catalyst, binary complex 15; Energy = -2449.845771; 6-31G(d) basis set.

N	2.236275	0.975474	-0.094574
C	1.477656	1.434753	0.918699
S	2.077391	1.930821	2.413629
C	3.687126	1.187934	-0.173699
C	4.374341	0.057969	-0.965903
C	5.870925	0.374965	-1.114735
C	6.125448	1.745594	-1.741638
C	5.456392	2.844395	-0.917269
C	3.959955	2.568533	-0.785943
N	4.208250	-1.292074	-0.427264
C	4.428848	-1.405340	1.003876
N	0.122655	1.497399	0.708398
C	-0.655675	0.961620	-0.331694
C	-1.803755	1.653427	-0.734000
C	-2.680324	1.065238	-1.636940
C	-2.423475	-0.188718	-2.182990
C	-1.265186	-0.854623	-1.795029
C	-0.385905	-0.298673	-0.876078
C	-3.969158	1.758324	-1.991396
F	-3.938562	3.059150	-1.686532
C	-1.010209	-2.235032	-2.337938
F	-0.970507	-2.230995	-3.677521
C	2.987754	-1.980691	-0.801073
F	-4.229329	1.649628	-3.302963
F	-5.003537	1.211582	-1.341030
F	0.146524	-2.746011	-1.898093
F	-1.988004	-3.081627	-1.981125
H	1.775785	0.879346	-0.996484
H	-0.374278	2.050182	1.402750
H	3.494078	2.610195	-1.781715
H	3.470076	3.326014	-0.164074
H	5.908311	2.878202	0.082993
H	5.615638	3.826861	-1.373058
H	7.202480	1.924781	-1.822717
H	5.721831	1.762524	-2.763506
H	6.346057	0.346509	-0.125073
H	6.322615	-0.425623	-1.707431
H	4.056187	1.178850	0.855411
H	3.943087	0.045338	-1.979205
H	2.131109	-1.711134	-0.163996
H	2.736399	-1.774460	-1.846012
H	3.130922	-3.063363	-0.696798
H	4.474183	-2.466520	1.272075
H	3.625774	-0.936754	1.602247
H	5.380070	-0.948947	1.289863
H	-2.027667	2.627813	-0.310564
H	-3.113857	-0.638231	-2.890077
H	0.465028	-0.873673	-0.532753
C	-2.282042	-0.821076	1.719733
O	-3.280299	-0.767618	2.753615
C	-2.379119	0.276643	2.702541
N	-2.968018	1.520753	2.072453
O	-2.296556	2.540095	2.169878
O	-4.003286	1.425159	1.457700
C	-1.520989	0.576956	3.898119

H	-1.239182	-0.370925	4.357409
H	-2.098110	1.162749	4.618356
H	-0.621394	1.135210	3.628151
C	-1.236334	-1.883658	1.741918
C	0.681489	-3.906382	1.583065
C	-1.555523	-3.114045	1.161074
C	0.057959	-1.659146	2.218836
C	1.007684	-2.676773	2.150542
C	-0.600311	-4.121842	1.080292
H	-2.552220	-3.273159	0.758521
H	0.342408	-0.690718	2.622342
H	2.009056	-2.499006	2.529868
H	-0.855153	-5.071140	0.620204
H	1.428698	-4.691589	1.522236
H	-2.723863	-0.622072	0.741499

SR epoxide:Catalyst, binary complex 16; Energy = -2449.844361; 6-31G(d) basis set.

N	0.271487	0.145553	1.377208
C	0.237670	1.353335	0.809972
S	-1.171763	2.251802	0.566883
C	-0.901001	-0.667655	1.668872
C	-0.542953	-2.152854	1.513704
C	-1.831218	-2.976772	1.685711
C	-2.462043	-2.715357	3.057623
C	-2.744470	-1.225943	3.266312
C	-1.478006	-0.392904	3.059281
N	0.230187	-2.391021	0.289923
C	0.793200	-3.733195	0.245639
N	1.445790	1.887634	0.426902
C	2.663064	1.241141	0.161471
C	3.837495	1.999027	0.261527
C	5.061524	1.429025	-0.049110
C	5.159382	0.096935	-0.444713
C	3.989880	-0.642353	-0.539854
C	2.743083	-0.090725	-0.256382
C	6.308716	2.267952	-0.000715
F	6.640383	2.719845	-1.219200
C	4.037508	-2.092498	-0.932860
F	3.858479	-2.893691	0.129243
C	-0.494778	-2.101609	-0.941319
F	6.160809	3.337566	0.791727
F	7.354486	1.564257	0.453620
F	3.067698	-2.393781	-1.811841
F	5.207338	-2.424703	-1.490459
H	1.168921	-0.302334	1.523686
H	1.388284	2.868123	0.182356
H	-0.726179	-0.647067	3.819821
H	-1.692324	0.676937	3.145329
H	-3.502069	-0.898005	2.542331
H	-3.153215	-1.049625	4.266853
H	-3.384279	-3.296910	3.161449
H	-1.775679	-3.066607	3.840909
H	-2.544430	-2.703865	0.895928
H	-1.611237	-4.043785	1.570990
H	-1.664309	-0.396992	0.933633
H	0.135084	-2.416975	2.342871
H	-0.897261	-1.082852	-0.918171
H	0.203442	-2.164851	-1.782439
H	-1.320437	-2.805752	-1.136953
H	0.029926	-4.520344	0.132592
H	1.359816	-3.925338	1.162138
H	1.480569	-3.804541	-0.600359
H	3.785479	3.032390	0.589815
H	6.121790	-0.347138	-0.672477
H	1.853510	-0.709359	-0.363615
C	-3.715205	0.546613	-1.049491
O	-3.689520	-0.498101	-0.059823
C	-4.372183	-0.753684	-1.250117
N	-3.591718	-1.763126	-2.064759
O	-2.786947	-1.361800	-2.879979
O	-3.812479	-2.930556	-1.804687
C	-5.835822	-1.063270	-1.213589
H	-5.997553	-2.023590	-0.720797
H	-6.238544	-1.107864	-2.228628
H	-6.348335	-0.273686	-0.662076

C	-4.487413	1.774689	-0.714337
C	-5.932040	4.086701	-0.133777
C	-5.144444	1.897593	0.509688
C	-4.540447	2.816932	-1.641043
C	-5.266035	3.968245	-1.352337
C	-5.865811	3.053123	0.797131
H	-5.069396	1.093811	1.236089
H	-4.010897	2.726624	-2.586017
H	-5.307114	4.775754	-2.076588
H	-6.369641	3.149151	1.753877
H	-6.493693	4.987427	0.093224
H	-2.759318	0.698406	-1.546431

SR epoxide:Catalyst, binary complex 17; Energy = -2449.840230; 6-31G(d) basis set.

N	1.776388	-2.489775	-1.088388
C	0.722174	-3.148222	-1.591732
S	0.803712	-4.714344	-2.173904
C	2.009406	-1.044165	-1.136339
C	3.366885	-0.755549	-0.475018
C	3.650741	0.753866	-0.506465
C	3.602380	1.311319	-1.930903
C	2.273785	0.976705	-2.610492
C	1.998642	-0.525148	-2.579818
N	3.452549	-1.384594	0.844210
C	2.739188	-0.664778	1.889696
N	-0.476180	-2.442447	-1.613343
C	-1.067536	-1.816023	-0.503459
C	-2.328221	-1.227843	-0.685781
C	-2.986602	-0.645496	0.386582
C	-2.416976	-0.626084	1.657896
C	-1.176990	-1.227164	1.832503
C	-0.496454	-1.825120	0.773434
C	-4.369149	-0.068497	0.217165
F	-5.182530	-0.524104	1.186542
C	-0.574319	-1.263318	3.211353
F	0.286352	-2.277822	3.355889
C	4.821707	-1.647251	1.257120
F	-4.377885	1.264464	0.306252
F	-4.914109	-0.406924	-0.955965
F	0.107740	-0.133527	3.495373
F	-1.515480	-1.385719	4.154226
H	2.598959	-3.061046	-0.929647
H	-1.145782	-2.858117	-2.251071
H	2.772328	-1.063589	-3.144165
H	1.032621	-0.748130	-3.041018
H	1.452957	1.490477	-2.092949
H	2.267036	1.334963	-3.645507
H	3.758398	2.396014	-1.907639
H	4.425068	0.882778	-2.519751
H	2.905212	1.274045	0.109171
H	4.629208	0.949509	-0.051705
H	1.221635	-0.528623	-0.570477
H	4.123177	-1.256685	-1.100324
H	5.406660	-0.729110	1.442299
H	4.810212	-2.227408	2.184823
H	5.335240	-2.237320	0.492398
H	1.742869	-0.371958	1.544595
H	3.258484	0.253536	2.214373
H	2.615936	-1.316980	2.759312
H	-2.789308	-1.227661	-1.669471
H	-2.949344	-0.191062	2.497033
H	0.454970	-2.318508	0.946265
C	-0.497748	1.966971	-0.238542
O	-1.860638	2.437988	-0.082359
C	-1.318063	2.434531	-1.354007
N	-1.874292	1.317520	-2.208856
O	-1.073281	0.578481	-2.751365
O	-3.081084	1.249193	-2.302713
C	-1.264299	3.713658	-2.137960
H	-2.270433	3.945269	-2.498004
H	-0.587777	3.617813	-2.991250
H	-0.927737	4.518004	-1.483193
C	0.614347	2.728704	0.397612
C	2.781639	3.952077	1.665116
C	1.452376	3.587332	-0.316801

C	0.868782	2.486042	1.749629
C	1.946988	3.096311	2.382326
C	2.532194	4.197844	0.317106
H	1.287450	3.758760	-1.376321
H	0.226613	1.802905	2.297814
H	2.139651	2.896747	3.431818
H	3.183812	4.857090	-0.247914
H	3.627350	4.423710	2.155497
H	-0.440129	0.882344	-0.118571

SR epoxide:Catalyst, binary complex 18; Energy = -2449.838535; 6-31G(d) basis set.

N	-3.393523	0.393199	1.151383
C	-3.186271	-0.596741	2.051227
S	-4.348467	-1.092652	3.143837
C	-2.901091	0.342722	-0.235475
C	-3.666766	-0.750208	-1.026645
C	-5.122828	-0.300220	-1.210978
C	-5.234673	1.060649	-1.904051
C	-4.485737	2.134869	-1.111712
C	-3.029045	1.718781	-0.891324
N	-2.963361	-0.996243	-2.290187
C	-1.741783	-1.761232	-2.057145
N	-1.945778	-1.206453	2.020691
C	-0.686947	-0.593616	1.894637
C	-0.509609	0.787036	1.776118
C	0.776548	1.315112	1.699014
C	1.900795	0.506749	1.759997
C	1.710110	-0.870966	1.860694
C	0.441837	-1.425943	1.920868
C	0.910675	2.807196	1.561814
F	2.149866	3.168771	1.217533
C	2.924856	-1.754385	1.824307
F	2.615265	-3.051250	1.807011
C	-3.767727	-1.708040	-3.275329
F	0.069247	3.283525	0.629043
F	0.609526	3.434621	2.708413
F	3.653664	-1.503558	0.710756
F	3.736630	-1.532860	2.863498
H	-4.305747	0.820557	1.268700
H	-1.935909	-2.065536	2.558537
H	-2.485005	2.459331	-0.293868
H	-2.532465	1.647270	-1.864818
H	-4.516453	3.094079	-1.638148
H	-4.991928	2.303063	-0.149951
H	-4.803818	0.999247	-2.911339
H	-6.288286	1.335738	-2.017858
H	-5.692552	-1.065974	-1.743813
H	-5.580468	-0.240830	-0.214253
H	-1.843425	0.087157	-0.194903
H	-3.670815	-1.672766	-0.410982
H	-3.141314	-1.918868	-4.146032
H	-4.155240	-2.670349	-2.893986
H	-4.610889	-1.101796	-3.612236
H	-1.954018	-2.773542	-1.667457
H	-1.082887	-1.267227	-1.341116
H	-1.180722	-1.856570	-2.989316
H	-1.367751	1.449714	1.751066
H	2.896213	0.931623	1.690792
H	0.321225	-2.503508	1.960901
C	1.695750	-0.313993	-1.425679
O	1.324206	-0.995078	-2.633140
C	2.403257	-1.505819	-1.923341
N	2.038945	-2.782744	-1.191743
O	2.907462	-3.621687	-1.081127
O	0.909949	-2.873827	-0.747841
C	3.751974	-1.563625	-2.572296
H	3.780217	-2.383142	-3.293836
H	4.532017	-1.726786	-1.827445
H	3.924371	-0.619355	-3.089618
C	2.259156	1.062832	-1.539707
C	3.233560	3.669519	-1.706507
C	1.441406	2.085747	-2.022215
C	3.559751	1.352079	-1.122422
C	4.047195	2.653176	-1.211427
C	1.929117	3.386421	-2.106018

H	0.425334	1.856498	-2.333731
H	4.184845	0.558106	-0.722512
H	5.060399	2.873010	-0.890289
H	1.290142	4.179323	-2.481391
H	3.612985	4.684257	-1.773179
H	0.971678	-0.481684	-0.628184

SR epoxide:Catalyst, binary complex 19; Energy = -2449.847707; 6-31G(d) basis set.

N	-3.436703	-0.963327	1.039066
C	-3.707654	-1.664894	-0.089373
S	-5.234748	-2.278383	-0.420111
C	-2.561394	0.211617	1.114008
C	-3.258429	1.443615	0.508412
C	-2.357429	2.677007	0.669209
C	-1.988486	2.914428	2.134014
C	-1.286643	1.687119	2.715692
C	-2.155072	0.438148	2.570476
N	-3.684822	1.148159	-0.856352
C	-4.873284	1.874018	-1.263677
N	-2.667595	-1.919428	-0.947954
C	-1.293329	-2.025262	-0.675672
C	-0.395103	-1.910659	-1.738826
C	0.972774	-2.010199	-1.506794
C	1.478973	-2.198603	-0.227283
C	0.572327	-2.303993	0.822911
C	-0.798947	-2.254648	0.612772
C	1.898128	-1.866620	-2.682734
F	1.783553	-0.651274	-3.250489
C	1.077124	-2.372065	2.236590
F	0.216307	-3.005663	3.045841
C	-2.639069	1.248802	-1.858226
F	3.178970	-2.038940	-2.350397
F	1.602857	-2.757739	-3.643095
F	2.257705	-2.984771	2.328422
F	1.229264	-1.128550	2.743094
H	-4.266400	-0.879042	1.618588
H	-2.976114	-2.303145	-1.832784
H	-3.065045	0.550951	3.178266
H	-1.627157	-0.447003	2.943672
H	-0.338992	1.525516	2.181295
H	-1.034792	1.844475	3.769437
H	-1.344719	3.796607	2.219531
H	-2.896675	3.123782	2.716349
H	-1.433684	2.524075	0.094155
H	-2.855187	3.556214	0.241261
H	-1.654858	0.019669	0.533362
H	-4.177015	1.607017	1.092669
H	-2.985451	0.768799	-2.780157
H	-2.358463	2.289925	-2.095747
H	-1.733974	0.727013	-1.527857
H	-5.677723	1.696545	-0.544404
H	-5.205469	1.500552	-2.237275
H	-4.712386	2.963618	-1.354229
H	-0.767762	-1.732076	-2.744520
H	2.546888	-2.222317	-0.048963
H	-1.485923	-2.367870	1.443776
C	2.227451	1.127774	0.255283
O	2.865176	0.326764	-0.737431
C	3.696125	1.078171	0.082123
N	4.396831	0.219603	1.106880
O	3.869211	-0.828597	1.421089
O	5.429821	0.659651	1.569134
C	4.555350	2.156367	-0.500552
H	5.437416	1.721352	-0.975810
H	4.878919	2.849785	0.276686
H	3.968952	2.692639	-1.248044
C	1.460941	2.313248	-0.225169
C	0.097267	4.567687	-1.133569
C	0.999313	2.363556	-1.540563
C	1.237238	3.389171	0.637630
C	0.561025	4.516227	0.180479
C	0.314506	3.490935	-1.990522
H	1.190286	1.522844	-2.201134
H	1.602934	3.347196	1.661197
H	0.398025	5.355658	0.849634

H	-0.044335	3.529449	-3.014535
H	-0.430792	5.447369	-1.488252
H	1.817703	0.543679	1.081553

SR epoxide:Catalyst, binary complex 20; Energy = -2449.845250; 6-31G(d) basis set.

N	3.541580	-0.680976	-1.093273
C	2.355770	-1.313532	-1.120542
S	2.103767	-2.665290	-2.096317
C	3.925289	0.455085	-0.268794
C	5.459262	0.581090	-0.302443
C	5.884117	1.691215	0.670864
C	5.246318	3.027642	0.275982
C	3.722299	2.921948	0.183573
C	3.307804	1.777442	-0.742312
N	6.100589	-0.722873	-0.146231
C	5.905233	-1.340879	1.156682
N	1.393569	-0.782449	-0.301483
C	0.105206	-1.328122	-0.088930
C	-0.809208	-1.439189	-1.135668
C	-2.108185	-1.851286	-0.864906
C	-2.509363	-2.175876	0.427729
C	-1.581978	-2.074546	1.455251
C	-0.279894	-1.654968	1.207556
C	-3.095208	-1.906986	-1.996487
F	-2.940057	-0.855980	-2.822608
C	-2.012571	-2.310150	2.873414
F	-3.058018	-3.144977	2.946490
C	7.508729	-0.702858	-0.507737
F	-2.967567	-3.010258	-2.739869
F	-4.362450	-1.869284	-1.548720
F	-1.023126	-2.828827	3.614619
F	-2.381405	-1.162411	3.464811
H	4.313106	-1.194296	-1.509214
H	1.688075	-0.126964	0.416491
H	3.654481	1.965829	-1.766526
H	2.217776	1.694751	-0.793821
H	3.293765	2.746059	1.178855
H	3.292660	3.861782	-0.175038
H	5.530264	3.805299	0.992599
H	5.644690	3.336272	-0.700288
H	5.576985	1.423371	1.690778
H	6.976144	1.781028	0.676837
H	3.619625	0.277446	0.777191
H	5.718545	0.911577	-1.320405
H	8.138349	-0.151327	0.210835
H	7.879574	-1.730880	-0.558153
H	7.629273	-0.246069	-1.494509
H	4.838305	-1.425232	1.382825
H	6.398727	-0.793795	1.977203
H	6.317447	-2.353520	1.129722
H	-0.507589	-1.180877	-2.144995
H	-3.529204	-2.483138	0.631284
H	0.431068	-1.561825	2.022698
C	-2.287059	2.190179	0.926358
O	-1.681360	0.896129	0.835475
C	-1.103350	1.902740	0.090302
N	0.212027	2.359988	0.668459
O	0.780487	1.633997	1.464742
O	0.625090	3.426315	0.263448
C	-1.042208	1.850651	-1.409592
H	-0.179563	1.256720	-1.728221
H	-0.949693	2.860466	-1.812605
H	-1.952474	1.384052	-1.789122
C	-3.638249	2.349035	0.322439
C	-6.155172	2.667564	-0.829490
C	-4.241813	1.282445	-0.344603
C	-4.301334	3.572263	0.424520
C	-5.556890	3.730533	-0.154601
C	-5.497787	1.442601	-0.921115
H	-3.727037	0.328190	-0.392776
H	-3.835274	4.398827	0.954738
H	-6.069756	4.683876	-0.075975
H	-5.958309	0.606229	-1.437714
H	-7.135363	2.793558	-1.278394
H	-2.107900	2.691251	1.877921

SR epoxide:Catalyst, binary complex 21; Energy = -2449.836854; 6-31G(d) basis set.

N	1.210285	-2.909883	-0.479748
C	0.395684	-3.294972	-1.489852
S	0.724185	-4.650603	-2.422609
C	1.551835	-1.525166	-0.111410
C	2.262719	-1.558965	1.262129
C	3.640064	-2.222943	1.096558
C	4.502169	-1.504917	0.055467
C	3.796672	-1.460719	-1.302678
C	2.410838	-0.828245	-1.173765
N	2.368543	-0.191792	1.782184
C	3.264980	-0.085811	2.925407
N	-0.723395	-2.543139	-1.760150
C	-1.557975	-1.802175	-0.905290
C	-1.481127	-1.861872	0.492763
C	-2.309284	-1.050215	1.255798
C	-3.242910	-0.194632	0.671826
C	-3.352264	-0.196024	-0.711539
C	-2.524687	-0.989964	-1.498949
C	-2.234435	-1.097416	2.758559
F	-1.932861	0.102338	3.271856
C	-4.370415	0.658972	-1.416144
F	-5.054609	1.434807	-0.575712
C	1.063069	0.340438	2.150259
F	-3.407918	-1.464359	3.290205
F	-1.306457	-1.965179	3.190563
F	-3.788625	1.448896	-2.334001
F	-5.254994	-0.104582	-2.078321
H	1.969849	-3.572259	-0.373572
H	-1.155102	-2.819940	-2.634480
H	1.878744	-0.848008	-2.133346
H	2.517228	0.221504	-0.867731
H	4.392637	-0.888986	-2.022011
H	3.705310	-2.478474	-1.708369
H	4.691781	-0.476346	0.387080
H	5.471594	-2.006473	-0.033836
H	4.147810	-2.285819	2.062511
H	3.498629	-3.268681	0.792474
H	0.616847	-0.980466	-0.011292
H	1.650762	-2.179648	1.949206
H	1.177619	1.341734	2.575562
H	0.406222	0.447695	1.282195
H	0.548653	-0.287395	2.897345
H	3.007367	-0.785614	3.741073
H	3.204042	0.929846	3.326855
H	4.302117	-0.260684	2.629704
H	-0.774798	-2.530104	0.973528
H	-3.864182	0.454141	1.280058
H	-2.606260	-0.947689	-2.582289
C	0.873241	3.341659	0.127705
O	-0.011100	3.994485	-0.805284
C	-0.313147	2.688737	-0.440052
N	-1.534649	2.628589	0.451364
O	-2.600577	2.794048	-0.107005
O	-1.382992	2.391548	1.633553
C	-0.372602	1.608401	-1.474551
H	-0.463023	0.634405	-0.985077
H	0.537403	1.618418	-2.074729
H	-1.247204	1.761223	-2.112109
C	2.251445	3.019205	-0.332448
C	4.819645	2.290002	-1.145425
C	2.608500	3.098535	-1.681004
C	3.196269	2.613032	0.608877
C	4.475883	2.246700	0.203743
C	3.887202	2.727342	-2.085597
H	1.886091	3.466571	-2.403651
H	2.929477	2.580653	1.661377
H	5.203192	1.926649	0.944363
H	4.158648	2.787387	-3.134845
H	5.816473	1.998861	-1.462264
H	0.777945	3.708855	1.148715

SR epoxide:Catalyst, binary complex 22; Energy = -2449.847955; 6-31G(d) basis set.

N	-3.936426	0.448650	0.130983

C	-3.001837	1.408968	0.294735
S	-3.424439	3.035778	0.340554
C	-3.737858	-0.906136	-0.389308
C	-4.804032	-1.853993	0.190760
C	-4.603031	-3.258585	-0.394698
C	-4.609614	-3.256108	-1.924518
C	-3.542195	-2.309182	-2.473576
C	-3.742305	-0.898517	-1.922196
N	-4.862384	-1.913475	1.651349
C	-5.703873	-0.916367	2.292690
N	-1.730920	0.930076	0.481250
C	-0.521684	1.637123	0.423558
C	-0.310144	2.660184	-0.504027
C	0.927401	3.291150	-0.559065
C	1.975231	2.908840	0.268713
C	1.762550	1.865728	1.164473
C	0.528213	1.233823	1.257733
C	1.103827	4.424427	-1.532011
F	0.594805	4.119352	-2.734700
C	2.922568	1.424950	2.011721
F	2.571712	0.554767	2.959561
C	-3.575410	-2.004979	2.313552
F	0.478501	5.531856	-1.112848
F	2.395842	4.736008	-1.705550
F	3.875304	0.843834	1.253887
F	3.508865	2.471369	2.612463
H	-4.870093	0.829004	0.019751
H	-1.649747	-0.034953	0.788709
H	-4.700848	-0.490709	-2.273184
H	-2.952211	-0.222990	-2.269273
H	-2.546224	-2.666225	-2.178212
H	-3.564968	-2.290917	-3.568108
H	-4.452600	-4.272295	-2.301273
H	-5.596804	-2.933650	-2.283395
H	-3.643178	-3.660214	-0.040997
H	-5.387013	-3.907769	0.006168
H	-2.760390	-1.275956	-0.067087
H	-5.787494	-1.493254	-0.147893
H	-3.023329	-1.045433	2.326706
H	-3.729119	-2.303423	3.355688
H	-2.942585	-2.758945	1.837050
H	-6.658985	-0.842277	1.764046
H	-5.248232	0.086532	2.341774
H	-5.914133	-1.236879	3.319269
H	-1.108060	2.959246	-1.172957
H	2.938416	3.404222	0.211062
H	0.384310	0.427431	1.971137
C	2.196997	-2.589167	0.217591
O	2.062184	-1.357590	0.923258
C	1.592694	-1.370983	-0.378721
N	0.085943	-1.418083	-0.414702
O	-0.493751	-1.784815	0.597620
O	-0.458026	-1.098274	-1.449865
C	2.185444	-0.481239	-1.427338
H	1.739405	0.516007	-1.372137
H	2.010884	-0.893544	-2.422119
H	3.258156	-0.407132	-1.244846
C	3.566626	-3.038306	-0.148353
C	6.111005	-3.918510	-0.859266
C	4.685136	-2.274636	0.188002
C	3.722149	-4.246891	-0.829583
C	4.993078	-4.683115	-1.188659
C	5.955339	-2.718620	-0.168997
H	4.551749	-1.345949	0.734410
H	2.849102	-4.844893	-1.078255
H	5.111403	-5.622223	-1.719726
H	6.825709	-2.127497	0.097440
H	7.102935	-4.261585	-1.135902
H	1.495287	-3.354744	0.548462

SR epoxide:Catalyst, binary complex 23; Energy = -2449.842719; 6-31G(d) basis set.

N	3.050241	-0.211455	-1.619885
C	2.222334	-1.284142	-1.559788
S	2.393020	-2.609355	-2.578018
C	3.569740	0.505674	-0.448436

C	4.628395	-0.351760	0.273563
C	5.260988	0.440050	1.428260
C	5.849780	1.765060	0.940625
C	4.771163	2.611341	0.262102
C	4.131715	1.853580	-0.901505
N	4.056058	-1.644877	0.633930
C	3.221028	-1.640961	1.821646
N	1.184038	-1.233621	-0.666011
C	0.479703	-0.123891	-0.177338
C	-0.328228	-0.311078	0.949616
C	-1.059505	0.752093	1.464604
C	-1.001953	2.014418	0.884895
C	-0.207851	2.183462	-0.244355
C	0.522159	1.134665	-0.788797
C	-1.842114	0.565870	2.736087
F	-1.080505	0.853766	3.807104
C	-0.212246	3.510917	-0.948702
F	-1.243498	3.602466	-1.805318
C	5.028286	-2.721230	0.674779
F	-2.907617	1.369337	2.789550
F	-2.259984	-0.697739	2.889294
F	-0.328763	4.528541	-0.086683
F	0.907632	3.703648	-1.660974
H	3.745241	-0.332151	-2.350632
H	0.712758	-2.125388	-0.550774
H	4.887963	1.677684	-1.680584
H	3.329197	2.443536	-1.358156
H	3.995007	2.865124	0.997099
H	5.189079	3.556724	-0.097850
H	6.293384	2.312041	1.778954
H	6.659541	1.566905	0.225062
H	4.494005	0.650432	2.185811
H	6.027427	-0.176330	1.913126
H	2.745223	0.694465	0.244811
H	5.417176	-0.557767	-0.466047
H	5.773239	-2.610876	1.483145
H	4.505045	-3.670080	0.828242
H	5.554393	-2.778925	-0.282383
H	3.794294	-1.577868	2.762627
H	2.634031	-2.565926	1.843393
H	2.515751	-0.803623	1.795898
H	-0.377931	-1.291125	1.417366
H	-1.566077	2.842988	1.299489
H	1.124590	1.288550	-1.677248
C	-4.101664	-1.359356	-0.096105
O	-3.923218	-0.159549	0.671547
C	-4.102032	-0.011777	-0.695672
N	-5.495545	0.492046	-1.020195
O	-6.377064	0.255886	-0.221983
O	-5.630019	1.079821	-2.075441
C	-3.036260	0.635318	-1.526743
H	-2.067948	0.237978	-1.217951
H	-3.045510	1.716954	-1.372365
H	-3.196180	0.435371	-2.587058
C	-2.942966	-2.296704	-0.189547
C	-0.801586	-4.087084	-0.288046
C	-2.255882	-2.502542	-1.385695
C	-2.569566	-3.009141	0.954080
C	-1.498622	-3.896481	0.906637
C	-1.187018	-3.396519	-1.436733
H	-2.556147	-1.969322	-2.283030
H	-3.112277	-2.854353	1.881644
H	-1.211000	-4.444351	1.798634
H	-0.641593	-3.540588	-2.364160
H	0.036769	-4.776557	-0.330065
H	-5.081062	-1.806623	0.070079

SR epoxide:Catalyst, binary complex 24; Energy = -2449.849638; 6-31G(d) basis set.

N	2.979247	-0.047979	1.368399
C	3.212271	1.291346	1.365027
S	4.599557	1.962080	2.022183
C	2.457096	-0.800685	0.220164
C	3.474828	-0.772490	-0.941726
C	3.029312	-1.695299	-2.086336
C	2.822540	-3.126174	-1.591888

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C          1.773885       -3.148570       -0.481442
C          2.166956       -2.232522        0.678808
N          3.768847        0.603143       -1.324696
C          5.103454        0.789018       -1.862930
N          2.230807        2.102924        0.852144
C          0.837833        1.948543        0.862454
C          0.087306        2.840630        0.091736
C         -1.301528        2.803731        0.131547
C         -1.974176        1.879328        0.917287
C         -1.216682        0.982927        1.666859
C          0.171995        1.001892        1.653033
C         -2.060827        3.827216       -0.665071
F         -3.361052        3.528284       -0.766115
C         -1.922893        0.012289        2.575071
F         -3.114359       -0.345273        2.074643
C          2.763001        1.236887       -2.156524
F         -1.974232        5.043107       -0.103979
F         -1.570103        3.945163       -1.910654
F         -1.205802       -1.106078        2.763561
F         -2.148221        0.543991        3.784284
H          3.732150       -0.537104        1.843334
H          2.556443        3.049859        0.701570
H          3.075271       -2.636077        1.150437
H          1.388572       -2.224664        1.452017
H          0.814758       -2.815913       -0.908048
H          1.616385       -4.164903       -0.107204
H          2.515290       -3.775990       -2.417443
H          3.771623       -3.523267       -1.207587
H          2.085987       -1.324872       -2.512747
H          3.774709       -1.656919       -2.889621
H          1.518033       -0.335917       -0.104962
H          4.410017       -1.182352       -0.530993
H          2.956510        2.314844       -2.186723
H          2.750753        0.864995       -3.195852
H          1.763219        1.095757       -1.729277
H          5.258602        0.297946       -2.840151
H          5.839991        0.403098       -1.152793
H          5.290266        1.859698       -1.991373
H          0.595211        3.567490       -0.537120
H         -3.057050        1.841527        0.930224
H          0.737489        0.305509        2.263483
C         -1.651071       -1.955970       -0.077743
O         -2.661877       -2.633942        0.656675
C         -1.995199       -3.379820       -0.304422
N         -1.007035       -4.333958        0.320465
O         -0.550055       -4.037823        1.405054
O         -0.702997       -5.312582       -0.334025
C         -2.732473       -3.945194       -1.477082
H         -3.401347       -3.176141       -1.866181
H         -3.319169       -4.814724       -1.171892
H         -2.033155       -4.248198       -2.257019
C         -2.066471       -0.877044       -1.012679
C         -2.776603        1.221246       -2.702957
C         -1.088877       -0.218175       -1.760354
C         -3.401076       -0.484137       -1.110158
C         -3.752321        0.564525       -1.955963
C         -1.442460        0.828394       -2.605219
H         -0.048790       -0.529015       -1.680072
H         -4.147289       -0.986843       -0.501986
H         -4.788805        0.880656       -2.021168
H         -0.676958        1.347361       -3.174885
H         -3.051352        2.052886       -3.343710
H         -0.746890       -1.770239        0.504392

SR epoxide:Catalyst, binary complex 25; Energy = -2449.847864; 6-31G(d) basis set.
N          1.803412        0.125425        1.120376
C          1.282379        0.274029        2.354933
S          2.031189        1.102205        3.614411
C          3.007099        0.833436        0.671362
C          3.747451        0.061832       -0.438713
C          4.997365        0.859621       -0.839062
C          4.645921        2.271797       -1.309186
C          3.878917        3.031303       -0.227729
C          2.640512        2.247648        0.205856
N          4.099082       -1.326490       -0.140304
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C	3.147376	-2.296102	-0.639614
N	0.047188	-0.281248	2.579584
C	-0.706412	-1.082855	1.698891
C	-2.040008	-0.763468	1.431879
C	-2.768636	-1.553750	0.553960
C	-2.190696	-2.652627	-0.079479
C	-0.867944	-2.968548	0.206269
C	-0.132142	-2.209711	1.111511
C	-4.179825	-1.180616	0.188123
F	-4.657150	-0.199345	0.957479
C	-0.196884	-4.122105	-0.488543
F	0.712672	-4.711370	0.295926
C	4.509550	-1.583590	1.228669
F	-4.248111	-0.776669	-1.087732
F	-5.002669	-2.233510	0.307087
F	-1.076079	-5.049311	-0.877461
F	0.455794	-3.709698	-1.593960
H	1.193228	-0.214531	0.379508
H	-0.358573	-0.028713	3.471988
H	1.933955	2.165436	-0.635406
H	2.124635	2.758383	1.026482
H	4.530066	3.183125	0.643734
H	3.586859	4.024850	-0.583706
H	5.553972	2.814888	-1.591432
H	4.020005	2.202963	-2.210829
H	5.680487	0.914548	0.020527
H	5.515915	0.300058	-1.623197
H	3.657009	0.909077	1.548393
H	3.086498	0.037371	-1.315996
H	3.686822	-1.523834	1.962769
H	4.946074	-2.585439	1.287319
H	5.281851	-0.868669	1.528576
H	2.140763	-2.212474	-0.197367
H	3.512322	-3.308425	-0.437369
H	3.040200	-2.189228	-1.725119
H	-2.495315	0.108816	1.888836
H	-2.766599	-3.254193	-0.775533
H	0.877768	-2.497351	1.384079
C	-2.058241	2.342583	-1.398811
O	-2.796498	1.624216	-0.413202
C	-2.081093	2.731475	0.028875
N	-2.993289	3.899504	0.322975
O	-2.589595	4.714358	1.129180
O	-4.043997	3.954016	-0.279966
C	-0.959316	2.574548	1.006254
H	-0.331396	3.466459	1.014696
H	-0.357618	1.715409	0.702214
H	-1.342842	2.410873	2.016993
C	-0.878154	1.664142	-2.003714
C	1.299755	0.396030	-3.199511
C	-0.631629	0.312976	-1.753141
C	-0.035322	2.378386	-2.856140
C	1.055134	1.745615	-3.448224
C	0.454895	-0.320849	-2.351824
H	-1.322121	-0.240465	-1.124468
H	-0.235438	3.426908	-3.061146
H	1.707864	2.304719	-4.111326
H	0.624225	-1.379599	-2.173369
H	2.142973	-0.098901	-3.672955
H	-2.687062	2.933520	-2.063394

SR epoxide:Catalyst, binary complex 26; Energy = -2449.844461; 6-31G(d) basis set.

N	-3.304271	-0.147972	1.192957
C	-3.531890	-1.446081	0.870009
S	-5.015838	-2.184249	1.114935
C	-2.536695	0.803336	0.379558
C	-3.329028	1.193921	-0.882473
C	-2.578408	2.287379	-1.660902
C	-2.323640	3.518168	-0.789302
C	-1.516114	3.136514	0.450152
C	-2.205910	2.024349	1.242951
N	-3.680918	0.000374	-1.644809
C	-4.897050	0.153605	-2.423328
N	-2.477389	-2.182542	0.378101
C	-1.105211	-2.090837	0.645538

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C         -0.561629       -1.237534        1.612074
C          0.814912       -1.187972        1.794465
C          1.683899       -2.002461        1.077839
C          1.128423       -2.882454        0.154580
C         -0.242291       -2.926377       -0.074586
C          1.327174       -0.192030        2.797726
F          0.819775       -0.425036        4.018257
C          2.015932       -3.754576       -0.691490
F          1.541048       -5.006786       -0.767578
C         -2.606576       -0.553225       -2.449072
F          2.656076       -0.196616        2.904371
F          0.945795        1.056759        2.461355
F          2.081810       -3.287421       -1.949136
F          3.261725       -3.815515       -0.216529
H         -4.135010        0.267682        1.604188
H         -2.782386       -3.073112        0.003679
H         -3.147157        2.413010        1.659477
H         -1.584778        1.714685        2.090344
H         -0.511010        2.816376        0.141096
H         -1.366494        4.006424        1.098097
H         -1.790218        4.285196       -1.361420
H         -3.284223        3.955366       -0.483397
H         -1.612682        1.891622       -2.004949
H         -3.150854        2.552355       -2.557882
H         -1.604871        0.322036        0.069491
H         -4.278896        1.624566       -0.530141
H         -1.702650       -0.684826       -1.844819
H         -2.908300       -1.543070       -2.806803
H         -2.347766        0.062064       -3.328101
H         -5.717029        0.459868       -1.767707
H         -5.162345       -0.811170       -2.866174
H         -4.804489        0.889023       -3.242108
H         -1.211500       -0.614807        2.217513
H          2.756930       -1.937950        1.217113
H         -0.644926       -3.609573       -0.817872
C          3.183005        1.590601       -0.667244
O          2.901905        0.523450        0.244067
C          2.376709        0.412265       -1.031524
N          3.091988       -0.606830       -1.874042
O          2.651418       -0.759076       -2.996604
O          4.048365       -1.176442       -1.394532
C          0.893788        0.417152       -1.245079
H          0.503829       -0.603670       -1.209180
H          0.642988        0.858034       -2.212521
H          0.450373        1.006094       -0.440178
C          2.505213        2.893111       -0.398057
C          1.237721        5.319218        0.114647
C          2.349397        3.332122        0.916705
C          2.021273        3.663675       -1.456540
C          1.384983        4.875264       -1.198364
C          1.720280        4.547793        1.170230
H          2.709520        2.711697        1.731051
H          2.140852        3.313310       -2.478917
H          1.006238        5.472496       -2.022130
H          1.601492        4.890439        2.193422
H          0.742894        6.264839        0.314188
H          4.220834        1.606278       -1.000936

SR epoxide:Catalyst, binary complex 27; Energy = -2449.838416; 6-31G(d) basis set.
N         -0.487059       -1.944407       -0.656334
C         -0.051216       -1.593689       -1.873198
S         -0.864961       -1.921742       -3.310826
C         -1.748298       -2.620841       -0.366315
C         -1.543795       -3.622490        0.786590
C         -2.888289       -4.279890        1.128707
C         -3.966885       -3.247941        1.466131
C         -4.159018       -2.264412        0.312335
C         -2.834770       -1.592552       -0.041929
N         -0.515390       -4.638678        0.562721
C         -0.560800       -5.278032       -0.741602
N          1.152603       -0.932347       -1.923014
C          1.924414       -0.418549       -0.861602
C          3.312006       -0.567608       -0.904918
C          4.097603       -0.022692        0.103431
C          3.526745        0.655631        1.173541
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C	2.144213	0.803433	1.205089
C	1.339656	0.289166	0.195509
C	5.584552	-0.250901	0.067284
F	6.057317	-0.206158	-1.185351
C	1.522157	1.580419	2.335065
F	0.244464	1.219167	2.536918
C	0.844711	-4.265395	0.907367
F	6.244057	0.662128	0.789209
F	5.901581	-1.455959	0.563802
F	2.183878	1.367574	3.482819
F	1.540822	2.896037	2.109563
H	0.117171	-1.770286	0.138900
H	1.537006	-0.862349	-2.857273
H	-2.490547	-0.981933	0.805360
H	-2.954535	-0.920657	-0.900124
H	-4.538932	-2.801592	-0.567181
H	-4.902840	-1.500981	0.566167
H	-4.908339	-3.755039	1.701635
H	-3.669877	-2.693422	2.367988
H	-3.224796	-4.881781	0.273570
H	-2.723785	-4.971007	1.960497
H	-2.030668	-3.166913	-1.272011
H	-1.229681	-3.050381	1.674451
H	0.854687	-3.726088	1.859995
H	1.444729	-5.173718	1.032581
H	1.350706	-3.646601	0.143899
H	0.081121	-6.164581	-0.725153
H	-0.215603	-4.622727	-1.561769
H	-1.577145	-5.608233	-0.973086
H	3.772609	-1.108916	-1.726045
H	4.145403	1.063339	1.965173
H	0.267784	0.462706	0.220888
C	-1.755023	3.469533	-0.103480
O	-0.515954	2.808551	0.147782
C	-0.928831	2.879132	-1.178781
N	-0.129276	3.896583	-1.955196
O	0.368104	4.812634	-1.334907
O	-0.066008	3.733456	-3.158140
C	-1.236158	1.632188	-1.947686
H	-0.320794	1.186855	-2.345370
H	-1.904907	1.846177	-2.782979
H	-1.722383	0.923099	-1.272742
C	-3.001426	2.799122	0.361912
C	-5.352248	1.568816	1.215478
C	-2.945173	1.757203	1.285626
C	-4.235262	3.231418	-0.129439
C	-5.407067	2.613635	0.293549
C	-4.122375	1.146202	1.713128
H	-1.980925	1.441268	1.673118
H	-4.275987	4.048879	-0.844923
H	-6.363636	2.948285	-0.094907
H	-4.077261	0.337643	2.437934
H	-6.267672	1.089575	1.548824
H	-1.692419	4.551536	0.007276

SR epoxide:Catalyst, binary complex 28; Energy = -2449.845011; 6-31G(d) basis set.

N	-0.923077	-0.596014	-0.074850
C	0.150472	0.161765	0.235736
S	-0.040070	1.579535	1.133032
C	-1.088048	-1.623745	-1.108891
C	-0.733549	-3.031856	-0.588354
C	-1.248694	-4.145727	-1.511180
C	-2.744405	-4.005659	-1.786553
C	-3.010875	-2.661690	-2.460054
C	-2.556121	-1.522358	-1.553376
N	0.717106	-3.119554	-0.301837
C	1.539528	-3.484680	-1.455697
N	1.332601	-0.367827	-0.189688
C	2.605969	0.203387	-0.073123
C	2.860318	1.544945	-0.376863
C	4.159588	2.027771	-0.299430
C	5.226388	1.205874	0.055354
C	4.962818	-0.126870	0.338262
C	3.667111	-0.629512	0.282887
C	4.409637	3.484883	-0.574803

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F          5.668284        3.700871       -0.984726
C          6.082779       -1.070532        0.670108
F          6.401027       -1.843926       -0.381891
C          1.011323       -3.984830        0.835873
F          3.587952        3.956467       -1.523457
F          4.218755        4.235122        0.519012
F          7.194947       -0.423999        1.037165
F          5.745574       -1.902552        1.668027
H         -1.783249       -0.266927        0.347099
H          1.289954       -1.406997       -0.230133
H         -3.180015       -1.533325       -0.647329
H         -2.704682       -0.549730       -2.034190
H         -2.473572       -2.620618       -3.416841
H         -4.075180       -2.539834       -2.685717
H         -3.088534       -4.832084       -2.416354
H         -3.306287       -4.058854       -0.843567
H         -0.721192       -4.105604       -2.472812
H         -1.019528       -5.119670       -1.062327
H         -0.428108       -1.372240       -1.951551
H         -1.245465       -3.125963        0.379152
H          0.725256       -5.033251        0.655602
H          2.085700       -3.959804        1.041343
H          0.483174       -3.619768        1.720416
H          1.425857       -4.538035       -1.750027
H          2.592035       -3.313954       -1.207468
H          1.290640       -2.853312       -2.313823
H          2.048051        2.197102       -0.673367
H          6.236153        1.595874        0.104762
H          3.475878       -1.669736        0.534084
C         -5.490006        1.330601        0.887877
O         -4.957820        2.566407        1.353844
C         -4.861244        2.331244       -0.008468
N         -5.878009        3.140178       -0.785669
O         -6.873839        3.503689       -0.196410
O         -5.633913        3.338489       -1.960075
C         -3.525130        2.254663       -0.678563
H         -3.606374        1.736025       -1.634698
H         -2.819949        1.735577       -0.026539
H         -3.139636        3.261069       -0.858600
C         -4.810926        0.072465        1.300341
C         -3.612598       -2.324512        2.086791
C         -5.429575       -1.148372        1.019088
C         -3.595907        0.091917        1.989234
C         -2.999033       -1.106812        2.378312
C         -4.831622       -2.343164        1.409149
H         -6.385560       -1.161599        0.501778
H         -3.125153        1.041444        2.230446
H         -2.052026       -1.080872        2.910037
H         -5.321138       -3.287718        1.192143
H         -3.150387       -3.256054        2.400604
H         -6.579369        1.307101        0.875709

SR epoxide:Catalyst, binary complex 29; Energy = -2449.846088; 6-31G(d) basis set.
N         -2.554397       -1.692953       -0.829010
C         -2.017967       -0.951870       -1.808444
S         -2.834953        0.089650       -2.852082
C         -3.857232       -1.528205       -0.171966
C         -3.987068       -0.134480        0.471869
C         -5.349156       -0.000127        1.169307
C         -6.503548       -0.299821        0.212023
C         -6.367309       -1.715612       -0.349670
C         -5.037233       -1.875930       -1.087157
N         -2.821161        0.139909        1.322021
C         -2.492781        1.555613        1.391315
N         -0.663418       -1.126206       -1.991601
C          0.318437       -1.411540       -1.021612
C          0.149351       -1.091772        0.328412
C          1.197345       -1.337310        1.213791
C          2.411877       -1.854859        0.790432
C          2.567679       -2.141584       -0.561725
C          1.532460       -1.949311       -1.461925
C          0.993703       -0.992328        2.660670
F          2.123316       -1.067944        3.368172
C          3.920377       -2.555190       -1.062489
F          3.844546       -3.235637       -2.215634
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C	-2.891101	-0.438870	2.655712
F	0.517547	0.264701	2.801161
F	0.094539	-1.800518	3.245525
F	4.693445	-1.481232	-1.288473
F	4.565914	-3.324806	-0.176471
H	-1.908662	-2.303839	-0.343557
H	-0.329627	-0.738949	-2.865677
H	-5.019396	-1.215640	-1.958323
H	-4.909374	-2.900860	-1.452260
H	-6.427751	-2.438332	0.476663
H	-7.193625	-1.942929	-1.031023
H	-7.461082	-0.182568	0.730451
H	-6.494838	0.422055	-0.615754
H	-5.403356	-0.704531	2.010648
H	-5.441247	1.007540	1.592400
H	-3.841217	-2.269481	0.638123
H	-3.951911	0.593141	-0.347333
H	-3.645524	0.042453	3.300112
H	-3.120110	-1.508280	2.600966
H	-1.917664	-0.330363	3.139841
H	-1.541825	1.675589	1.920570
H	-3.255310	2.155663	1.919643
H	-2.369377	1.954137	0.380022
H	-0.779979	-0.631997	0.677435
H	3.227764	-2.002413	1.487665
H	1.667556	-2.190089	-2.511942
C	1.816278	1.867165	0.234769
O	2.320401	0.945583	-0.726259
C	3.143101	2.017575	-0.406923
N	4.291400	1.579081	0.471238
O	5.315177	2.229305	0.400543
O	4.106480	0.626479	1.201774
C	3.520429	3.015895	-1.454950
H	4.271052	2.593999	-2.127133
H	3.925809	3.918562	-0.996598
H	2.624025	3.268376	-2.023589
C	0.652078	2.704498	-0.164757
C	-1.516340	4.300122	-0.889805
C	-0.037859	2.448748	-1.349357
C	0.242938	3.749205	0.667956
C	-0.836468	4.547175	0.303055
C	-1.121227	3.247193	-1.711043
H	0.270246	1.621299	-1.981822
H	0.771537	3.936614	1.599471
H	-1.147780	5.361925	0.949319
H	-1.661853	3.028256	-2.625805
H	-2.360917	4.921090	-1.171604
H	1.821879	1.478057	1.251976

SR epoxide:Catalyst, binary complex 30; Energy = -2449.843144; 6-31G(d) basis set.

N	-0.438799	1.173121	-0.727949
C	0.261898	1.384404	-1.867735
S	-0.461298	1.932895	-3.278057
C	0.030745	1.510083	0.621608
C	-0.022164	3.039003	0.807975
C	0.294470	3.418936	2.261400
C	-0.662094	2.716281	3.226272
C	-0.552303	1.199050	3.070669
C	-0.846313	0.770582	1.632758
N	0.788057	3.687470	-0.216859
C	2.216544	3.691140	0.039924
N	1.597340	1.060974	-1.847228
C	2.230245	0.050158	-1.105018
C	3.623203	0.093327	-0.975620
C	4.285654	-0.904997	-0.275092
C	3.592296	-1.953369	0.325462
C	2.211462	-1.983193	0.189829
C	1.527171	-1.009315	-0.528136
C	5.776417	-0.818815	-0.094375
F	6.092399	-0.239246	1.074097
C	1.392022	-3.080756	0.809560
F	0.508759	-2.580670	1.696465
C	0.310776	5.005363	-0.590643
F	6.341943	-2.032462	-0.095133
F	6.354270	-0.095970	-1.062445

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F          0.671571       -3.735313       -0.112348
F          2.145025       -3.975249        1.454384
H         -1.421009        1.404081       -0.853815
H          2.101393        1.397672       -2.658683
H         -1.900262        0.981038        1.398011
H         -0.695630       -0.308104        1.511978
H          0.462358        0.880724        3.346678
H         -1.240752        0.688837        3.752282
H         -0.447112        3.011565        4.258499
H         -1.694115        3.028023        3.009515
H          1.325305        3.126218        2.504096
H          0.237138        4.508544        2.372567
H          1.065488        1.173525        0.738157
H         -1.064171        3.331986        0.608534
H          0.414308        5.756365        0.212893
H          0.877750        5.358061       -1.457686
H         -0.742525        4.945324       -0.881654
H          2.518074        4.390924        0.838411
H          2.739482        3.980529       -0.877898
H          2.561431        2.688535        0.315400
H          4.181031        0.909675       -1.424619
H          4.117182       -2.725986        0.875265
H          0.448925       -1.067614       -0.633339
C         -4.668509       -1.283123       -0.323919
O         -4.384972       -1.749981       -1.638537
C         -3.601812       -2.269358       -0.618693
N         -3.997512       -3.691787       -0.288623
O         -5.134099       -4.028845       -0.545224
O         -3.150001       -4.386726        0.236307
C         -2.123648       -2.039482       -0.604070
H         -1.703364       -2.305865        0.367168
H         -1.933316       -0.984036       -0.812672
H         -1.641375       -2.651186       -1.371266
C         -4.384803        0.147292       -0.021412
C         -3.949329        2.840362        0.571887
C         -4.706725        0.649005        1.241418
C         -3.849811        0.998136       -0.991438
C         -3.636892        2.344374       -0.693746
C         -4.483859        1.990503        1.539740
H         -5.137592       -0.011942        1.989189
H         -3.618280        0.608439       -1.979872
H         -3.225935        3.001392       -1.456296
H         -4.734879        2.373858        2.523934
H         -3.785447        3.889714        0.799390
H         -5.587898       -1.694012        0.092194

SR epoxide:Catalyst, binary complex 31; Energy = -2449.846158; 6-31G(d) basis set.
N         -1.573912       -0.426906        0.969993
C         -0.892223       -0.711160        2.083802
S         -1.516351       -1.573137        3.389868
C         -2.992536       -0.666332        0.760460
C         -3.577258        0.433927       -0.135437
C         -5.119940        0.320141       -0.123073
C         -5.593976       -1.135648        0.054205
C         -4.605119       -2.104481       -0.597970
C         -3.237263       -2.041011        0.109336
N         -3.027569        1.756392        0.178168
C         -3.285825        2.213017        1.538309
N          0.419981       -0.299620        2.108891
C          1.033461        0.724956        1.369484
C          2.419629        0.663389        1.183244
C          3.069050        1.668808        0.482705
C          2.370423        2.750876       -0.048893
C          0.998770        2.805575        0.154732
C          0.322671        1.817376        0.864642
C          4.546149        1.555151        0.222946
F          4.786817        0.985665       -0.967245
C          0.194652        3.948659       -0.398417
F          0.957008        5.008805       -0.683517
C         -3.452788        2.755611       -0.791518
F          5.133739        2.759542        0.207854
F          5.159962        0.811822        1.150992
F         -0.443752        3.606611       -1.534343
F         -0.754151        4.346473        0.464152
H         -1.085275       -0.006686        0.183561
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H          0.950678       -0.690782        2.877338
H         -2.433904       -2.221257       -0.616771
H         -3.153650       -2.807844        0.886597
H         -4.991231       -3.127799       -0.578441
H         -4.488465       -1.834159       -1.656048
H         -5.676339       -1.377555        1.121012
H         -6.595272       -1.256657       -0.369929
H         -5.530689        0.942173        0.680426
H         -5.509048        0.723582       -1.064405
H         -3.461441       -0.638178        1.749304
H         -3.229879        0.217240       -1.156028
H         -4.532631        2.975205       -0.741219
H         -2.905849        3.684979       -0.616111
H         -3.218333        2.405466       -1.803092
H         -2.912497        1.484032        2.265149
H         -4.351291        2.400642        1.748878
H         -2.745936        3.152407        1.695127
H          2.977505       -0.185270        1.564879
H          2.887913        3.535465       -0.589071
H         -0.751342        1.905755        1.001933
C          1.755308       -2.572818       -1.428360
O          2.285154       -2.083784       -0.196063
C          1.614034       -3.301116       -0.151084
N          2.577414       -4.456219       -0.002432
O          2.138403       -5.471659        0.500189
O          3.707412       -4.298634       -0.414450
C          0.358778       -3.441977        0.648845
H         -0.157651       -4.368166        0.393113
H         -0.287479       -2.593565        0.419459
H          0.578219       -3.444015        1.719658
C          0.605910       -1.816469       -2.006241
C         -1.518570       -0.379468       -3.098647
C          0.530908       -0.434504       -1.825566
C         -0.380611       -2.478303       -2.738640
C         -1.440845       -1.758706       -3.285331
C         -0.533924        0.284148       -2.366156
H          1.317675        0.070940       -1.271844
H         -0.321313       -3.555035       -2.876478
H         -2.208517       -2.276035       -3.852334
H         -0.590091        1.358798       -2.216817
H         -2.344322        0.180122       -3.529206
H          2.523098       -2.934626       -2.111570

SR epoxide:Catalyst, binary complex 32; Energy = -2449.841762; 6-31G(d) basis set.
N          2.334574       -0.568749       -0.833509
C          2.325492       -1.904730       -0.969280
S          3.666324       -2.921561       -1.019133
C          3.492855        0.320292       -0.674737
C          4.277371        0.061983        0.625976
C          5.404118        1.098701        0.759502
C          6.325296        1.078569       -0.461780
C          5.526638        1.354784       -1.736616
C          4.403345        0.329613       -1.907345
N          3.363840       -0.022802        1.768923
C          3.890591       -0.839174        2.850382
N          1.079851       -2.487231       -1.062371
C         -0.192587       -1.907881       -1.170165
C         -1.266238       -2.579171       -0.565844
C         -2.543064       -2.053586       -0.638332
C         -2.789899       -0.840208       -1.281532
C         -1.721834       -0.181326       -1.866969
C         -0.434136       -0.715942       -1.852946
C         -3.695737       -2.786789       -0.008805
F         -4.416895       -3.444605       -0.927745
C         -1.898527        1.187904       -2.461489
F         -1.433304        1.260852       -3.712219
C          2.897460        1.257763        2.276946
F         -3.286194       -3.685973        0.894958
F         -4.532896       -1.939586        0.608151
F         -3.175788        1.577185       -2.464698
F         -1.205923        2.097073       -1.738614
H          1.456020       -0.164680       -0.530386
H          1.116139       -3.496324       -0.989282
H          4.832933       -0.666466       -2.046488
H          3.798706        0.554745       -2.792592
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H          5.100157        2.366464       -1.682498
H          6.180338        1.332407       -2.614388
H          7.123693        1.818497       -0.342694
H          6.807087        0.094928       -0.541345
H          4.971097        2.103867        0.859125
H          5.970634        0.903106        1.677881
H          3.042908        1.320081       -0.602720
H          4.734600       -0.928003        0.524152
H          2.547868        1.894114        1.456438
H          2.050337        1.087133        2.951285
H          3.669614        1.815507        2.833058
H          3.110382       -0.980382        3.606794
H          4.765707       -0.389045        3.351141
H          4.174765       -1.821123        2.461489
H         -1.083287       -3.495256       -0.013521
H         -3.787794       -0.415198       -1.302249
H          0.368570       -0.199256       -2.368669
C         -2.414230        1.632741        1.046254
O         -3.048546        2.586784        1.905498
C         -1.905975        3.001368        1.235219
N         -2.226956        3.917327        0.075069
O         -3.319110        3.808518       -0.438329
O         -1.344921        4.675069       -0.278780
C         -0.702972        3.425124        2.022046
H         -0.550507        2.707946        2.829800
H         -0.869006        4.418195        2.446494
H          0.183817        3.461954        1.388102
C         -1.760261        0.444069        1.666732
C         -0.582779       -1.850340        2.733104
C         -0.399662        0.198037        1.480793
C         -2.532097       -0.465728        2.392166
C         -1.944166       -1.611078        2.920607
C          0.195465       -0.944060        2.016197
H          0.198159        0.919327        0.923188
H         -3.592060       -0.276143        2.533917
H         -2.550594       -2.318940        3.476890
H          1.261806       -1.106394        1.862662
H         -0.127666       -2.743854        3.149885
H         -2.991958        1.464868        0.137755

SR epoxide:Catalyst, binary complex 33; Energy = -2449.848252; 6-31G(d) basis set.
N         -1.608816       -1.001760        0.020270
C         -0.359697       -1.192235       -0.456833
S          0.007608       -2.189836       -1.754145
C         -2.779930       -1.753119       -0.411458
C         -3.849392       -1.628988        0.687224
C         -5.038383       -2.530704        0.327304
C         -5.633174       -2.114416       -1.023189
C         -4.572416       -2.113067       -2.126473
C         -3.363571       -1.259391       -1.737341
N         -3.263509       -1.800192        2.022082
C         -2.670968       -3.111659        2.254896
N          0.570808       -0.444311        0.225431
C          1.962281       -0.405596        0.017502
C          2.594346        0.834575        0.005340
C          3.979861        0.914441       -0.096974
C          4.753625       -0.228270       -0.226350
C          4.108740       -1.463796       -0.232509
C          2.731425       -1.568230       -0.095467
C          4.602308        2.279828       -0.053654
F          5.935086        2.234721       -0.142134
C          4.918265       -2.717823       -0.413983
F          6.178100       -2.558359        0.017659
C         -4.193079       -1.458119        3.087721
F          4.152908        3.057521       -1.049524
F          4.293551        2.914043        1.093455
F          4.388330       -3.751398        0.254894
F          4.988102       -3.077327       -1.703195
H         -1.688015       -0.674908        0.983445
H          0.206262        0.293120        0.823393
H         -3.663883       -0.208960       -1.624129
H         -2.594755       -1.301005       -2.513585
H         -4.236633       -3.142430       -2.311477
H         -4.999581       -1.745401       -3.064569
H         -6.461893       -2.778817       -1.288897
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H         -6.054651       -1.104276       -0.928726
H         -4.705401       -3.576032        0.277579
H         -5.802911       -2.470910        1.109766
H         -2.492126       -2.806925       -0.537383
H         -4.207518       -0.585555        0.663176
H         -5.001953       -2.195688        3.216177
H         -3.649056       -1.392153        4.035699
H         -4.651533       -0.484415        2.884278
H         -3.410742       -3.928533        2.250259
H         -2.181625       -3.106511        3.233708
H         -1.908593       -3.324465        1.500060
H          2.004351        1.743130        0.079453
H          5.832273       -0.164097       -0.309315
H          2.253398       -2.539442       -0.065870
C         -2.407009        2.858297        0.300043
O         -1.927544        3.900010       -0.542443
C         -2.170490        2.676427       -1.153316
N         -3.441151        2.732897       -1.976794
O         -4.304017        3.505780       -1.617096
O         -3.509606        1.986070       -2.933065
C         -1.059296        1.921867       -1.812979
H         -1.364612        0.899918       -2.044736
H         -0.203057        1.896764       -1.136314
H         -0.766895        2.423118       -2.738658
C         -1.472719        2.334710        1.333829
C          0.254532        1.298145        3.272761
C         -1.919290        1.353479        2.223175
C         -0.166584        2.817044        1.438256
C          0.692198        2.302977        2.410798
C         -1.054928        0.824215        3.178169
H         -2.940497        0.984821        2.155531
H          0.165060        3.600011        0.761764
H          1.709377        2.677339        2.481284
H         -1.405772        0.040226        3.842377
H          0.929761        0.888933        4.016961
H         -3.447132        2.982853        0.599625

SR epoxide:Catalyst, binary complex 34; Energy = -2449.846428; 6-31G(d) basis set.
N         -1.408633       -2.079606       -1.337897
C         -1.185165       -0.905513       -1.940763
S         -2.341063        0.116851       -2.622923
C         -2.666602       -2.591472       -0.779532
C         -3.194780       -1.676739        0.343823
C         -4.483806       -2.269778        0.934860
C         -5.537097       -2.519462       -0.145595
C         -4.988315       -3.474046       -1.206820
C         -3.725862       -2.894791       -1.846150
N         -2.132086       -1.397555        1.317586
C         -2.340945       -0.149778        2.037966
N          0.139549       -0.551373       -2.065223
C          1.219628       -0.844202       -1.212811
C          2.511496       -0.699455       -1.725852
C          3.610064       -0.835175       -0.886830
C          3.454488       -1.155520        0.455999
C          2.163559       -1.329137        0.942765
C          1.042583       -1.165931        0.138795
C          4.972662       -0.562220       -1.458543
F          5.174740       -1.257326       -2.589864
C          1.940340       -1.661443        2.391452
F          0.983961       -0.892996        2.934878
C         -1.870886       -2.482472        2.253992
F          5.115499        0.733203       -1.771820
F          5.951106       -0.884085       -0.605403
F          1.533138       -2.936116        2.538233
F          3.048373       -1.511187        3.122699
H         -0.580097       -2.587493       -1.052217
H          0.280797        0.202471       -2.726177
H         -3.976294       -1.973064       -2.376584
H         -3.299348       -3.588748       -2.578605
H         -4.763380       -4.443272       -0.739277
H         -5.738126       -3.661850       -1.982170
H         -6.447624       -2.928182        0.305332
H         -5.812228       -1.568134       -0.620560
H         -4.257295       -3.226168        1.426168
H         -4.869738       -1.597092        1.710036
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H          -2.383717       -3.550784       -0.327214
H          -3.442559       -0.715698       -0.124688
H          -2.690202       -2.641642        2.974757
H          -1.698378       -3.422848        1.720583
H          -0.965934       -2.250856        2.820135
H          -1.438412        0.081522        2.612368
H          -3.195272       -0.189864        2.736466
H          -2.507008        0.663384        1.325099
H           2.652867       -0.457526       -2.776230
H           4.312321       -1.242436        1.111423
H           0.039151       -1.207766        0.569369
C          -0.202329        2.683712        1.047138
O          -0.149223        1.365015        0.507215
C           0.852851        2.239263        0.103898
N           2.171266        1.903295        0.768191
O           2.132606        1.464462        1.900232
O           3.182249        2.107249        0.124837
C           0.989955        2.655647       -1.328831
H           1.632889        1.956950       -1.868621
H           1.444458        3.646581       -1.392530
H          -0.003092        2.682711       -1.781644
C          -1.326236        3.558664        0.615250
C          -3.421381        5.219628       -0.172999
C          -2.239408        3.121256       -0.345138
C          -1.469734        4.823095        1.190035
C          -2.513430        5.652943        0.791895
C          -3.284385        3.953104       -0.736803
H          -2.132483        2.130419       -0.781138
H          -0.766098        5.156664        1.948716
H          -2.621125        6.636242        1.238873
H          -3.992289        3.605084       -1.482883
H          -4.237470        5.866669       -0.479261
H           0.092033        2.733466        2.094636

SR epoxide:Catalyst, binary complex 35; Energy = -2449.840447; 6-31G(d) basis set.
N           2.944299        1.193163       -1.721613
C           1.627874        1.378260       -1.929562
S           1.026517        1.616295       -3.483859
C           3.641992        0.831727       -0.493123
C           4.678658       -0.275227       -0.788889
C           5.421889       -0.629313        0.506158
C           6.070041        0.594864        1.156013
C           5.034548        1.684917        1.435906
C           4.288860        2.060712        0.156828
N           4.140015       -1.478542       -1.418907
C           2.897053       -1.963588       -0.846956
N           0.857218        1.359492       -0.797328
C          -0.547543        1.428112       -0.705520
C          -1.102778        2.190885        0.314993
C          -2.479489        2.171814        0.531285
C          -3.318177        1.415701       -0.268915
C          -2.747040        0.665922       -1.296457
C          -1.381834        0.666855       -1.529674
C          -3.012748        2.966937        1.687029
F          -4.343714        2.902868        1.778825
C          -3.620378       -0.286368       -2.059660
F          -3.048865       -0.703741       -3.194923
C           4.061687       -1.458780       -2.871923
F          -2.502327        2.519900        2.849226
F          -2.670576        4.260732        1.593224
F          -3.868245       -1.389976       -1.320571
F          -4.807471        0.247961       -2.362710
H           3.503004        1.284040       -2.561976
H           1.335662        1.464981        0.089875
H           4.987392        2.505303       -0.565060
H           3.518547        2.816839        0.353726
H           4.312051        1.319008        2.178167
H           5.510463        2.571480        1.866707
H           6.578219        0.303743        2.081336
H           6.840763        0.996757        0.484253
H           4.712100       -1.082429        1.212087
H           6.168005       -1.393327        0.269509
H           2.912275        0.395941        0.202647
H           5.416323        0.146246       -1.488858
H           3.965477       -2.487746       -3.235516
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H	3.203701	-0.887598	-3.265943
H	4.984796	-1.043708	-3.287704
H	2.023964	-1.347463	-1.133238
H	2.951767	-1.995824	0.245971
H	2.711287	-2.982131	-1.204034
H	-0.461862	2.796976	0.951323
H	-4.386932	1.389272	-0.088346
H	-0.955111	0.070037	-2.325623
C	-1.439511	-2.012786	1.952072
O	-2.174994	-1.121268	1.116596
C	-1.800628	-2.335594	0.557493
N	-2.967539	-3.283113	0.438084
O	-2.859895	-4.171564	-0.383821
O	-3.907146	-3.111828	1.184519
C	-0.845620	-2.397341	-0.593043
H	-0.116138	-1.594224	-0.466464
H	-1.374738	-2.274120	-1.540741
H	-0.329182	-3.359574	-0.605793
C	-0.049580	-1.603169	2.306656
C	2.521949	-0.821782	3.046888
C	0.918367	-2.567349	2.589349
C	0.269365	-0.247388	2.390950
C	1.555407	0.142416	2.759606
C	2.202902	-2.175955	2.958938
H	0.665661	-3.622700	2.526081
H	-0.507845	0.487356	2.202303
H	1.796477	1.199374	2.851943
H	2.954211	-2.927518	3.181066
H	3.518621	-0.521189	3.356874
H	-2.045730	-2.474818	2.730883

SR epoxide:Catalyst, binary complex 36; Energy = -2449.836438; 6-31G(d) basis set.

N	2.908588	0.310041	-0.447165
C	2.282738	-0.861569	-0.658850
S	2.943093	-2.248320	-1.357764
C	4.346386	0.585584	-0.568051
C	5.200108	-0.296593	0.364604
C	6.665336	0.161162	0.289252
C	7.185579	0.109078	-1.149113
C	6.323658	0.981098	-2.064644
C	4.856568	0.547929	-2.011749
N	4.616229	-0.347358	1.706360
C	4.981423	-1.554737	2.426700
N	0.969967	-0.915408	-0.263707
C	0.113494	0.098401	0.193276
C	-0.834954	-0.238206	1.166092
C	-1.753606	0.707817	1.597106
C	-1.745182	2.002716	1.088231
C	-0.804523	2.325079	0.118036
C	0.119202	1.391467	-0.341621
C	-2.708665	0.365036	2.708508
F	-3.859000	1.035695	2.599681
C	-0.860320	3.676921	-0.536982
F	-1.299641	4.620061	0.304434
C	4.864310	0.831893	2.518547
F	-2.987570	-0.944337	2.747735
F	-2.178619	0.685755	3.901456
F	0.340129	4.058677	-0.992763
F	-1.696418	3.667065	-1.589671
H	2.448215	0.910207	0.228267
H	0.574815	-1.849657	-0.301560
H	4.756673	-0.467806	-2.404490
H	4.231500	1.202866	-2.628402
H	6.410378	2.030416	-1.748616
H	6.685645	0.929976	-3.096673
H	8.230745	0.434412	-1.184956
H	7.159644	-0.928402	-1.508440
H	6.751487	1.192279	0.660879
H	7.279495	-0.466533	0.945856
H	4.437763	1.625596	-0.226417
H	5.141643	-1.316327	-0.031548
H	4.605672	1.741283	1.966148
H	4.231047	0.791897	3.410598
H	5.912076	0.923542	2.853407
H	4.717303	-2.431100	1.827952

H	4.418843	-1.598250	3.365045
H	6.055967	-1.609289	2.678422
H	-0.849767	-1.244876	1.573302
H	-2.462676	2.738906	1.434225
H	0.814533	1.657264	-1.131005
C	-4.157735	-1.688512	-0.604249
O	-4.252354	-0.533784	0.241927
C	-4.226778	-0.311025	-1.126970
N	-5.600011	0.057453	-1.654404
O	-6.563451	-0.339314	-1.034540
O	-5.632727	0.709781	-2.679245
C	-3.124988	0.502930	-1.732704
H	-2.178665	0.175149	-1.300028
H	-3.273282	1.562446	-1.510875
H	-3.097797	0.374756	-2.815533
C	-2.892184	-2.479560	-0.549923
C	-0.563799	-4.013905	-0.385800
C	-2.031004	-2.565040	-1.644153
C	-2.595861	-3.183247	0.621143
C	-1.432515	-3.942872	0.704703
C	-0.867716	-3.330097	-1.562708
H	-2.268413	-2.037024	-2.563444
H	-3.272414	-3.120724	1.468180
H	-1.203466	-4.482300	1.618402
H	-0.187245	-3.378561	-2.407301
H	0.350504	-4.596134	-0.322344
H	-5.088597	-2.254184	-0.627481

SR epoxide:Catalyst, binary complex 37; Energy = -2449.849140; 6-31G(d) basis set.

N	-1.722688	-1.114201	0.345067
C	-0.483245	-1.459105	-0.059157
S	-0.188854	-2.441582	-1.388859
C	-2.955879	-1.660835	-0.202529
C	-4.052095	-1.500315	0.863358
C	-5.336905	-2.176536	0.364580
C	-5.798800	-1.517124	-0.939622
C	-4.702936	-1.569270	-2.006305
C	-3.394024	-0.963213	-1.494745
N	-3.561806	-1.882148	2.189361
C	-3.222117	-3.292253	2.321860
N	0.486144	-0.877890	0.728340
C	1.871641	-0.790182	0.510733
C	2.646430	-1.829324	-0.010410
C	4.014930	-1.638642	-0.174318
C	4.640967	-0.449940	0.180587
C	3.862818	0.563278	0.728352
C	2.495347	0.400873	0.900951
C	4.822053	-2.750803	-0.785385
F	6.121452	-2.651408	-0.471296
C	4.492565	1.881115	1.087207
F	4.447829	2.740214	0.060545
C	-4.451685	-1.454833	3.256217
F	4.396559	-3.954083	-0.374695
F	4.738033	-2.742322	-2.123834
F	3.868509	2.461643	2.120684
F	5.783460	1.733521	1.422430
H	-1.833134	-0.781667	1.302086
H	0.134970	-0.121137	1.307616
H	-3.526964	0.108165	-1.286059
H	-2.602788	-1.066276	-2.243399
H	-4.524468	-2.614656	-2.292719
H	-5.026808	-1.043801	-2.910820
H	-6.712245	-1.998099	-1.305063
H	-6.048516	-0.466246	-0.735550
H	-5.154403	-3.245821	0.192872
H	-6.121549	-2.099513	1.125922
H	-2.794650	-2.725309	-0.423230
H	-4.257558	-0.422231	0.933998
H	-5.401666	-2.014091	3.286093
H	-3.952660	-1.592234	4.220304
H	-4.682428	-0.390773	3.136946
H	-4.096348	-3.958795	2.238889
H	-2.767042	-3.454127	3.303377
H	-2.489425	-3.579667	1.561798
H	2.188783	-2.772290	-0.275833

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H           5.709879       -0.322735        0.053501
H           1.911064        1.201111        1.350112
C          -1.059382        2.985052        0.145633
O          -0.358070        1.889850        0.747330
C           0.030888        2.263194       -0.538944
N           1.346916        3.011930       -0.520048
O           1.659933        3.567980        0.513874
O           1.979564        3.020402       -1.554268
C          -0.108628        1.311587       -1.686066
H          -0.113216        1.856327       -2.631626
H          -1.048389        0.766963       -1.570890
H           0.721682        0.600039       -1.699553
C          -2.489959        2.765351       -0.217039
C          -5.190940        2.472212       -0.845347
C          -2.953098        3.102623       -1.489409
C          -3.379886        2.276727        0.740618
C          -4.729851        2.139423        0.427334
C          -4.300757        2.949621       -1.805032
H          -2.258119        3.485243       -2.232256
H          -3.013661        2.010135        1.729184
H          -5.423920        1.768906        1.176668
H          -4.654686        3.206857       -2.798131
H          -6.243352        2.360208       -1.087538
H          -0.795373        3.940949        0.597297

SR epoxide:Catalyst, binary complex 38; Energy = -2449.846882; 6-31G(d) basis set.
N           1.183536       -2.644714        0.398816
C          -0.135151       -2.429904        0.558561
S          -1.104129       -3.553273        1.364782
C           2.169807       -1.835978       -0.306043
C           3.560399       -2.390611        0.052391
C           4.640700       -1.520910       -0.607932
C           4.487247       -1.567523       -2.130485
C           3.092892       -1.102187       -2.552357
C           1.980596       -1.869982       -1.830406
N           3.679092       -2.618108        1.491244
C           3.598717       -1.412784        2.301433
N          -0.601725       -1.253514        0.042880
C          -1.929587       -0.781913        0.130668
C          -2.999934       -1.501151       -0.394014
C          -4.273320       -0.941091       -0.369322
C          -4.495751        0.333829        0.137936
C          -3.416672        1.040078        0.658695
C          -2.146886        0.481075        0.681276
C          -5.434692       -1.745604       -0.882417
F          -5.957076       -2.522653        0.077373
C          -3.650390        2.418666        1.206861
F          -4.232199        3.214713        0.301182
C           4.846374       -3.410180        1.841394
F          -6.423204       -0.957430       -1.330570
F          -5.072074       -2.553967       -1.888167
F          -4.456145        2.396616        2.278432
F          -2.502888        3.010403        1.585187
H           1.567737       -3.387928        0.973584
H           0.075285       -0.520253       -0.151765
H           1.984729       -2.921616       -2.143765
H           0.998504       -1.463425       -2.098388
H           3.009929       -0.033369       -2.321979
H           2.963065       -1.201494       -3.634975
H           5.250997       -0.943837       -2.607630
H           4.650904       -2.596577       -2.478005
H           4.556008       -0.481109       -0.259508
H           5.633973       -1.879671       -0.316216
H           2.122863       -0.789245        0.039589
H           3.618911       -3.391513       -0.405195
H           5.799192       -2.866738        1.723782
H           4.765973       -3.723328        2.886654
H           4.881558       -4.307760        1.216777
H           4.428361       -0.707761        2.120678
H           3.618036       -1.699045        3.356962
H           2.652792       -0.893086        2.117877
H          -2.833294       -2.480340       -0.827073
H          -5.488748        0.771180        0.119513
H          -1.315981        1.017085        1.127999
C           1.745051        1.858042       -0.798877
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O          0.893905        1.327528        0.223701
C          0.582896        2.600556       -0.258472
N         -0.645756        2.518359       -1.145175
O         -0.781496        1.505905       -1.804550
O         -1.406977        3.460918       -1.122273
C          0.602306        3.785172        0.651491
H          0.561714        4.704594        0.065826
H          1.526354        3.767081        1.230711
H         -0.257370        3.758996        1.323381
C          3.160721        2.096847       -0.413186
C          5.853080        2.384573        0.250752
C          4.104281        2.354707       -1.410823
C          3.568542        1.976825        0.916502
C          4.913551        2.124057        1.245737
C          5.446988        2.501337       -1.077681
H          3.787455        2.428676       -2.448399
H          2.836159        1.743105        1.683972
H          5.227956        2.024750        2.280032
H          6.177233        2.697493       -1.856069
H          6.902001        2.491313        0.508190
H          1.575948        1.402393       -1.773485

SR epoxide:Catalyst, binary complex 39; Energy = -2449.846153; 6-31G(d) basis set.
N         -2.199119       -1.536460       -0.158636
C         -1.039399       -1.622795        0.524381
S         -0.913087       -1.912490        2.168895
C         -3.532641       -1.718737        0.400333
C         -4.529945       -1.292134       -0.695087
C         -5.966289       -1.410986       -0.171081
C         -6.265751       -2.848103        0.262216
C         -5.252325       -3.320679        1.306015
C         -3.816557       -3.171266        0.798040
N         -4.153395        0.004020       -1.271969
C         -4.566047        1.149879       -0.471069
N          0.046094       -1.430395       -0.306416
C          1.400775       -1.279471        0.035498
C          1.814268       -0.467562        1.097361
C          3.168158       -0.264911        1.312594
C          4.134802       -0.847632        0.496519
C          3.710218       -1.641081       -0.557486
C          2.357012       -1.870409       -0.787390
C          3.615690        0.631860        2.432569
F          4.062457       -0.066563        3.484807
C          4.706327       -2.150943       -1.555944
F          5.934729       -2.257598       -1.037813
C         -4.615231        0.166965       -2.643602
F          4.626251        1.427023        2.038669
F          2.626912        1.423959        2.866233
F          4.360990       -3.346832       -2.049661
F          4.793537       -1.308270       -2.606236
H         -2.217054       -0.921747       -0.975645
H         -0.130279       -1.586239       -1.292245
H         -3.663693       -3.803244       -0.087741
H         -3.101263       -3.491026        1.558730
H         -5.372495       -2.728126        2.223161
H         -5.441382       -4.364143        1.577810
H         -7.284573       -2.917414        0.657346
H         -6.218317       -3.508101       -0.614764
H         -6.098687       -0.740144        0.688052
H         -6.670611       -1.084398       -0.945512
H         -3.644381       -1.078310        1.290389
H         -4.408900       -2.022921       -1.509266
H         -5.713723        0.226370       -2.726719
H         -4.195051        1.091341       -3.050829
H         -4.266611       -0.670142       -3.255253
H         -5.659405        1.285475       -0.451209
H         -4.127641        2.053791       -0.902949
H         -4.221141        1.045077        0.563086
H          1.084874        0.007698        1.739503
H          5.190210       -0.660008        0.662618
H          2.046492       -2.496662       -1.619210
C         -0.605957        3.186426       -1.026052
O         -1.699780        2.337731       -1.374585
C         -1.546824        2.641104       -0.025882
N         -2.585624        3.625172        0.445532
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O	-3.055920	4.384517	-0.377357
O	-2.865066	3.596534	1.627514
C	-1.217230	1.566525	0.957010
H	-0.484579	0.916530	0.477626
H	-2.099385	0.979389	1.223750
H	-0.788721	1.990506	1.867383
C	0.766522	2.619895	-1.170278
C	3.352384	1.636629	-1.502634
C	1.003581	1.569627	-2.056202
C	1.821133	3.163803	-0.433645
C	3.111226	2.669249	-0.597048
C	2.298883	1.085076	-2.226852
H	0.171557	1.150911	-2.615408
H	1.630966	3.974322	0.265480
H	3.927023	3.085692	-0.015256
H	2.492864	0.275054	-2.924069
H	4.357961	1.250424	-1.637648
H	-0.758803	4.225833	-1.315365

SR epoxide:Catalyst, binary complex 40; Energy = -2449.843902; 6-31G(d) basis set.

N	1.392862	-3.014788	0.214836
C	0.320863	-3.710058	-0.239112
S	0.275673	-5.379706	-0.294810
C	1.935893	-1.819495	-0.471762
C	3.200987	-1.343537	0.287219
C	3.932076	-0.261218	-0.522077
C	4.281135	-0.715026	-1.938273
C	3.020319	-1.133473	-2.692537
C	2.271499	-2.215634	-1.920955
N	3.028075	-0.896656	1.664202
C	2.775961	-1.927312	2.655339
N	-0.756402	-2.966907	-0.680027
C	-1.349341	-1.869987	-0.029827
C	-0.957209	-1.440521	1.241209
C	-1.628967	-0.388674	1.846223
C	-2.715160	0.233799	1.239276
C	-3.105903	-0.215340	-0.016029
C	-2.426273	-1.243343	-0.660461
C	-1.164730	0.132123	3.176805
F	-0.605906	1.351801	3.053585
C	-4.323226	0.362451	-0.681132
F	-4.622642	1.580672	-0.200931
C	2.184315	0.271575	1.846006
F	-2.184173	0.266944	4.036292
F	-0.250916	-0.662103	3.747865
F	-4.144102	0.487722	-2.005046
F	-5.401903	-0.409417	-0.501079
H	2.120135	-3.649202	0.533671
H	-1.408382	-3.532464	-1.211348
H	2.894167	-3.121490	-1.882485
H	1.341952	-2.484613	-2.433978
H	2.362804	-0.267340	-2.842842
H	3.271311	-1.505989	-3.691309
H	4.803381	0.088224	-2.469124
H	4.972598	-1.567240	-1.890879
H	3.310471	0.641338	-0.584344
H	4.828341	0.018795	0.040316
H	1.174969	-1.027279	-0.464997
H	3.878914	-2.212804	0.332404
H	1.149639	0.141353	1.489153
H	2.135692	0.508464	2.912950
H	2.609748	1.141733	1.336658
H	3.011120	-1.528261	3.648215
H	3.439125	-2.779988	2.471857
H	1.740815	-2.301188	2.684040
H	-0.132120	-1.924798	1.748110
H	-3.241784	1.045149	1.730175
H	-2.732285	-1.561299	-1.653843
C	0.791192	1.811746	-1.099121
O	-0.193270	1.108868	-0.346766
C	-0.629697	1.723210	-1.513087
N	-0.872233	0.701903	-2.601151
O	-0.224781	-0.328079	-2.558689
O	-1.685768	0.988930	-3.453781
C	-1.639083	2.826519	-1.473516

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H         -2.641079        2.432824       -1.297161
H         -1.639318        3.368805       -2.419874
H         -1.372153        3.508962       -0.665634
C          1.384407        3.029374       -0.487475
C          2.543625        5.298680        0.638310
C          2.441145        3.669831       -1.137486
C          0.921216        3.513303        0.737969
C          1.501591        4.648073        1.296394
C          3.015415        4.806579       -0.577034
H          2.814234        3.276343       -2.080173
H          0.129714        2.979985        1.256654
H          1.144194        5.020437        2.251109
H          3.834635        5.304260       -1.085870
H          2.994847        6.182891        1.077159
H          1.472445        1.154612       -1.638161

SR epoxide:Catalyst, binary complex 41; Energy = -2449.846158; 6-31G(d) basis set.
N         -2.191569       -1.553154       -0.146390
C         -1.034447       -1.629843        0.542618
S         -0.914618       -1.882508        2.193477
C         -3.527181       -1.722605        0.411455
C         -4.520552       -1.303457       -0.690180
C         -5.958959       -1.417580       -0.170769
C         -6.260941       -2.850580        0.274195
C         -5.252992       -3.313269        1.327646
C         -3.815149       -3.170118        0.824154
N         -4.141374       -0.011336       -1.274938
C         -4.561130        1.140695       -0.486315
N          0.054726       -1.461333       -0.288532
C          1.406860       -1.293195        0.055809
C          2.371727       -1.905725       -0.741920
C          3.721619       -1.661126       -0.511445
C          4.135646       -0.827027        0.516193
C          3.161323       -0.221165        1.304501
C          1.809538       -0.443208        1.090243
C          4.728658       -2.197356       -1.485061
F          4.835372       -1.378405       -2.551701
C          3.583146        0.729682        2.389800
F          2.625412        1.627201        2.661329
C         -4.594789        0.140120       -2.650726
F          5.949077       -2.298599       -0.947073
F          4.384029       -3.402142       -1.957416
F          3.870439        0.094988        3.534140
F          4.685086        1.412915        2.034851
H         -2.203934       -0.951619       -0.972843
H         -0.117116       -1.643252       -1.270647
H         -3.659289       -3.811873       -0.054036
H         -3.102747       -3.482062        1.590997
H         -5.376954       -2.711251        2.238095
H         -5.444024       -4.353810        1.609159
H         -7.281857       -2.916010        0.664537
H         -6.208971       -3.518849       -0.596268
H         -6.094778       -0.739269        0.681903
H         -6.659979       -1.097558       -0.950947
H         -3.637812       -1.072354        1.294361
H         -4.397349       -2.040276       -1.498589
H         -5.692912        0.195817       -2.741316
H         -4.174628        1.062693       -3.062041
H         -4.239911       -0.700455       -3.254009
H         -5.654539        1.277233       -0.478841
H         -4.117506        2.041516       -0.919655
H         -4.227433        1.043135        0.552132
H          2.069533       -2.561239       -1.553963
H          5.188888       -0.625756        0.678660
H          1.073035        0.053172        1.708018
C         -0.601041        3.180857       -1.048814
O         -1.705408        2.346920       -1.399310
C         -1.546483        2.641436       -0.049596
N         -2.574428        3.633243        0.428701
O         -2.845437        3.606970        1.612754
O         -3.044971        4.395581       -0.391178
C         -1.224959        1.559515        0.927752
H         -0.506738        0.899928        0.439978
H         -2.112788        0.984810        1.201876
H         -0.781433        1.975231        1.834895
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C	0.763409	2.596597	-1.200643
C	3.332648	1.576954	-1.552649
C	1.830722	3.124552	-0.470675
C	0.978933	1.541857	-2.087030
C	2.265755	1.038662	-2.267033
C	3.112360	2.611416	-0.643833
H	1.657130	3.934556	0.233314
H	0.136700	1.133403	-2.638406
H	2.441934	0.225024	-2.964888
H	3.937613	3.012249	-0.063833
H	4.331377	1.175626	-1.693822
H	-0.741638	4.223508	-1.332709

SR epoxide:Catalyst, binary complex 42; Energy = -2449.845345; 6-31G(d) basis set.

N	1.104893	-0.838472	-0.412503
C	-0.001335	-0.073683	-0.298903
S	0.139648	1.579168	-0.002706
C	1.215719	-2.178589	-0.979627
C	2.707055	-2.392084	-1.323306
C	2.865527	-3.710743	-2.090083
C	2.389090	-4.877764	-1.219118
C	0.948287	-4.667076	-0.749673
C	0.775428	-3.317875	-0.044726
N	3.290519	-1.192556	-1.932095
C	2.743880	-0.850816	-3.239014
N	-1.183379	-0.741672	-0.435623
C	-2.488481	-0.223259	-0.291192
C	-2.891817	0.949400	-0.934054
C	-4.204078	1.380258	-0.796594
C	-5.133697	0.659653	-0.051055
C	-4.722128	-0.512326	0.566848
C	-3.406807	-0.954402	0.458412
C	-4.634124	2.670115	-1.438720
F	-4.596892	3.690164	-0.569523
C	-5.712776	-1.347423	1.327920
F	-6.732353	-0.611832	1.787623
C	4.745730	-1.234428	-1.970824
F	-3.849483	2.999988	-2.472721
F	-5.894459	2.591876	-1.892921
F	-6.237978	-2.312321	0.555590
F	-5.142332	-1.957305	2.376633
H	1.952378	-0.290620	-0.543670
H	-1.130447	-1.751747	-0.430226
H	1.380286	-3.265837	0.866971
H	-0.266814	-3.211490	0.279610
H	0.276084	-4.708131	-1.618103
H	0.645618	-5.475523	-0.076988
H	2.473960	-5.820446	-1.769222
H	3.045478	-4.957959	-0.342641
H	2.280335	-3.677961	-3.018971
H	3.914419	-3.853925	-2.372485
H	0.618036	-2.228665	-1.906143
H	3.223514	-2.503102	-0.357958
H	5.139295	-1.941497	-2.718740
H	5.127510	-0.237013	-2.212193
H	5.134144	-1.523071	-0.988814
H	2.974063	-1.600992	-4.012504
H	3.168138	0.105758	-3.559475
H	1.658401	-0.728626	-3.176670
H	-2.186198	1.510287	-1.533011
H	-6.157497	1.005403	0.041102
H	-3.092059	-1.858481	0.971945
C	3.797167	0.620416	1.218829
O	4.244129	0.310131	2.535844
C	2.869833	0.413988	2.358925
N	2.225564	-0.955341	2.353436
O	2.927122	-1.896639	2.030063
O	1.050798	-1.023428	2.646520
C	2.086221	1.447386	3.102652
H	1.072366	1.505190	2.707551
H	2.575732	2.413656	2.972455
H	2.056563	1.195958	4.166193
C	4.124697	1.960367	0.666304
C	4.745442	4.443848	-0.433087
C	4.743383	2.934189	1.450084

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C          3.829626        2.225438       -0.673004
C          4.135305        3.467333       -1.218715
C          5.051710        4.174782        0.898924
H          4.993977        2.706822        2.482171
H          3.356254        1.455322       -1.279534
H          3.897281        3.673874       -2.257418
H          5.535905        4.930465        1.509607
H          4.984927        5.412566       -0.860691
H          3.882711       -0.216473        0.523891

SR epoxide:Catalyst, binary complex 43; Energy = -2449.843222; 6-31G(d) basis set.
N         -3.883483        0.411854       -0.442046
C         -2.924762        1.347540       -0.324964
S         -3.314730        2.985083       -0.451300
C         -3.774654       -1.038136       -0.286033
C         -5.110956       -1.604005        0.216894
C         -5.058250       -3.142067        0.184565
C         -4.665062       -3.721447       -1.171745
C         -3.302950       -3.176673       -1.593088
C         -3.347281       -1.653404       -1.628444
N         -5.474739       -1.201115        1.585574
C         -6.917595       -1.217864        1.761650
N         -1.678995        0.856874       -0.058616
C         -0.477659        1.566146        0.129581
C         -0.117198        2.658673       -0.661104
C          1.104289        3.287636       -0.439338
C          1.990415        2.833968        0.529535
C          1.637343        1.716894        1.280539
C          0.413313        1.085918        1.096294
C          1.448474        4.501347       -1.258498
F          1.044767        4.366329       -2.528999
C          2.634020        1.195856        2.276389
F          3.723483        0.703794        1.651316
C         -4.930243        0.026085        2.149355
F          0.863236        5.604203       -0.773676
F          2.770693        4.727793       -1.274624
F          3.074577        2.174430        3.080822
F          2.137243        0.226639        3.046854
H         -4.801992        0.790076       -0.639992
H         -1.590708       -0.147188        0.067393
H         -4.069186       -1.322653       -2.387340
H         -2.373845       -1.236791       -1.907797
H         -2.536727       -3.503286       -0.876800
H         -3.009879       -3.561059       -2.575588
H         -4.648869       -4.814929       -1.116134
H         -5.416024       -3.450809       -1.926752
H         -4.327622       -3.451150        0.943424
H         -6.025816       -3.539240        0.506593
H         -3.022731       -1.269466        0.483305
H         -5.880195       -1.258106       -0.504771
H         -5.314029        0.951684        1.686496
H         -5.201392        0.047894        3.209759
H         -3.839671        0.040903        2.093030
H         -7.340301       -2.159404        1.402613
H         -7.417390       -0.390894        1.223975
H         -7.158308       -1.125965        2.825013
H         -0.785925        3.010390       -1.436255
H          2.943526        3.328093        0.685455
H          0.152483        0.217971        1.694791
C          2.319877       -2.601781       -0.047277
O          2.039022       -1.461176        0.760520
C          1.868818       -1.301771       -0.604392
N          0.405544       -1.285292       -0.969879
O         -0.382438       -1.780002       -0.175408
O          0.102956       -0.781339       -2.028827
C          2.681594       -0.311330       -1.379009
H          2.243631        0.686592       -1.288640
H          2.715913       -0.587982       -2.433672
H          3.691910       -0.301558       -0.969003
C          3.735181       -3.046403       -0.152699
C          6.371061       -3.914280       -0.381795
C          4.756009       -2.345210        0.490845
C          4.031901       -4.188014       -0.899461
C          5.349514       -4.617582       -1.017647
C          6.072356       -2.782247        0.373474
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H          4.508505       -1.471518        1.086231
H          3.231435       -4.738824       -1.386873
H          5.578983       -5.503472       -1.601085
H          6.866005       -2.240471        0.878075
H          7.398571       -4.252825       -0.470178
H          1.559386       -3.379238        0.023028

SR epoxide:Catalyst, binary complex 44; Energy = -2449.844802; 6-31G(d) basis set.
N         -2.864986       -0.435464       -0.719555
C         -1.976102       -1.107703       -1.459549
S         -2.283905       -2.577077       -2.229927
C         -4.238546       -0.833958       -0.430034
C         -4.516784       -0.637270        1.076124
C         -5.980634       -0.989629        1.374742
C         -6.951473       -0.183460        0.509934
C         -6.665754       -0.400434       -0.976461
C         -5.216841       -0.039941       -1.301569
N         -3.617494       -1.350132        1.983434
C         -3.430455       -2.757270        1.674557
N         -0.725535       -0.543313       -1.572132
C         -0.253272        0.593794       -0.879249
C          0.849735        0.470108       -0.034040
C          1.316215        1.579300        0.661781
C          0.699099        2.819628        0.535511
C         -0.388664        2.934621       -0.322379
C         -0.862159        1.840614       -1.040385
C          2.448758        1.387792        1.634019
F          2.058361        0.662831        2.693825
C         -1.054723        4.267843       -0.531251
F         -2.390632        4.142539       -0.534770
C         -2.343249       -0.712585        2.266261
F          3.475606        0.719755        1.073778
F          2.922485        2.549060        2.090186
F         -0.728847        5.143050        0.425772
F         -0.710801        4.807846       -1.707703
H         -2.554610        0.410412       -0.254061
H         -0.027658       -1.197680       -1.907562
H         -5.056390        1.033792       -1.124513
H         -4.983996       -0.234967       -2.354061
H         -6.842545       -1.453942       -1.231517
H         -7.346073        0.195522       -1.593208
H         -7.983255       -0.462150        0.747725
H         -6.848344        0.884955        0.745733
H         -6.144973       -2.059311        1.188696
H         -6.159760       -0.818233        2.440296
H         -4.318778       -1.896748       -0.679338
H         -4.392925        0.435363        1.297325
H         -1.575580       -0.867096        1.485991
H         -2.485172        0.364528        2.405538
H         -1.940266       -1.118347        3.201745
H         -2.901612       -3.235602        2.506017
H         -2.845900       -2.925567        0.752387
H         -4.394514       -3.260166        1.561547
H          1.322306       -0.499403        0.087937
H          1.056067        3.676992        1.093946
H         -1.692859        1.953618       -1.732000
C          4.504137       -1.848345        0.053433
O          5.165651       -2.134504       -1.176676
C          4.852917       -0.803992       -0.938695
N          6.073351       -0.003740       -0.543596
O          6.024260        1.196180       -0.730855
O          6.999691       -0.606912       -0.044299
C          3.932225       -0.063204       -1.858988
H          4.449194        0.170317       -2.792938
H          3.598536        0.865354       -1.397134
H          3.068238       -0.691502       -2.079139
C          3.110722       -2.333571        0.234315
C          0.453509       -3.109815        0.598366
C          2.389795       -2.884922       -0.828826
C          2.509576       -2.209334        1.489296
C          1.181027       -2.590215        1.667748
C          1.064216       -3.270553       -0.646466
H          2.878519       -3.020998       -1.789279
H          3.071907       -1.787990        2.318212
H          0.713432       -2.472866        2.640735
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H          0.496827       -3.690950       -1.472293
H         -0.585500       -3.398397        0.728357
H          5.158798       -1.905991        0.922302

SR epoxide:Catalyst, binary complex 45; Energy = -2449.843254; 6-31G(d) basis set.
N         -3.891668        0.505055       -0.418249
C         -2.909442        1.414091       -0.289833
S         -3.247904        3.061026       -0.441270
C         -3.820841       -0.950102       -0.289707
C         -5.176815       -1.492304        0.186420
C         -5.163035       -3.030274        0.118801
C         -4.766295       -3.588927       -1.245120
C         -3.384626       -3.071352       -1.636081
C         -3.390212       -1.547133       -1.639081
N         -5.542166       -1.111383        1.560948
C         -6.986385       -1.109064        1.728244
N         -1.684685        0.891871        0.011824
C         -0.462218        1.566344        0.190046
C          0.406308        1.086086        1.175672
C          1.650074        1.681495        1.349471
C          2.045745        2.760321        0.566376
C          1.181233        3.211639       -0.423861
C         -0.060981        2.621831       -0.631216
C          2.618070        1.163825        2.374922
F          2.100126        0.194816        3.131881
C          1.642304        4.285975       -1.368332
F          0.629265        5.041079       -1.804510
C         -4.984212        0.098604        2.148508
F          3.725507        0.672861        1.782188
F          3.033672        2.143694        3.190883
F          2.543611        5.095296       -0.795448
F          2.229674        3.749007       -2.452329
H         -4.794599        0.907200       -0.639451
H         -1.629492       -0.110173        0.166239
H         -4.092955       -1.182376       -2.400303
H         -2.402856       -1.148790       -1.894580
H         -2.636876       -3.432699       -0.916910
H         -3.087822       -3.442083       -2.622679
H         -4.780200       -4.683412       -1.214358
H         -5.499170       -3.281192       -2.003671
H         -4.451233       -3.375959        0.879560
H         -6.144690       -3.410318        0.417762
H         -3.085791       -1.217561        0.484167
H         -5.930059       -1.110242       -0.533994
H         -5.350522        1.036654        1.696782
H         -5.264173        0.107942        3.206783
H         -3.893190        0.098110        2.101199
H         -7.421192       -2.038969        1.354047
H         -7.470355       -0.267254        1.199201
H         -7.231923       -1.028270        2.791345
H          0.113516        0.247339        1.800003
H          3.012275        3.230499        0.716380
H         -0.717370        2.977664       -1.414967
C          2.273629       -2.587219       -0.036738
O          2.003495       -1.447216        0.775674
C          1.828176       -1.282881       -0.588177
N          0.363805       -1.257334       -0.949406
O         -0.424379       -1.754384       -0.157097
O          0.062486       -0.745768       -2.005147
C          2.646680       -0.298907       -1.365573
H          2.209511        0.700731       -1.293254
H          2.691881       -0.587429       -2.416796
H          3.653288       -0.284880       -0.946117
C          3.685808       -3.040134       -0.150494
C          6.315996       -3.921388       -0.394973
C          3.973924       -4.175192       -0.910448
C          4.712375       -2.352520        0.498373
C          6.025821       -2.796118        0.373500
C          5.288681       -4.611363       -1.036232
H          3.169161       -4.715906       -1.402007
H          4.470961       -1.484213        1.103847
H          6.823720       -2.264569        0.882263
H          5.511640       -5.492182       -1.629815
H          7.341187       -4.265247       -0.489513
H          1.508710       -3.360144        0.035107
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SR epoxide:Catalyst, binary complex 46; Energy = -2449.846387; 6-31G(d) basis set.

N	0.372866	1.570758	1.086710
C	0.744037	1.275774	2.349696
S	-0.175529	1.693228	3.692288
C	1.237280	1.923606	-0.042254
C	0.350900	2.521781	-1.147021
C	1.227774	2.873607	-2.360836
C	2.344501	3.849748	-1.984593
C	3.198608	3.283857	-0.849938
C	2.324874	2.931013	0.353068
N	-0.806225	1.660440	-1.428121
C	-0.449319	0.418855	-2.109359
N	1.942261	0.627254	2.495753
C	2.500984	-0.260270	1.538459
C	3.850173	-0.146495	1.216511
C	4.404391	-0.994010	0.261039
C	3.632969	-1.960065	-0.369934
C	2.287340	-2.073100	-0.026827
C	1.710527	-1.235011	0.920848
C	5.838984	-0.785710	-0.133159
F	6.331066	-1.828037	-0.812233
C	1.437119	-3.114279	-0.706471
F	0.752378	-2.599041	-1.739062
C	-1.841351	2.364722	-2.175324
F	5.969730	0.299026	-0.915188
F	6.620553	-0.587045	0.937317
F	2.189644	-4.111555	-1.197805
F	0.549481	-3.653348	0.133603
H	-0.585737	1.885608	1.002001
H	2.243102	0.524758	3.457687
H	1.833324	3.832785	0.742758
H	2.933752	2.525575	1.166215
H	3.722615	2.379735	-1.192555
H	3.969181	4.002303	-0.552096
H	2.962297	4.068282	-2.861728
H	1.902957	4.801862	-1.660022
H	1.679022	1.956200	-2.759601
H	0.603147	3.295550	-3.155956
H	1.723746	1.025221	-0.444212
H	-0.063257	3.459846	-0.744495
H	-1.543189	2.609205	-3.208580
H	-2.735395	1.735762	-2.223191
H	-2.098505	3.296934	-1.661364
H	-0.042070	0.588838	-3.119166
H	-1.339906	-0.206171	-2.200064
H	0.283943	-0.141258	-1.522330
H	4.458556	0.612503	1.700311
H	4.072251	-2.622354	-1.107000
H	0.656983	-1.327217	1.177423
C	-4.321747	-1.095010	-0.318035
O	-3.537000	-0.303516	-1.209339
C	-3.271340	-0.151601	0.142390
N	-1.997729	-0.855644	0.548206
O	-1.542411	-0.567711	1.638294
O	-1.546919	-1.695861	-0.202810
C	-3.471082	1.171939	0.811936
H	-4.475533	1.534580	0.588524
H	-2.736865	1.880512	0.417849
H	-3.344740	1.080300	1.890787
C	-5.771765	-0.785395	-0.205596
C	-8.494295	-0.242257	0.050658
C	-6.331695	0.306140	-0.870949
C	-6.580208	-1.611981	0.577150
C	-7.937438	-1.337461	0.708250
C	-7.691098	0.575534	-0.741102
H	-5.700576	0.929275	-1.497850
H	-6.144769	-2.470023	1.082789
H	-8.561122	-1.980543	1.320889
H	-8.124906	1.422909	-1.262669
H	-9.554201	-0.030559	0.150613
H	-4.043621	-2.148611	-0.319914

SR epoxide:Catalyst, binary complex 47; Energy = -2449.841008; 6-31G(d) basis set.

N	-1.671459	-2.455719	0.911421

```
C         -0.354546       -2.462485        0.644440
S          0.425327       -3.898605        0.236884
C         -2.537132       -1.336946        1.287003
C         -3.924141       -1.466557        0.617150
C         -4.932416       -0.510213        1.285302
C         -4.929987       -0.525699        2.811785
C         -3.538013       -0.219901        3.348237
C         -2.580262       -1.279088        2.822715
N         -3.864788       -1.155005       -0.825953
C         -5.187048       -1.274837       -1.445204
N          0.252405       -1.233542        0.709312
C          1.615735       -0.922786        0.531814
C          2.164462        0.042187        1.376600
C          3.477757        0.454279        1.200862
C          4.271703       -0.089856        0.199380
C          3.709696       -1.045145       -0.639538
C          2.391185       -1.460965       -0.496440
C          4.057855        1.505873        2.102607
F          4.794096        2.390185        1.408964
C          4.504244       -1.549808       -1.810395
F          4.144059       -2.786706       -2.168416
C         -2.933551       -1.978511       -1.597922
F          3.105051        2.196782        2.745770
F          4.863217        0.978069        3.034838
F          4.325054       -0.762615       -2.889304
F          5.819110       -1.560038       -1.554382
H         -2.094651       -3.376614        0.891545
H         -0.262262       -0.500346        1.182403
H         -2.891736       -2.266086        3.190948
H         -1.557199       -1.122542        3.186459
H         -3.221518        0.775363        3.007445
H         -3.524728       -0.211344        4.442801
H         -5.660403        0.204383        3.174962
H         -5.252285       -1.508857        3.181805
H         -4.700813        0.500597        0.927600
H         -5.938533       -0.753865        0.936827
H         -2.117752       -0.403531        0.896071
H         -4.269442       -2.512857        0.771146
H         -3.100291       -3.062451       -1.466923
H         -3.067756       -1.736496       -2.655624
H         -1.893844       -1.765623       -1.343723
H         -5.630146       -2.274278       -1.286055
H         -5.085272       -1.106528       -2.519149
H         -5.869874       -0.515566       -1.067243
H          1.559854        0.486116        2.161909
H          5.297308        0.236917        0.062618
H          1.967321       -2.188026       -1.176790
C         -1.683193        1.380678       -0.913458
O         -2.562953        1.836184        0.140217
C         -2.799530        2.301232       -1.146026
N         -4.030093        1.686729       -1.761940
O         -3.908726        1.194243       -2.865060
O         -5.063314        1.805332       -1.136623
C         -2.742248        3.769249       -1.444837
H         -2.807560        3.928958       -2.523840
H         -1.799359        4.178449       -1.079440
H         -3.576581        4.273960       -0.951422
C         -0.263901        1.821534       -0.856287
C          2.398549        2.652228       -0.842289
C          0.645891        1.275910       -1.764791
C          0.170690        2.761289        0.081804
C          1.500252        3.177247        0.084759
C          1.973160        1.692560       -1.759314
H          0.312317        0.519208       -2.471389
H         -0.535753        3.156856        0.806250
H          1.839398        3.900780        0.819632
H          2.680148        1.251113       -2.455086
H          3.437015        2.968407       -0.829982
H         -1.869897        0.348361       -1.207010

SR epoxide:Catalyst, binary complex 48; Energy = -2449.849450; 6-31G(d) basis set.
N         -1.559331       -0.554756        1.122424
C         -1.107377       -1.287652        2.148889
S         -2.013051       -2.294118        3.147703
C         -2.848917       -0.652103        0.436144
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C	-3.102121	-2.055630	-0.150443
C	-4.415980	-2.045405	-0.948846
C	-5.593650	-1.587980	-0.085808
C	-5.326331	-0.194673	0.486041
C	-4.030991	-0.188595	1.298987
N	-1.928981	-2.539001	-0.884936
C	-1.828684	-3.990751	-0.885800
N	0.239947	-1.128336	2.404977
C	1.266263	-1.004422	1.440455
C	1.149261	-1.568809	0.164226
C	2.235952	-1.503786	-0.703245
C	3.425701	-0.878881	-0.342174
C	3.512209	-0.303947	0.919892
C	2.447737	-0.362606	1.811002
C	2.117283	-2.117610	-2.069841
F	1.542561	-1.277225	-2.952032
C	4.784448	0.379592	1.338165
F	4.544973	1.399762	2.171755
C	-1.808521	-2.012791	-2.236250
F	3.308977	-2.452712	-2.573966
F	1.356765	-3.225266	-2.050462
F	5.603815	-0.468114	1.983952
F	5.460239	0.853708	0.286438
H	-0.888070	0.094001	0.720876
H	0.520325	-1.525999	3.293695
H	-4.126622	-0.860448	2.156949
H	-3.818987	0.810145	1.698350
H	-5.248861	0.527571	-0.340052
H	-6.160888	0.129890	1.116396
H	-6.515799	-1.590681	-0.676446
H	-5.738561	-2.295913	0.740835
H	-4.322190	-1.362154	-1.804237
H	-4.600409	-3.045794	-1.358515
H	-2.759090	0.056001	-0.401289
H	-3.229194	-2.730956	0.702725
H	-1.942925	-0.926361	-2.234797
H	-0.807190	-2.229042	-2.619626
H	-2.541474	-2.443823	-2.939141
H	-0.881737	-4.281337	-1.350911
H	-2.645609	-4.483758	-1.441475
H	-1.833437	-4.356008	0.145287
H	0.220804	-2.062836	-0.131636
H	4.257245	-0.822952	-1.035153
H	2.520812	0.108469	2.786148
C	0.206122	3.112767	0.058462
O	0.348919	1.778038	0.553175
C	0.703893	1.998885	-0.777986
N	2.201139	1.957972	-0.950826
O	2.881697	2.369509	-0.033758
O	2.617881	1.506276	-1.998909
C	-0.059590	1.328888	-1.875423
H	0.199782	0.270166	-1.931888
H	0.168478	1.791835	-2.837013
H	-1.126251	1.443816	-1.668675
C	-1.179661	3.629042	-0.122242
C	-3.764605	4.590149	-0.519570
C	-1.384892	4.789840	-0.869237
C	-2.266922	2.956639	0.435369
C	-3.558496	3.437998	0.235452
C	-2.676533	5.266689	-1.068572
H	-0.535288	5.315152	-1.297934
H	-2.093305	2.070062	1.039943
H	-4.403625	2.918243	0.677896
H	-2.834587	6.167660	-1.652835
H	-4.771014	4.965604	-0.674859
H	0.959533	3.793126	0.451537

SR epoxide:Catalyst, binary complex 49; Energy = -2449.843421; 6-31G(d) basis set.

N	1.245153	-2.961827	-0.284771
C	-0.076039	-2.711236	-0.185371
S	-1.172700	-3.993123	-0.088158
C	2.398654	-2.067455	-0.279772
C	3.395188	-2.499965	0.822570
C	4.635871	-1.597799	0.779488
C	5.299758	-1.589756	-0.597822

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C          4.309114       -1.157492       -1.678624
C          3.063517       -2.043587       -1.662246
N          2.851602       -2.560497        2.176518
C          2.181546       -3.799381        2.542669
N         -0.434058       -1.400881       -0.141022
C         -1.731127       -0.864421        0.013611
C         -2.795606       -1.233613       -0.806323
C         -4.003201       -0.553853       -0.694666
C         -4.165013        0.501176        0.196962
C         -3.096942        0.850578        1.013970
C         -1.891704        0.163227        0.942296
C         -5.166924       -0.975307       -1.548167
F         -5.925792       -1.890543       -0.927141
C         -3.269172        1.961647        2.009056
F         -3.961835        2.983646        1.495719
C          2.067177       -1.408264        2.577741
F         -5.966013        0.062490       -1.837815
F         -4.766461       -1.516262       -2.706104
F         -3.927485        1.552149        3.103333
F         -2.082750        2.442106        2.427300
H          1.454080       -3.952917       -0.322952
H          0.289530       -0.689639       -0.124724
H          3.339124       -3.074093       -1.927798
H          2.327707       -1.711364       -2.403509
H          4.020139       -0.113309       -1.500457
H          4.776097       -1.193095       -2.668505
H          6.167031       -0.920710       -0.590353
H          5.674173       -2.597110       -0.827361
H          4.350043       -0.569611        1.040330
H          5.329084       -1.942739        1.552555
H          2.070180       -1.050159       -0.033617
H          3.725204       -3.520222        0.572493
H          1.060308       -1.380465        2.121142
H          1.933091       -1.427020        3.664057
H          2.586453       -0.479485        2.321199
H          1.164476       -3.903311        2.130294
H          2.103821       -3.848414        3.634529
H          2.781310       -4.653124        2.212846
H         -2.668874       -2.022839       -1.536844
H         -5.100389        1.048752        0.243247
H         -1.061003        0.438717        1.585679
C          1.558081        1.918368       -1.014839
O          0.944058        1.217555        0.075337
C          0.482300        2.511141       -0.188024
N         -0.888537        2.460027       -0.833568
O         -1.690566        3.300738       -0.484047
O         -1.090008        1.574047       -1.638349
C          0.623624        3.585642        0.841042
H          0.438869        4.560723        0.387763
H          1.638085        3.561564        1.239945
H         -0.097197        3.430526        1.644760
C          2.995076        2.268362       -0.865249
C          5.726556        2.794934       -0.681180
C          3.666849        2.062133        0.340839
C          3.693344        2.738266       -1.979023
C          5.055216        3.005637       -1.884349
C          5.031507        2.323114        0.430193
H          3.123201        1.671772        1.197201
H          3.173670        2.879770       -2.923108
H          5.594871        3.367433       -2.753634
H          5.551903        2.149012        1.366839
H          6.791298        2.993347       -0.611847
H          1.247051        1.546665       -1.989574

SR epoxide:Catalyst, binary complex 50; Energy = -2449.841241; 6-31G(d) basis set.
N          0.942914       -2.722518       -1.743949
C         -0.258547       -2.132196       -1.990067
S         -1.455810       -2.905227       -2.874398
C          1.695079       -2.580038       -0.495444
C          0.996708       -3.341668        0.653267
C          1.872095       -3.323450        1.917029
C          3.269505       -3.881404        1.647633
C          3.956638       -3.071578        0.547755
C          3.121369       -3.083592       -0.732087
N         -0.372401       -2.853547        0.838545
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C	-1.287058	-3.885006	1.301329
N	-0.329436	-0.837323	-1.567430
C	-1.466768	-0.108985	-1.192947
C	-2.611573	-0.716274	-0.676312
C	-3.624376	0.077755	-0.153491
C	-3.528506	1.466125	-0.121900
C	-2.388939	2.052592	-0.655761
C	-1.374896	1.281093	-1.206565
C	-4.807374	-0.623062	0.450218
F	-5.542089	-1.256265	-0.474007
C	-2.177844	3.536262	-0.605880
F	-0.977038	3.833475	-0.058528
C	-0.477765	-1.656886	1.659372
F	-4.410793	-1.560228	1.332752
F	-5.619054	0.220208	1.100046
F	-2.174074	4.085286	-1.829757
F	-3.110002	4.162828	0.115830
H	0.989210	-3.653371	-2.145914
H	0.538913	-0.405681	-1.270517
H	3.067619	-4.114286	-1.112360
H	3.586879	-2.479761	-1.519543
H	4.089165	-2.034816	0.891846
H	4.956870	-3.465693	0.340723
H	3.866547	-3.865469	2.565214
H	3.195746	-4.931235	1.332722
H	1.975399	-2.288044	2.270218
H	1.370594	-3.882247	2.716059
H	1.745144	-1.518701	-0.220263
H	0.911545	-4.385791	0.316267
H	0.151824	-0.858527	1.252985
H	-1.509235	-1.294830	1.634962
H	-0.204555	-1.822041	2.716265
H	-1.287950	-4.721157	0.596266
H	-2.299783	-3.470656	1.338380
H	-1.042159	-4.269000	2.307817
H	-2.676116	-1.798764	-0.640992
H	-4.308458	2.068378	0.327861
H	-0.485586	1.754389	-1.612392
C	2.049441	2.153668	0.068616
O	1.316448	0.913614	0.160402
C	1.573784	1.592741	1.344005
N	0.339504	2.242582	1.911322
O	0.515336	3.305215	2.472362
O	-0.709317	1.646061	1.802089
C	2.394704	0.955365	2.423889
H	1.810300	0.172480	2.917144
H	2.680246	1.709415	3.160409
H	3.293898	0.518571	1.985786
C	3.470385	2.058502	-0.364159
C	6.138659	1.907616	-1.160037
C	4.212633	3.226721	-0.543432
C	4.063270	0.816462	-0.596799
C	5.394923	0.741842	-0.993481
C	5.545232	3.148686	-0.935637
H	3.748031	4.194823	-0.376178
H	3.474430	-0.089589	-0.481440
H	5.847664	-0.228165	-1.176063
H	6.119335	4.059613	-1.071632
H	7.177028	1.851089	-1.470643
H	1.459386	2.973720	-0.342564

SR epoxide:Catalyst, binary complex 51; Energy = -2449.845124; 6-31G(d) basis set.

N	3.043632	0.654191	-1.176942
C	2.314073	-0.268345	-1.817956
S	2.895320	-1.676042	-2.538308
C	4.408629	0.534797	-0.661132
C	4.608954	-0.683044	0.262343
C	6.010010	-0.581340	0.890854
C	7.095497	-0.547447	-0.188542
C	6.874964	0.624898	-1.145361
C	5.475945	0.571471	-1.762168
N	3.498125	-0.849385	1.206932
C	3.486774	-2.182078	1.793931
N	0.972778	0.021141	-1.926174
C	0.188550	0.834312	-1.087778

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C          0.481573        0.999661        0.268715
C         -0.346937        1.793346        1.056864
C         -1.476244        2.408347        0.534802
C         -1.772258        2.210333       -0.811632
C         -0.952198        1.440369       -1.624161
C          0.000748        1.943040        2.511353
F          0.022583        0.750600        3.134286
C         -2.974915        2.890009       -1.405319
F         -3.464596        2.203397       -2.447938
C          3.441657        0.161057        2.253994
F          1.221865        2.478507        2.668346
F         -0.868579        2.719328        3.163985
F         -3.959480        3.014442       -0.502563
F         -2.683862        4.121996       -1.842955
H          2.556927        1.502065       -0.913534
H          0.475591       -0.602527       -2.550664
H          5.371422       -0.321660       -2.386511
H          5.296384        1.442590       -2.401370
H          6.996455        1.568249       -0.594416
H          7.629949        0.621383       -1.938303
H          8.085209       -0.480628        0.275354
H          7.070155       -1.487239       -0.755999
H          6.078688        0.332509        1.497721
H          6.173053       -1.427684        1.567801
H          4.540376        1.440977       -0.055155
H          4.589202       -1.573192       -0.376138
H          4.280069        0.100168        2.967922
H          3.430608        1.167142        1.822117
H          2.512302        0.037091        2.820453
H          2.556981       -2.325290        2.354559
H          4.326079       -2.361214        2.487120
H          3.525773       -2.933763        0.999549
H          1.329103        0.472552        0.704952
H         -2.120544        3.014398        1.161264
H         -1.190406        1.304640       -2.674713
C         -3.856897       -2.592927        0.368332
O         -4.501987       -2.068212        1.525244
C         -4.719865       -1.389270        0.335013
N         -6.102483       -1.654544       -0.210028
O         -6.647983       -2.685869        0.122094
O         -6.558199       -0.822028       -0.970051
C         -4.265961        0.026838        0.172917
H         -4.248849        0.303627       -0.882264
H         -3.260749        0.114517        0.589620
H         -4.937662        0.707630        0.701159
C         -2.373078       -2.498725        0.295792
C          0.406228       -2.363485        0.116549
C         -1.720359       -2.971139       -0.846433
C         -1.632932       -1.965004        1.350547
C         -0.244027       -1.906762        1.259436
C         -0.334407       -2.896859       -0.937913
H         -2.301049       -3.399094       -1.660216
H         -2.147819       -1.609985        2.238733
H          0.330805       -1.487501        2.080342
H          0.180439       -3.248097       -1.828113
H          1.486378       -2.280731        0.030563
H         -4.311537       -3.511959       -0.000436

SR epoxide:Catalyst, binary complex 52; Energy = -2449.844994; 6-31G(d) basis set.
N          3.399774       -0.134983        0.781146
C          2.307861       -0.905906        0.987985
S          2.256242       -2.546034        0.649484
C          4.671198       -0.620924        0.264507
C          5.462101        0.594074       -0.250269
C          6.775218        0.111124       -0.881773
C          7.613773       -0.660227        0.142822
C          6.823164       -1.830344        0.732947
C          5.493791       -1.358193        1.325836
N          4.615349        1.457602       -1.082677
C          5.168380        2.793607       -1.253563
N          1.280006       -0.175968        1.538155
C         -0.103600       -0.375489        1.564105
C         -0.852956        0.628118        2.196937
C         -2.235542        0.570467        2.211265
C         -2.922777       -0.475437        1.599018
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C	-2.172077	-1.451791	0.963458
C	-0.778946	-1.432571	0.950336
C	-3.022016	1.714325	2.782748
F	-4.126878	1.296269	3.408951
C	-2.855066	-2.510048	0.144876
F	-2.398659	-3.736550	0.411199
C	4.271667	0.879694	-2.376579
F	-2.305843	2.440725	3.650226
F	-3.420318	2.551108	1.804017
F	-4.180051	-2.509929	0.313407
F	-2.628360	-2.290803	-1.171985
H	3.241184	0.849376	0.568084
H	1.552963	0.748144	1.853563
H	5.675321	-0.672161	2.164029
H	4.915519	-2.203467	1.708118
H	6.621913	-2.567776	-0.055656
H	7.413108	-2.341502	1.500232
H	8.538121	-1.017689	-0.322303
H	7.907884	0.022000	0.952044
H	6.551280	-0.543500	-1.734510
H	7.339386	0.966426	-1.270419
H	4.472719	-1.318551	-0.561333
H	5.716867	1.200705	0.632845
H	3.878794	-0.133081	-2.248921
H	3.491137	1.489106	-2.843988
H	5.129066	0.835263	-3.067102
H	4.423901	3.429523	-1.743532
H	6.081835	2.810490	-1.870226
H	5.401312	3.225662	-0.276109
H	-0.348699	1.468396	2.665591
H	-4.007534	-0.505467	1.589368
H	-0.229990	-2.212513	0.440353
C	-3.003025	1.077186	-1.275774
O	-3.850366	1.661703	-2.277697
C	-3.644269	0.288933	-2.340998
N	-4.855966	-0.489223	-1.860062
O	-5.099350	-1.534266	-2.426170
O	-5.489686	-0.022014	-0.934620
C	-3.027928	-0.284150	-3.581125
H	-2.185548	0.346579	-3.867333
H	-3.766841	-0.282600	-4.385788
H	-2.690845	-1.307750	-3.418534
C	-1.549519	1.413899	-1.252700
C	1.159256	2.058699	-1.025142
C	-1.163784	2.670345	-0.778302
C	-0.573310	0.475782	-1.593878
C	0.777397	0.799209	-1.484211
C	0.185879	2.992555	-0.667735
H	-1.925688	3.388803	-0.488519
H	-0.870205	-0.518641	-1.914891
H	1.530499	0.058319	-1.740296
H	0.478054	3.973116	-0.304634
H	2.217139	2.301760	-0.940914
H	-3.499672	1.067203	-0.310092

SR epoxide:Catalyst, binary complex 53; Energy = -2449.843981; 6-31G(d) basis set.

N	-3.746850	-0.359260	0.625075
C	-4.021525	-1.106820	-0.457719
S	-5.592783	-1.602459	-0.811903
C	-2.604827	0.506404	0.939067
C	-2.970726	2.013506	0.849325
C	-1.731754	2.846402	1.219951
C	-1.152098	2.487048	2.588224
C	-0.846315	0.993507	2.676759
C	-2.089560	0.175250	2.346045
N	-3.521693	2.480435	-0.414853
C	-4.947666	2.275098	-0.607633
N	-3.002419	-1.439300	-1.319642
C	-1.649202	-1.697750	-1.022507
C	-1.259005	-2.221398	0.210952
C	0.089387	-2.426331	0.476176
C	1.063330	-2.191419	-0.491088
C	0.651330	-1.731113	-1.737376
C	-0.687793	-1.463222	-2.004451
C	0.490095	-2.883885	1.851549

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F          -0.445982       -3.668023        2.402330
C           1.654882       -1.462068       -2.823692
F           2.797528       -2.129077       -2.635236
C          -2.762226        2.129096       -1.600771
F           1.642755       -3.562434        1.839874
F           0.653737       -1.838862        2.685979
F           1.175127       -1.800150       -4.026967
F           1.966535       -0.150422       -2.893910
H          -4.567225       -0.211262        1.204279
H          -3.347346       -1.826494       -2.190180
H          -2.888483        0.399627        3.068297
H          -1.880502       -0.894901        2.432749
H          -0.056566        0.735729        1.958562
H          -0.474474        0.725198        3.671760
H          -0.243893        3.071592        2.768315
H          -1.870523        2.753069        3.376507
H          -0.948913        2.702262        0.465480
H          -2.021202        3.900989        1.179855
H          -1.815880        0.316790        0.207209
H          -3.742274        2.201398        1.611865
H          -2.851007        1.063821       -1.882522
H          -3.127791        2.724379       -2.443936
H          -1.702868        2.366056       -1.465650
H          -5.231407        1.245581       -0.879189
H          -5.293221        2.936537       -1.410333
H          -5.484021        2.551671        0.305607
H          -2.011447       -2.466351        0.953260
H           2.112323       -2.380488       -0.282364
H          -0.989599       -1.074962       -2.972942
C           2.215883        1.511015       -0.160519
O           1.488302        2.218806        0.841960
C           2.509481        2.913396        0.208701
N           1.962394        3.920715       -0.773339
O           0.860291        3.711900       -1.238625
O           2.683276        4.858377       -1.050320
C           3.687591        3.398328        0.993116
H           3.417398        4.284233        1.572409
H           4.513435        3.650098        0.327276
H           3.996390        2.601621        1.671705
C           3.074179        0.381031        0.291118
C           4.577899       -1.835151        1.064759
C           3.981471       -0.192985       -0.601632
C           2.931945       -0.144186        1.575947
C           3.678970       -1.255577        1.958261
C           4.733033       -1.298089       -0.212923
H           4.085233        0.210606       -1.604453
H           2.220804        0.306567        2.261319
H           3.543697       -1.678920        2.948366
H           5.431753       -1.745588       -0.912713
H           5.154915       -2.705288        1.361575
H           1.654261        1.365153       -1.082962

SR epoxide:Catalyst, binary complex 54; Energy = -2449.844056; 6-31G(d) basis set.
N          -0.930475        2.549637        0.116701
C          -2.064882        3.051164        0.626427
S          -2.287787        4.666532        1.059425
C           0.273726        3.332784       -0.182171
C           1.482500        2.356558       -0.236357
C           2.517978        2.848476       -1.248923
C           1.941844        2.813903       -2.675342
C           0.441217        3.167900       -2.685957
C           0.102004        4.088614       -1.514210
N           2.100705        2.027307        1.050259
C           2.851273        3.112028        1.662508
N          -3.095282        2.159709        0.787594
C          -2.971638        0.749311        0.754168
C          -2.051664        0.117773        1.591722
C          -1.877148       -1.257199        1.508180
C          -2.654395       -2.026884        0.649320
C          -3.593906       -1.391053       -0.151521
C          -3.744978       -0.008150       -0.123137
C          -0.752866       -1.909669        2.256166
F          -0.368752       -1.199532        3.322612
C          -4.457929       -2.207590       -1.071926
F          -5.631292       -2.516227       -0.497908
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C	1.169785	1.450474	2.002389
F	-1.059286	-3.143888	2.663923
F	0.337579	-2.026004	1.457666
F	-4.738157	-1.541829	-2.200656
F	-3.868721	-3.360228	-1.410819
H	-0.937522	1.588722	-0.216942
H	-3.972875	2.573602	1.074513
H	-0.921653	4.469386	-1.570663
H	0.764494	4.962678	-1.522322
H	0.160940	3.628692	-3.637886
H	-0.157642	2.250523	-2.598495
H	2.497242	3.520216	-3.301770
H	2.089326	1.818157	-3.104321
H	2.828829	3.869880	-0.998235
H	3.407157	2.212648	-1.172538
H	0.394179	4.050953	0.635817
H	1.100864	1.407663	-0.635634
H	0.605029	0.647615	1.514580
H	1.726133	1.017868	2.841276
H	0.441960	2.176550	2.410163
H	3.306072	2.742236	2.586413
H	2.228927	3.986492	1.922678
H	3.656844	3.441356	1.002943
H	-1.471300	0.713676	2.288090
H	-2.511520	-3.099777	0.584649
H	-4.444150	0.486007	-0.790446
C	2.345795	-0.939849	-0.524734
O	2.134478	-0.467642	-1.854741
C	1.525327	-1.670656	-1.518259
N	0.037578	-1.506621	-1.316813
O	-0.646501	-2.498969	-1.448756
O	-0.380007	-0.403500	-1.009927
C	1.894983	-2.935025	-2.228482
H	2.980783	-2.968318	-2.325507
H	1.440661	-2.961366	-3.221713
H	1.556946	-3.802465	-1.660864
C	3.708603	-1.387552	-0.139311
C	6.234295	-2.243671	0.658492
C	4.767352	-1.366695	-1.046202
C	3.914803	-1.825622	1.170110
C	5.175789	-2.258131	1.565646
C	6.030001	-1.794660	-0.644170
H	4.597730	-1.001583	-2.055111
H	3.083392	-1.827949	1.870966
H	5.334297	-2.602235	2.582778
H	6.856057	-1.772906	-1.348050
H	7.219281	-2.576982	0.969806
H	1.803122	-0.375292	0.228322

SR epoxide:Catalyst, binary complex 55; Energy = -2449.839662; 6-31G(d) basis set.

N	-1.009291	-2.826546	-0.086535
C	0.301582	-2.558689	-0.237212
S	1.331957	-3.734556	-0.878070
C	-2.107035	-1.997487	0.412088
C	-3.365081	-2.252334	-0.439792
C	-4.611203	-1.655989	0.240817
C	-4.783456	-2.064733	1.700243
C	-3.551840	-1.647721	2.498083
C	-2.312009	-2.307976	1.903978
N	-3.283053	-1.684646	-1.796585
C	-4.167617	-2.394745	-2.707454
N	0.699679	-1.306123	0.117634
C	1.981450	-0.740811	-0.060931
C	2.051948	0.524277	-0.636871
C	3.271248	1.186222	-0.721675
C	4.441312	0.585246	-0.280876
C	4.361678	-0.694443	0.263284
C	3.146864	-1.356660	0.396752
C	3.263912	2.594047	-1.238196
F	4.489997	3.051055	-1.504877
C	5.620821	-1.391147	0.698679
F	6.119465	-2.162502	-0.278473
C	-1.975794	-1.534309	-2.422780
F	2.528216	2.709654	-2.356441
F	2.707186	3.429761	-0.338339

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F          6.579935       -0.515925        1.035140
F          5.407777       -2.185965        1.756020
H         -1.252577       -3.775433       -0.346317
H         -0.002126       -0.618598        0.376593
H         -2.403039       -3.397432        2.009316
H         -1.400668       -2.016669        2.439564
H         -3.456967       -0.552978        2.456790
H         -3.646873       -1.920887        3.553951
H         -5.686436       -1.597641        2.107510
H         -4.920154       -3.152002        1.780845
H         -4.525369       -0.564941        0.177215
H         -5.499484       -1.930860       -0.335901
H         -1.854358       -0.938183        0.288483
H         -3.484185       -3.355868       -0.486180
H         -1.465455       -2.486665       -2.644412
H         -2.126521       -1.006357       -3.370286
H         -1.310523       -0.916265       -1.813727
H         -5.175188       -2.469238       -2.292899
H         -3.809925       -3.417445       -2.927505
H         -4.234157       -1.847763       -3.652766
H          1.148414        0.985003       -1.025156
H          5.392307        1.100665       -0.350221
H          3.096609       -2.335801        0.856593
C         -1.921218        1.610902        0.922902
O         -0.951638        1.192939       -0.043714
C         -0.751021        2.439773        0.544125
N          0.360022        2.375590        1.567585
O          0.645691        1.277568        2.006515
O          0.855150        3.429242        1.901652
C         -0.742759        3.677166       -0.295022
H          0.198695        3.750530       -0.845275
H         -0.849868        4.559597        0.336246
H         -1.576581        3.627372       -0.996747
C         -3.303751        1.833250        0.429309
C         -5.937460        2.104413       -0.429152
C         -4.319572        2.072403        1.358261
C         -3.606919        1.720101       -0.928180
C         -4.925270        1.858581       -1.353481
C         -5.634312        2.211399        0.928068
H         -4.080363        2.137974        2.416995
H         -2.818818        1.485867       -1.637431
H         -5.162331        1.755379       -2.407493
H         -6.422458        2.394157        1.651271
H         -6.965171        2.203092       -0.764059
H         -1.823035        1.089242        1.876738

SR epoxide:Catalyst, binary complex 56; Energy = -2449.841485; 6-31G(d) basis set.
N          0.930289        3.550939        1.510578
C          1.775196        2.498387        1.793594
S          2.318163        2.192683        3.346735
C         -0.355290        3.401495        0.787395
C         -0.290047        2.682890       -0.571412
C         -1.673450        2.757432       -1.238053
C         -2.735920        2.098512       -0.353329
C         -2.782563        2.749093        1.027599
C         -1.400302        2.715316        1.678164
N          0.842841        3.141951       -1.393020
C          0.890125        4.581017       -1.629660
N          2.162600        1.844759        0.669678
C          2.673857        0.560446        0.496184
C          2.489456       -0.484234        1.408303
C          2.905798       -1.766420        1.068720
C          3.508742       -2.048055       -0.153066
C          3.698176       -0.998011       -1.044371
C          3.293908        0.292585       -0.729782
C          2.705271       -2.868410        2.072649
F          2.693015       -4.074673        1.492131
C          4.379954       -1.233547       -2.362954
F          5.679624       -0.910510       -2.308890
C          0.971820        2.391056       -2.637502
F          3.674389       -2.879637        2.996041
F          1.541319       -2.723341        2.730650
F          4.302054       -2.514210       -2.743343
F          3.833131       -0.485259       -3.335463
H          0.795678        4.109055        2.348225
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H          1.953380        2.375430       -0.203090
H         -1.086567        1.674929        1.850034
H         -1.419324        3.209072        2.656415
H         -3.111371        3.792934        0.931024
H         -3.511784        2.247947        1.672958
H         -3.714231        2.152541       -0.844375
H         -2.489465        1.032547       -0.243941
H         -1.943798        3.804386       -1.432100
H         -1.638240        2.244509       -2.205280
H         -0.690614        4.431021        0.603595
H         -0.099107        1.616987       -0.376739
H          0.195417        2.636254       -3.377854
H          1.946669        2.605059       -3.086563
H          0.920023        1.317925       -2.420618
H          0.011802        4.952235       -2.180179
H          1.781120        4.806625       -2.221430
H          0.975836        5.112028       -0.679284
H          2.004074       -0.298992        2.358670
H          3.808735       -3.057736       -0.407550
H          3.439699        1.098847       -1.443705
C         -4.445512       -1.988243       -0.745432
O         -4.956262       -2.585599        0.442856
C         -5.389993       -1.298153        0.165303
N         -6.814229       -1.290570       -0.342496
O         -7.440612       -0.258645       -0.197100
O         -7.220746       -2.298650       -0.880079
C         -5.081960       -0.174399        1.104430
H         -5.272057        0.785903        0.623624
H         -4.030447       -0.235066        1.390992
H         -5.704673       -0.250078        1.999257
C         -2.995492       -1.657699       -0.789420
C         -0.273492       -1.064332       -0.936008
C         -2.177661       -1.846303        0.325875
C         -2.447777       -1.173264       -1.979338
C         -1.090880       -0.873409       -2.050462
C         -0.819171       -1.547751        0.252607
H         -2.606627       -2.252389        1.237188
H         -3.082868       -1.041661       -2.851967
H         -0.669247       -0.510055       -2.983236
H         -0.181452       -1.722910        1.114052
H          0.792497       -0.857656       -0.998232
H         -4.881740       -2.396347       -1.656576

SR epoxide:Catalyst, binary complex 57; Energy = -2449.841629; 6-31G(d) basis set.
N         -1.029567        3.620151       -1.374616
C         -1.886679        2.586182       -1.685542
S         -2.476124        2.359008       -3.234234
C          0.272502        3.429763       -0.691079
C          0.236645        2.657346        0.639594
C          1.636949        2.697506        1.272735
C          2.670379        2.066329        0.335394
C          2.687691        2.771057       -1.019389
C          1.289332        2.774096       -1.635846
N         -0.871257        3.091869        1.507571
C         -0.910018        4.524101        1.786002
N         -2.243870        1.878619       -0.583130
C         -2.716062        0.575193       -0.452136
C         -3.246921        0.227257        0.796503
C         -3.602964       -1.086322        1.065712
C         -3.467004       -2.081970        0.103850
C         -2.960629       -1.719885       -1.138875
C         -2.581102       -0.413910       -1.431635
C         -4.030106       -1.434999        2.462188
F         -4.693807       -2.594581        2.512746
C         -2.792629       -2.751554       -2.220096
F         -1.545378       -2.722485       -2.725477
C         -0.958475        2.310247        2.736757
F         -2.960800       -1.550139        3.270835
F         -4.814343       -0.487247        2.994566
F         -3.015584       -3.992360       -1.772617
F         -3.626292       -2.535146       -3.244808
H         -0.913513        4.219292       -2.186325
H         -2.011631        2.368044        0.307041
H          0.962914        1.744272       -1.843171
H          1.288059        3.308332       -2.592680
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H	3.027577	3.807697	-0.889339
H	3.396044	2.291187	-1.703065
H	3.661375	2.091965	0.802930
H	2.410989	1.007527	0.191028
H	1.919553	3.734225	1.501467
H	1.623012	2.145395	2.218470
H	0.620566	4.448231	-0.473151
H	0.033615	1.600247	0.410012
H	-0.161530	2.543387	3.458889
H	-1.920179	2.509272	3.219598
H	-0.906597	1.242758	2.493862
H	-0.012394	4.879782	2.315339
H	-1.779100	4.731683	2.415785
H	-1.029532	5.082424	0.855144
H	-3.363721	0.991468	1.560543
H	-3.741306	-3.107887	0.317613
H	-2.169891	-0.167303	-2.403487
C	4.436480	-1.965233	0.648751
O	4.915893	-2.552721	-0.557446
C	5.339201	-1.259372	-0.292017
N	6.779758	-1.231174	0.167037
O	7.219963	-2.234426	0.686699
O	7.384950	-0.189268	0.004097
C	4.984064	-0.139467	-1.219100
H	5.180997	0.823012	-0.745647
H	3.923562	-0.212060	-1.466941
H	5.574634	-0.208870	-2.135929
C	2.983375	-1.659824	0.743807
C	0.257092	-1.121275	0.990145
C	2.131738	-1.849187	-0.346013
C	2.467347	-1.201179	1.957846
C	1.107826	-0.929847	2.079142
C	0.771335	-1.576531	-0.223491
H	2.536242	-2.236619	-1.276439
H	3.129334	-1.069852	2.810222
H	0.709471	-0.590150	3.030969
H	0.107824	-1.749872	-1.065431
H	-0.810239	-0.942027	1.095425
H	4.909589	-2.368140	1.543730

SR epoxide:Catalyst, binary complex 58; Energy = -2449.844457; 6-31G(d) basis set.

N	3.381856	1.255726	0.229984
C	3.312766	1.569068	-1.073164
S	4.586666	2.318293	-1.872973
C	2.623303	0.291282	1.033963
C	3.413659	-1.032288	1.247361
C	2.608026	-1.927969	2.201212
C	2.331697	-1.267107	3.548653
C	1.554578	0.028333	3.331162
C	2.316119	0.953322	2.386743
N	3.784248	-1.786651	0.061910
C	2.687633	-2.218791	-0.783611
N	2.176528	1.220362	-1.779310
C	0.833289	1.394016	-1.401373
C	0.456181	2.117525	-0.271043
C	-0.891581	2.241380	0.051253
C	-1.884741	1.721752	-0.766276
C	-1.493985	1.049252	-1.922510
C	-0.155590	0.856118	-2.231977
C	-1.237753	2.949934	1.330466
F	-0.781534	2.267708	2.402700
C	-2.544998	0.526085	-2.861711
F	-2.879279	1.426815	-3.792831
C	4.913465	-1.295303	-0.711364
F	-0.671796	4.163007	1.388173
F	-2.554781	3.102147	1.491096
F	-2.127330	-0.574959	-3.507289
F	-3.670592	0.197489	-2.205429
H	4.242135	1.583377	0.658379
H	2.336296	1.280429	-2.778513
H	3.271975	1.235497	2.853229
H	1.756901	1.880220	2.231453
H	0.577446	-0.210539	2.889013
H	1.361416	0.542003	4.278414
H	1.769112	-1.950780	4.193589

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H          3.278547       -1.048636        4.060602
H          1.639559       -2.150682        1.735777
H          3.145320       -2.875090        2.311392
H          1.689948        0.050650        0.515542
H          4.355789       -0.766177        1.751884
H          5.658903       -0.857342       -0.040295
H          5.382375       -2.138892       -1.231409
H          4.656026       -0.541178       -1.469568
H          1.994467       -2.845810       -0.213389
H          3.089625       -2.839653       -1.590362
H          2.116517       -1.394472       -1.244596
H          1.210590        2.588938        0.349689
H         -2.932339        1.819849       -0.504345
H          0.127035        0.277352       -3.106226
C         -1.773613       -1.614600       -0.253069
O         -0.403227       -1.343055        0.043727
C         -0.805311       -2.674174        0.101946
N         -0.309472       -3.446361       -1.098800
O         -0.173918       -4.645366       -0.955562
O         -0.103443       -2.823894       -2.120515
C         -0.765150       -3.447740        1.383417
H         -1.491980       -4.261412        1.353339
H         -1.014899       -2.769519        2.201731
H          0.226208       -3.874749        1.550280
C         -2.798930       -1.107653        0.697892
C         -4.746764       -0.069269        2.398898
C         -4.148915       -1.354688        0.444791
C         -2.426809       -0.333768        1.796752
C         -3.399680        0.190872        2.641989
C         -5.119492       -0.843807        1.301037
H         -4.437987       -1.934504       -0.427688
H         -1.376397       -0.114791        1.958612
H         -3.102608        0.813451        3.480088
H         -6.168573       -1.040057        1.103868
H         -5.506450        0.339126        3.057824
H         -2.005661       -1.542865       -1.314830

SR epoxide:Catalyst, binary complex 59; Energy = -2449.841070; 6-31G(d) basis set.
N          1.560953       -1.063478       -0.014145
C          0.288454       -1.074798       -0.456741
S         -0.079921       -1.385310       -2.070205
C          1.985120       -1.195966        1.376774
C          3.343678       -1.922540        1.402348
C          3.721764       -2.222087        2.860714
C          3.844325       -0.914986        3.649086
C          2.555423       -0.094364        3.569892
C          2.125940        0.141363        2.118627
N          3.363891       -3.039739        0.462982
C          4.698945       -3.578229        0.267293
N         -0.648611       -0.788274        0.502931
C         -2.038604       -0.617059        0.323091
C         -2.815681       -1.546660       -0.370570
C         -4.185042       -1.341135       -0.477708
C         -4.805464       -0.243652        0.111811
C         -4.023198        0.658648        0.819444
C         -2.646864        0.484748        0.922817
C         -5.010745       -2.310649       -1.277753
F         -4.493497       -3.546142       -1.245609
C         -4.676309        1.811012        1.529468
F         -5.788626        2.212387        0.901613
C          2.407745       -4.098157        0.751080
F         -6.267421       -2.383151       -0.814536
F         -5.088286       -1.948182       -2.565462
F         -5.030089        1.476790        2.780975
F         -3.854429        2.864992        1.623568
H          2.235345       -1.411635       -0.694126
H         -0.296257       -0.418909        1.377253
H          2.866283        0.751014        1.582960
H          1.187690        0.711338        2.101113
H          1.753704       -0.631270        4.095095
H          2.679659        0.865602        4.080525
H          4.095079       -1.122746        4.694124
H          4.673055       -0.325059        3.234165
H          2.959904       -2.865451        3.321620
H          4.669634       -2.770292        2.893590
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H          1.247363       -1.817613        1.909051
H          4.080941       -1.205244        1.012753
H          1.389991       -3.697223        0.776885
H          2.449775       -4.835444       -0.055501
H          2.607598       -4.621232        1.701432
H          4.694909       -4.241494       -0.603342
H          5.071911       -4.154783        1.130545
H          5.399169       -2.759001        0.073555
H         -2.351764       -2.416798       -0.816543
H         -5.876905       -0.099666        0.025706
H         -2.047774        1.214195        1.461567
C          2.799150        3.003576       -1.381473
O          1.825720        3.521842       -2.283976
C          1.384009        3.232789       -1.002673
N          1.193604        4.483148       -0.175074
O          0.468949        4.385259        0.797345
O          1.799742        5.478553       -0.509991
C          0.325731        2.200236       -0.776351
H         -0.665323        2.628976       -0.945431
H          0.377376        1.830177        0.248711
H          0.479002        1.371374       -1.469217
C          3.358734        1.648858       -1.634398
C          4.489744       -0.867952       -2.063352
C          2.836893        0.806915       -2.615367
C          4.458537        1.233921       -0.877066
C          5.022972       -0.018748       -1.092571
C          3.401081       -0.450016       -2.825959
H          1.997200        1.137625       -3.219056
H          4.881140        1.902075       -0.130143
H          5.887359       -0.326733       -0.510558
H          2.978760       -1.104911       -3.580683
H          4.928210       -1.847178       -2.230912
H          3.504669        3.757757       -1.033473

SR epoxide:Catalyst, binary complex 60; Energy = -2449.844285; 6-31G(d) basis set.
N          1.399851       -1.823637        0.476164
C          0.843081       -2.976729        0.863034
S          1.693459       -4.374218        1.261480
C          2.821927       -1.489172        0.570341
C          3.281745       -0.687569       -0.665738
C          4.626015        0.014845       -0.394613
C          4.698703        0.769165        0.929696
C          4.391834       -0.163958        2.093858
C          2.994789       -0.734385        1.899275
N          3.423005       -1.527272       -1.864783
C          2.266824       -2.363392       -2.172481
N         -0.531806       -2.992001        0.876617
C         -1.382474       -1.873370        0.977580
C         -2.541475       -1.821119        0.205032
C         -3.399938       -0.732489        0.322704
C         -3.109333        0.322147        1.180203
C         -1.938349        0.267134        1.931564
C         -1.085601       -0.825182        1.855253
C         -4.669195       -0.704408       -0.484445
F         -5.698288       -1.228693        0.193375
C         -1.616373        1.411687        2.852923
F         -1.823179        2.592817        2.241591
C          3.767590       -0.727038       -3.032200
F         -5.015322        0.553669       -0.807729
F         -4.544680       -1.396821       -1.621432
F         -2.374828        1.404240        3.953524
F         -0.332539        1.390226        3.246025
H          0.787154       -1.087182        0.130520
H         -0.939367       -3.913279        0.974635
H          2.269732        0.094666        1.919813
H          2.718795       -1.425373        2.704598
H          5.129185       -0.977377        2.125278
H          4.451335        0.363143        3.051793
H          5.692116        1.218202        1.034478
H          3.972482        1.594754        0.923973
H          5.409537       -0.754512       -0.429566
H          4.828760        0.719148       -1.205687
H          3.377087       -2.432088        0.598515
H          2.521155        0.103567       -0.834697
H          3.060962        0.109817       -3.201987
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H          4.772093       -0.309617       -2.948457
H          3.750897       -1.363858       -3.919326
H          2.449657       -2.860207       -3.128936
H          1.321504       -1.794325       -2.260762
H          2.141435       -3.143168       -1.419236
H         -2.754462       -2.617501       -0.500828
H         -3.770116        1.180993        1.246518
H         -0.186556       -0.864840        2.462275
C          0.370036        1.208060       -1.786662
O         -0.436102        0.297342       -1.033237
C         -1.108458        1.187326       -1.865671
N         -1.637753        0.475329       -3.090904
O         -2.577950        0.995975       -3.656044
O         -1.074119       -0.543216       -3.432265
C         -2.040272        2.229009       -1.327751
H         -3.048817        1.826713       -1.228408
H         -2.072575        3.080146       -2.010550
H         -1.680447        2.560043       -0.352754
C          1.117982        2.230041       -1.004658
C          2.562994        4.106739        0.466454
C          2.084702        3.014187       -1.634627
C          0.895840        2.369665        0.365785
C          1.611395        3.309698        1.100255
C          2.802996        3.952619       -0.898481
H          2.277536        2.887201       -2.696981
H          0.173161        1.722136        0.850924
H          1.426242        3.409054        2.165443
H          3.554274        4.561958       -1.390589
H          3.126328        4.838757        1.036496
H          0.895466        0.732782       -2.615434

SR epoxide:Catalyst, binary complex 61; Energy = -2449.842825; 6-31G(d) basis set.
N         -1.088189       -2.059829        1.720054
C          0.197091       -1.655438        1.890125
S          1.244486       -2.470585        2.914538
C         -1.826650       -1.978870        0.462167
C         -1.281354       -2.982633       -0.579361
C         -2.149419       -2.948520       -1.849756
C         -3.630060       -3.189707       -1.548713
C         -4.138092       -2.164081       -0.534974
C         -3.308464       -2.235140        0.744963
N          0.154991       -2.789967       -0.805387
C          0.853056       -4.033689       -1.095553
N          0.503383       -0.480799        1.257048
C          1.775333       -0.049964        0.855002
C          2.021403        1.321506        0.767848
C          3.233701        1.771398        0.261073
C          4.220958        0.879942       -0.149891
C          3.960678       -0.480751       -0.048633
C          2.752973       -0.955825        0.448440
C          3.484273        3.242806        0.098833
F          4.705478        3.588902        0.524365
C          4.953733       -1.498188       -0.532310
F          6.033393       -0.931202       -1.084536
C          0.479133       -1.772880       -1.793839
F          3.410983        3.610351       -1.195847
F          2.591296        3.988611        0.764928
F          5.374800       -2.296390        0.455919
F          4.397575       -2.297606       -1.463549
H         -1.299811       -2.883135        2.274452
H         -0.268432        0.097771        0.942642
H         -3.410086       -3.239263        1.182175
H         -3.673757       -1.530381        1.498762
H         -4.051576       -1.157196       -0.974718
H         -5.198248       -2.312375       -0.306816
H         -4.212993       -3.139540       -2.473815
H         -3.766054       -4.199246       -1.138576
H         -2.049862       -1.963607       -2.326968
H         -1.769670       -3.684689       -2.568213
H         -1.720505       -0.965379        0.053760
H         -1.391014       -3.975391       -0.118640
H          1.562960       -1.625782       -1.808465
H          0.161351       -2.034219       -2.816759
H          0.020202       -0.815024       -1.520859
H          0.523331       -4.510802       -2.035283
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H	0.707331	-4.737963	-0.271886
H	1.925405	-3.829422	-1.181657
H	1.264624	2.029281	1.092476
H	5.165713	1.238414	-0.543352
H	2.548113	-2.020331	0.495026
C	-3.345588	1.467783	0.555084
O	-4.263281	2.290216	1.267315
C	-4.695667	1.789271	0.047297
N	-5.676486	0.653938	0.211530
O	-5.654045	0.036923	1.256311
O	-6.389686	0.411016	-0.741895
C	-5.014975	2.719489	-1.081056
H	-4.264743	3.511816	-1.091385
H	-6.004446	3.159966	-0.939907
H	-4.997834	2.187491	-2.033081
C	-2.136177	2.113323	-0.031080
C	0.129249	3.289505	-1.158754
C	-1.512476	1.521897	-1.134503
C	-1.627389	3.298118	0.502214
C	-0.495989	3.883110	-0.063675
C	-0.378716	2.106488	-1.693407
H	-1.933566	0.619502	-1.574923
H	-2.125707	3.756210	1.351046
H	-0.095704	4.800497	0.355851
H	0.101971	1.643571	-2.549828
H	1.019913	3.739167	-1.584595
H	-3.223598	0.483106	1.007604

SR epoxide:Catalyst, binary complex 62; Energy = -2449.836860; 6-31G(d) basis set.

N	1.443088	-1.462592	-0.731610
C	0.232649	-0.968497	-1.044290
S	-0.019343	-0.220104	-2.536164
C	1.911291	-2.044955	0.522268
C	3.163392	-2.897589	0.220876
C	3.739402	-3.452998	1.529878
C	4.042068	-2.342811	2.536782
C	2.780976	-1.538324	2.850053
C	2.191315	-0.956538	1.566169
N	2.973247	-3.965371	-0.757579
C	1.798767	-4.791788	-0.551554
N	-0.731098	-1.146309	-0.090710
C	-2.083197	-0.744176	-0.137617
C	-2.462185	0.522065	-0.584629
C	-3.799818	0.890828	-0.536622
C	-4.776326	0.030964	-0.045250
C	-4.383395	-1.223395	0.403270
C	-3.050200	-1.617733	0.356856
C	-4.176726	2.252165	-1.051645
F	-3.278945	3.178226	-0.678493
C	-5.394283	-2.169488	0.988185
F	-6.640010	-1.866387	0.605954
C	3.106360	-3.596475	-2.157866
F	-4.228264	2.277415	-2.389853
F	-5.375424	2.640940	-0.598226
F	-5.149792	-3.436330	0.621551
F	-5.371839	-2.144270	2.330435
H	2.157240	-1.230780	-1.412933
H	-0.501236	-1.755061	0.685310
H	2.895911	-0.240919	1.120360
H	1.265761	-0.406189	1.772867
H	2.041952	-2.193369	3.332235
H	2.998170	-0.731497	3.557343
H	4.463575	-2.769605	3.452492
H	4.801790	-1.668209	2.116968
H	3.025809	-4.158721	1.977233
H	4.639121	-4.024252	1.283900
H	1.143995	-2.734689	0.905664
H	3.915874	-2.213429	-0.199453
H	3.949132	-2.908650	-2.280975
H	3.322477	-4.496066	-2.744748
H	2.203625	-3.129916	-2.587466
H	1.878467	-5.687991	-1.174789
H	0.855836	-4.281587	-0.822439
H	1.733634	-5.117678	0.490487
H	-1.717910	1.207532	-0.968801

H	-5.816539	0.333173	-0.010802
H	-2.765445	-2.610509	0.693505
C	2.951915	3.312507	0.281266
O	1.981046	4.058203	-0.447389
C	1.518385	3.369835	0.661952
N	1.256197	4.305339	1.825203
O	1.857201	5.358315	1.842229
O	0.481169	3.914553	2.676601
C	0.474602	2.307593	0.511234
H	0.748495	1.650129	-0.317387
H	-0.490734	2.774902	0.294376
H	0.381302	1.728366	1.430076
C	3.580819	2.140100	-0.384438
C	4.853349	-0.018951	-1.614862
C	4.718881	1.569980	0.195231
C	3.083953	1.627732	-1.583720
C	3.721717	0.550205	-2.196813
C	5.349091	0.489443	-0.413211
H	5.115494	1.980345	1.120607
H	2.214461	2.081202	-2.050155
H	3.330882	0.165439	-3.135058
H	6.235886	0.055527	0.038429
H	5.362083	-0.844922	-2.103785
H	3.616673	3.938501	0.875600

SR epoxide:Catalyst, binary complex 63; Energy = -2449.845041; 6-31G(d) basis set.

N	-2.665027	-0.415369	0.310824
C	-1.569106	-0.821188	0.980243
S	-1.499577	-2.218421	1.909586
C	-4.001415	-0.968377	0.478863
C	-5.011133	0.072921	-0.036690
C	-6.431798	-0.417293	0.277834
C	-6.689559	-1.765019	-0.405194
C	-5.637263	-2.803118	-0.009615
C	-4.218287	-2.289277	-0.266604
N	-4.662234	1.427415	0.406643
C	-5.461561	2.448292	-0.252169
N	-0.520811	0.058937	0.848081
C	0.837127	-0.131686	1.152620
C	1.496976	-1.343248	0.935464
C	2.874800	-1.409116	1.093786
C	3.624676	-0.295443	1.458604
C	2.951239	0.894141	1.697227
C	1.569782	0.977013	1.572869
C	3.550203	-2.729926	0.854851
F	4.864667	-2.590634	0.642444
C	3.703881	2.150701	2.020238
F	4.955224	1.908338	2.421589
C	-4.674049	1.610701	1.852170
F	3.399837	-3.561356	1.894613
F	3.031387	-3.354868	-0.217998
F	3.780447	2.958105	0.943475
F	3.093880	2.861119	2.981662
H	-2.669143	0.533381	-0.062328
H	-0.742457	0.986934	0.495232
H	-4.062962	-2.117574	-1.340397
H	-3.475430	-3.017548	0.065997
H	-5.741588	-3.036979	1.058547
H	-5.801278	-3.738399	-0.554386
H	-7.694061	-2.124648	-0.159059
H	-6.662306	-1.620650	-1.494110
H	-6.553017	-0.523071	1.364235
H	-7.167639	0.320465	-0.060366
H	-4.164859	-1.154051	1.550503
H	-4.906468	0.098007	-1.134237
H	-4.001062	0.894343	2.332346
H	-4.309025	2.617210	2.080251
H	-5.677045	1.505608	2.296894
H	-5.036356	3.435652	-0.042806
H	-6.512874	2.463716	0.078544
H	-5.445677	2.288287	-1.335359
H	0.938943	-2.218101	0.624395
H	4.702763	-0.354972	1.549841
H	1.059221	1.911882	1.783713
C	1.697185	1.282342	-2.445904

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O          2.507453        0.527510       -1.536714
C          1.894206       -0.173750       -2.564952
N          2.890830       -0.549111       -3.645684
O          2.609780       -1.506706       -4.338725
O          3.879585        0.143537       -3.756902
C          0.910189       -1.262963       -2.264180
H          0.212632       -0.906458       -1.503033
H          1.439866       -2.141588       -1.887102
H          0.360559       -1.542379       -3.163782
C          0.449604        1.878738       -1.882493
C         -1.829053        3.030567       -0.748371
C         -0.816739        1.540709       -2.361042
C          0.574801        2.815762       -0.853312
C         -0.561373        3.388370       -0.285063
C         -1.953677        2.116118       -1.794343
H         -0.916178        0.820058       -3.168116
H          1.565044        3.069568       -0.483033
H         -0.458335        4.109258        0.520314
H         -2.940122        1.841578       -2.158712
H         -2.718882        3.457311       -0.296555
H          2.290198        1.907925       -3.112212

SR epoxide:Catalyst, binary complex 64; Energy = -2449.838181; 6-31G(d) basis set.
N          0.221972       -1.473244       -0.763948
C         -1.132321       -1.684537       -0.807272
S         -1.744022       -3.184946       -1.258347
C          1.009836       -0.757928        0.263428
C          0.484201        0.615794        0.712013
C          1.531574        1.258099        1.639913
C          1.802083        0.374558        2.860663
C          2.248547       -1.025711        2.444101
C          1.231416       -1.653620        1.490738
N          0.060555        1.443737       -0.429109
C         -0.457113        2.744817       -0.015205
N         -1.854940       -0.563470       -0.560632
C         -3.231194       -0.385104       -0.407901
C         -4.113484       -1.372008        0.049913
C         -5.451338       -1.051322        0.238149
C         -5.946995        0.226537       -0.005289
C         -5.060309        1.197836       -0.450489
C         -3.718521        0.902567       -0.652993
C         -6.413842       -2.107775        0.705761
F         -7.209163       -2.523589       -0.291584
C         -5.558507        2.579713       -0.764439
F         -4.613383        3.507442       -0.543871
C          1.062930        1.585615       -1.486492
F         -5.788531       -3.185516        1.193330
F         -7.220538       -1.636989        1.671075
F         -5.924461        2.696820       -2.049792
F         -6.625566        2.902454       -0.020906
H          0.706373       -2.311142       -1.067873
H         -1.292828        0.310822       -0.668146
H          0.269138       -1.806694        1.998579
H          1.575394       -2.639028        1.156159
H          3.218042       -0.959855        1.930079
H          2.390598       -1.664167        3.322005
H          2.550618        0.845925        3.507600
H          0.881841        0.297553        3.455596
H          2.457912        1.419949        1.074433
H          1.175942        2.239019        1.969620
H          1.987311       -0.589382       -0.205967
H         -0.422204        0.451940        1.315109
H          1.268840        0.612254       -1.937285
H          0.649353        2.234927       -2.262689
H          2.003487        2.027534       -1.127719
H         -1.175549        2.612273        0.801069
H         -0.975306        3.207569       -0.860620
H          0.330394        3.436626        0.317899
H         -3.754280       -2.369813        0.261180
H         -6.992575        0.460555        0.163973
H         -3.038657        1.675998       -0.999719
C          5.531640        0.621919       -0.750956
O          4.237538        0.443407       -0.174995
C          5.144388        1.195649        0.561051
N          4.813394        2.668979        0.503726
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O          5.262171        3.363522        1.392756
O          4.148989        3.059953       -0.435276
C          5.601798        0.738286        1.910748
H          6.497139        1.283158        2.211110
H          5.824381       -0.328459        1.862525
H          4.818396        0.912998        2.653259
C          6.407952       -0.576026       -0.854036
C          8.087309       -2.791850       -1.055267
C          7.666318       -0.448647       -1.445330
C          5.986435       -1.817480       -0.375669
C          6.826463       -2.922394       -0.477292
C          8.505386       -1.554011       -1.540330
H          7.988111        0.515600       -1.830244
H          4.996605       -1.913927        0.061981
H          6.493296       -3.887291       -0.108615
H          9.484264       -1.449332       -1.997165
H          8.741327       -3.654594       -1.132485
H          5.537396        1.317603       -1.589573

SR epoxide:Catalyst, binary complex 65; Energy = -2449.839954; 6-31G(d) basis set.
N          0.112540       -1.900741       -0.134684
C         -0.461138       -1.267992        0.900395
S         -1.839367       -1.777725        1.724943
C         -0.334081       -3.122249       -0.824548
C         -0.301317       -4.388392        0.062133
C         -0.681934       -5.601173       -0.801172
C         -2.034328       -5.417995       -1.491062
C         -2.026327       -4.168080       -2.370882
C         -1.677204       -2.931468       -1.541680
N          0.963123       -4.635411        0.752269
C          2.161391       -4.483618       -0.044979
N          0.138382       -0.096475        1.304959
C          1.333867        0.489969        0.851350
C          2.481562       -0.271621        0.611281
C          3.636638        0.346639        0.145917
C          3.691858        1.719173       -0.055274
C          2.560479        2.474616        0.237985
C          1.389257        1.878996        0.688584
C          4.855432       -0.505785       -0.078424
F          5.458432       -0.813078        1.077899
C          2.571300        3.959793       -0.014089
F          3.817961        4.453333        0.015111
C          1.108909       -4.024866        2.060145
F          4.531973       -1.667752       -0.669176
F          5.757586        0.107350       -0.852141
F          2.058842        4.244423       -1.217268
F          1.850396        4.619300        0.898591
H          0.859659       -1.406545       -0.608223
H         -0.458255        0.471865        1.896518
H         -2.459522       -2.747723       -0.798329
H         -1.613101       -2.041536       -2.180057
H         -1.285722       -4.295184       -3.173047
H         -2.998443       -4.026663       -2.854209
H         -2.275963       -6.304654       -2.086543
H         -2.820458       -5.318150       -0.730591
H          0.089165       -5.766307       -1.567179
H         -0.681764       -6.483903       -0.155071
H          0.428253       -3.266642       -1.601494
H         -1.067441       -4.276948        0.835747
H          0.184824       -4.144002        2.630959
H          1.917488       -4.529928        2.600691
H          1.350732       -2.947098        2.033459
H          3.006816       -4.932721        0.486430
H          2.430345       -3.429957       -0.254575
H          2.058979       -5.001647       -1.003015
H          2.483905       -1.339101        0.811585
H          4.596430        2.191571       -0.419964
H          0.521973        2.489518        0.928038
C         -2.950532        2.767783        0.185327
O         -1.806137        2.207131        0.833486
C         -1.814045        2.171604       -0.557693
N         -0.878774        3.206473       -1.141645
O         -0.651146        4.194048       -0.471434
O         -0.440267        2.983569       -2.251658
C         -1.799271        0.864161       -1.285301
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H	-2.201995	0.983768	-2.292437
H	-2.405228	0.146211	-0.727376
H	-0.774703	0.489837	-1.362083
C	-4.255044	2.068302	0.326726
C	-6.719780	0.789004	0.539432
C	-5.392511	2.645664	-0.241657
C	-4.353223	0.858568	1.012800
C	-5.586114	0.220719	1.115797
C	-6.621920	2.003105	-0.138554
H	-5.314822	3.596759	-0.762600
H	-3.467882	0.419214	1.463986
H	-5.656362	-0.722126	1.649470
H	-7.504427	2.452475	-0.582837
H	-7.680648	0.290643	0.622468
H	-2.966706	3.856350	0.219232

SR epoxide:Catalyst, binary complex 66; Energy = -2449.844210; 6-31G(d) basis set.

N	-3.282541	-0.627412	-0.454610
C	-2.215449	-1.213326	0.128661
S	-2.273665	-1.991768	1.614522
C	-4.632614	-0.647109	0.092851
C	-5.443586	0.479564	-0.566058
C	-6.842142	0.525650	0.066472
C	-7.563947	-0.813539	-0.114723
C	-6.738307	-1.967459	0.458302
C	-5.330778	-1.990269	-0.140570
N	-4.691438	1.739696	-0.569657
C	-5.246890	2.722951	-1.488443
N	-1.081355	-1.115989	-0.642194
C	0.239578	-1.442423	-0.290760
C	0.774438	-1.102619	0.954713
C	2.108034	-1.373406	1.226817
C	2.926946	-1.996914	0.290436
C	2.386337	-2.323330	-0.946211
C	1.054970	-2.050789	-1.245530
C	2.674952	-1.003036	2.569734
F	2.022825	0.034354	3.115427
C	3.279054	-2.890802	-2.011610
F	3.879498	-1.909914	-2.712431
C	-4.509280	2.327377	0.752968
F	2.588862	-2.020892	3.439340
F	3.969504	-0.674138	2.477787
F	4.251305	-3.650984	-1.495059
F	2.598671	-3.635091	-2.893361
H	-3.108489	0.139206	-1.101583
H	-1.225004	-0.882381	-1.617579
H	-5.382626	-2.173218	-1.222487
H	-4.730631	-2.789020	0.303894
H	-6.661448	-1.854605	1.548183
H	-7.238406	-2.923732	0.274377
H	-8.550299	-0.774569	0.359153
H	-7.732811	-0.987312	-1.186384
H	-6.747806	0.747843	1.137757
H	-7.426406	1.337224	-0.381619
H	-4.570569	-0.479159	1.176481
H	-5.562725	0.207841	-1.627108
H	-5.444213	2.727529	1.176953
H	-4.102462	1.586992	1.447777
H	-3.790181	3.149907	0.680595
H	-4.551665	3.564879	-1.575877
H	-6.219230	3.125674	-1.160428
H	-5.372826	2.274816	-2.478460
H	0.148400	-0.625901	1.697294
H	3.968290	-2.204155	0.513537
H	0.648754	-2.322055	-2.215559
C	2.687961	2.890754	0.373235
O	3.219488	1.778190	1.094568
C	3.692830	1.972905	-0.196364
N	5.093427	2.534828	-0.200750
O	5.760743	2.321690	-1.194630
O	5.443086	3.178211	0.765768
C	3.440771	0.954385	-1.263431
H	4.166930	0.142163	-1.201490
H	3.513876	1.411542	-2.252090
H	2.434831	0.553276	-1.117693

C	1.262341	2.792065	-0.053004
C	-1.393806	2.550144	-0.858086
C	0.838290	3.387481	-1.241933
C	0.356327	2.091114	0.740533
C	-0.971118	1.969778	0.337337
C	-0.488507	3.263242	-1.643644
H	1.548213	3.936212	-1.855826
H	0.707953	1.640824	1.663672
H	-1.677485	1.421614	0.957565
H	-0.815509	3.719545	-2.573042
H	-2.430788	2.439943	-1.167928
H	3.055376	3.850429	0.734918

SR epoxide:Catalyst, binary complex 67; Energy = -2449.845879; 6-31G(d) basis set.

N	1.488297	-1.807565	0.433270
C	1.037105	-2.994561	0.856729
S	2.003970	-4.331276	1.195074
C	2.885949	-1.372978	0.437808
C	3.210082	-0.548461	-0.826725
C	4.507997	0.259850	-0.639134
C	4.597827	1.025327	0.677555
C	4.445689	0.074399	1.857561
C	3.088036	-0.604254	1.754642
N	3.342258	-1.388432	-2.025824
C	2.213141	-2.279422	-2.274173
N	-0.328038	-3.096560	0.964603
C	-1.225386	-2.012493	1.077204
C	-2.361240	-1.963458	0.276289
C	-3.238967	-0.888528	0.394581
C	-2.997217	0.143613	1.289237
C	-1.848960	0.088796	2.076941
C	-0.970324	-0.980092	1.988197
C	-4.398119	-0.815711	-0.557434
F	-5.216683	0.206447	-0.276643
C	-1.580630	1.208145	3.044836
F	-1.874606	2.398910	2.492883
C	3.594926	-0.583503	-3.213374
F	-3.957811	-0.633394	-1.817853
F	-5.121701	-1.938986	-0.556738
F	-2.311303	1.101536	4.158837
F	-0.289283	1.249358	3.410611
H	0.804437	-1.112756	0.139007
H	-0.675895	-4.035788	1.108269
H	2.303754	0.165788	1.826199
H	2.920612	-1.313709	2.573675
H	5.246058	-0.677346	1.836382
H	4.526908	0.607162	2.810756
H	5.553387	1.559063	0.719519
H	3.803635	1.784398	0.718393
H	5.347758	-0.444030	-0.719054
H	4.604586	0.972608	-1.462350
H	3.506418	-2.274574	0.429849
H	2.381255	0.180400	-0.955334
H	2.842117	0.216902	-3.358318
H	4.581615	-0.119201	-3.178287
H	3.568903	-1.229369	-4.093669
H	2.366309	-2.764777	-3.241485
H	1.239259	-1.753824	-2.308010
H	2.165626	-3.065788	-1.518812
H	-2.539067	-2.744690	-0.456755
H	-3.680121	0.983413	1.363163
H	-0.081993	-1.018097	2.611438
C	0.165383	1.270907	-1.734072
O	-0.602792	0.293516	-1.026374
C	-1.311875	1.196631	-1.811979
N	-1.801622	0.553562	-3.086879
O	-2.676994	1.145086	-3.685111
O	-1.265691	-0.476195	-3.437524
C	-2.281915	2.172737	-1.218037
H	-3.276366	1.728581	-1.141800
H	-2.347832	3.058613	-1.851849
H	-1.931991	2.462402	-0.225779
C	0.877551	2.286901	-0.912413
C	2.229744	4.175906	0.629289
C	0.679370	2.339086	0.467222

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C          1.777688        3.164718       -1.518279
C          2.448031        4.109980       -0.746669
C          1.349169        3.283704        1.238162
H          0.007444        1.621855        0.925994
H          1.953793        3.107294       -2.589634
H          3.145150        4.794619       -1.219163
H          1.182346        3.314485        2.310336
H          2.755937        4.914176        1.226099
H          0.704143        0.858018       -2.587765

SR epoxide:Catalyst, binary complex 68; Energy = -2449.840166; 6-31G(d) basis set.
N         -1.003935       -0.004009        0.350917
C          0.116535       -0.366065       -0.326200
S          0.131490       -0.451786       -2.003114
C         -1.028433        0.836556        1.551893
C         -0.599917        2.277120        1.195902
C         -0.821413        3.222951        2.386316
C         -2.278613        3.191041        2.847550
C         -2.667930        1.772130        3.260868
C         -2.456652        0.794815        2.105694
N          0.745254        2.298562        0.615231
C          1.819621        2.300994        1.596734
N          1.150238       -0.771312        0.471512
C          2.512727       -0.784124        0.134750
C          3.347676       -1.741658        0.708776
C          4.714195       -1.708844        0.451085
C          5.268459       -0.739589       -0.376717
C          4.420618        0.208356       -0.940019
C          3.054511        0.197749       -0.695427
C          5.608104       -2.708388        1.128836
F          4.982800       -3.877634        1.326847
C          4.960819        1.297968       -1.821778
F          4.516282        2.504192       -1.419959
C          0.922337        3.374466       -0.348079
F          6.714564       -2.950884        0.415461
F          6.005603       -2.271736        2.335906
F          6.298821        1.339274       -1.810263
F          4.572221        1.149587       -3.094162
H         -1.756104        0.232152       -0.291159
H          0.924950       -0.995666        1.433095
H         -3.146650        1.053914        1.287325
H         -2.689848       -0.231751        2.407784
H         -2.057288        1.465271        4.120952
H         -3.713182        1.734897        3.584450
H         -2.429400        3.888543        3.677831
H         -2.930870        3.520006        2.026099
H         -0.178579        2.921677        3.224281
H         -0.520644        4.239090        2.104215
H         -0.343783        0.426181        2.305389
H         -1.284590        2.588943        0.393837
H          0.842506        4.380962        0.098773
H          1.914386        3.289384       -0.803599
H          0.175096        3.281658       -1.142464
H          1.868524        3.228548        2.190523
H          2.776116        2.184612        1.077974
H          1.709333        1.457076        2.286818
H          2.929890       -2.514978        1.346320
H          6.333645       -0.720914       -0.575541
H          2.403360        0.953125       -1.122497
C         -5.658942       -0.988328       -1.082313
O         -5.112407       -2.036123       -1.876505
C         -5.086298       -2.227497       -0.504191
N         -6.142072       -3.216492       -0.061261
O         -7.107921       -3.363124       -0.779653
O         -5.956623       -3.771241        1.004677
C         -3.786056       -2.377800        0.220683
H         -3.928628       -2.231361        1.291836
H         -3.078411       -1.639071       -0.157407
H         -3.376724       -3.376817        0.052831
C         -4.942606        0.316137       -1.058389
C         -3.677895        2.805208       -1.028244
C         -5.520192        1.389680       -0.376349
C         -3.730817        0.492243       -1.730740
C         -3.101295        1.736499       -1.714454
C         -4.887391        2.629264       -0.357019
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H	-6.471944	1.256100	0.131562
H	-3.289242	-0.337192	-2.278004
H	-2.156097	1.858051	-2.237678
H	-5.343934	3.459785	0.172570
H	-3.188902	3.775363	-1.023124
H	-6.747148	-0.942831	-1.115597

SR epoxide:Catalyst, binary complex 69; Energy = -2449.843944; 6-31G(d) basis set.

N	2.288953	-1.568332	0.975645
C	1.073204	-1.613349	0.397974
S	0.824815	-1.958570	-1.232161
C	3.553862	-1.513436	0.252228
C	4.620551	-0.983714	1.231690
C	5.918195	-0.728222	0.453891
C	6.417546	-2.031020	-0.179912
C	5.341403	-2.668766	-1.062657
C	4.024360	-2.860318	-0.304273
N	4.103957	0.125285	2.039367
C	4.923303	0.395038	3.210437
N	0.055867	-1.330289	1.276412
C	-1.321402	-1.181369	0.999622
C	-1.980393	-0.089120	1.560447
C	-3.341907	0.094183	1.340209
C	-4.061574	-0.794093	0.555740
C	-3.393336	-1.887949	0.012490
C	-2.039112	-2.101728	0.232181
C	-4.008342	1.282183	1.973895
F	-4.190516	1.091759	3.293702
C	-4.137249	-2.814082	-0.906494
F	-5.432950	-2.908653	-0.570608
C	3.861920	1.345808	1.281408
F	-3.258809	2.387024	1.849453
F	-5.207496	1.535731	1.441410
F	-4.090554	-2.385647	-2.175085
F	-3.624588	-4.053317	-0.888771
H	2.370420	-1.105724	1.882763
H	0.335784	-0.977701	2.185087
H	4.162794	-3.558850	0.531773
H	3.257221	-3.274537	-0.961356
H	5.156701	-2.023327	-1.932704
H	5.691089	-3.629900	-1.452873
H	7.326603	-1.843234	-0.761031
H	6.691523	-2.733316	0.619340
H	5.732201	0.016688	-0.332375
H	6.680858	-0.311537	1.121788
H	3.438882	-0.813676	-0.590073
H	4.815024	-1.795058	1.950312
H	3.233053	1.137613	0.410406
H	3.330698	2.061854	1.916649
H	4.789520	1.827769	0.931043
H	5.907442	0.826244	2.961989
H	5.082419	-0.530183	3.772102
H	4.401322	1.106285	3.858023
H	-1.425790	0.641736	2.140585
H	-5.114975	-0.631589	0.358538
H	-1.541396	-2.962676	-0.194355
C	-0.144413	1.637267	-0.919683
O	-0.882178	2.269797	0.146708
C	-1.375933	2.403503	-1.149219
N	-2.627984	1.566809	-1.332476
O	-2.520098	0.450216	-1.793661
O	-3.668899	2.090061	-0.980609
C	-1.530286	3.765287	-1.751176
H	-0.583668	4.301352	-1.672438
H	-2.310889	4.312530	-1.219484
H	-1.804219	3.682108	-2.805943
C	1.215329	2.166200	-1.214418
C	3.795246	3.072603	-1.776470
C	1.693124	3.333174	-0.614969
C	2.037098	1.447316	-2.086922
C	3.323107	1.901698	-2.367138
C	2.979023	3.785967	-0.900225
H	1.061344	3.867806	0.088758
H	1.670770	0.524730	-2.528167
H	3.956919	1.336235	-3.043788

H	3.347255	4.693160	-0.430787
H	4.799016	3.425348	-1.993125
H	-0.246836	0.551604	-0.951073

SR epoxide:Catalyst, binary complex 70; Energy = -2449.839639; 6-31G(d) basis set.

N	1.361932	-0.878217	0.104369
C	0.114988	-0.758967	-0.390090
S	-0.260250	-1.237331	-1.958447
C	1.775685	-0.828456	1.507635
C	2.611946	-2.084725	1.847770
C	3.088189	-2.007356	3.304887
C	3.858027	-0.718726	3.594565
C	2.997319	0.505024	3.284347
C	2.523525	0.471608	1.832071
N	1.951122	-3.362530	1.594159
C	2.080335	-3.899539	0.249153
N	-0.790181	-0.192515	0.471908
C	-2.175690	-0.036310	0.251429
C	-2.965864	-1.113243	-0.157108
C	-4.332310	-0.932587	-0.312657
C	-4.937482	0.294311	-0.049261
C	-4.141620	1.349045	0.372911
C	-2.765138	1.195889	0.518016
C	-5.179032	-2.073222	-0.805483
F	-5.344314	-2.024719	-2.134583
C	-4.770653	2.668905	0.720747
F	-5.066751	2.743984	2.028004
C	0.583204	-3.461340	2.067787
F	-4.630548	-3.260397	-0.516062
F	-6.403036	-2.046104	-0.257781
F	-3.948518	3.692337	0.448691
F	-5.909916	2.868464	0.046762
H	2.037933	-1.238939	-0.564380
H	-0.414604	0.348749	1.241476
H	3.388379	0.545041	1.158984
H	1.883443	1.336244	1.615866
H	2.124781	0.513426	3.952116
H	3.548094	1.431997	3.472330
H	4.186109	-0.702887	4.638818
H	4.765571	-0.689533	2.974837
H	2.219819	-2.063766	3.975915
H	3.700502	-2.891318	3.504909
H	0.868755	-0.877783	2.123445
H	3.505950	-2.059234	1.206643
H	-0.140663	-2.898806	1.448669
H	0.277586	-4.512229	2.056007
H	0.503883	-3.105455	3.099207
H	1.427546	-3.417549	-0.499370
H	1.825785	-4.965082	0.269750
H	3.118720	-3.809928	-0.083571
H	-2.509964	-2.077946	-0.344919
H	-6.007919	0.421323	-0.168840
H	-2.153741	2.040537	0.822187
C	3.915591	1.928499	-1.269304
O	3.437920	2.937321	-2.153614
C	2.665990	2.698433	-1.028814
N	2.851575	3.779495	0.016656
O	3.847779	4.465156	-0.056879
O	2.001194	3.856933	0.885003
C	1.243008	2.259931	-1.188711
H	1.194248	1.365386	-1.811221
H	0.672758	3.060550	-1.668279
H	0.793206	2.042378	-0.221039
C	3.924116	0.517163	-1.732387
C	3.919091	-2.171130	-2.489509
C	4.688000	-0.415220	-1.022541
C	3.191545	0.104518	-2.846025
C	3.182417	-1.238235	-3.215513
C	4.684396	-1.754948	-1.399354
H	5.291522	-0.090667	-0.177692
H	2.634465	0.835533	-3.423799
H	2.588949	-1.554644	-4.066296
H	5.282443	-2.472566	-0.844981
H	3.905820	-3.217828	-2.776961
H	4.778583	2.245372	-0.683030

SR epoxide:Catalyst, binary complex 71; Energy = -2449.851170; 6-31G(d) basis set.

N	3.013168	0.712498	-0.708756
C	1.815370	1.199553	-0.342056
S	1.599472	2.137689	1.039458
C	4.264653	0.928713	0.006796
C	5.203841	-0.258366	-0.244735
C	6.496976	-0.052991	0.562014
C	7.178041	1.265424	0.183829
C	6.231878	2.450138	0.382154
C	4.933175	2.246369	-0.399119
N	4.511124	-1.533136	-0.039729
C	3.978747	-1.725365	1.303005
N	0.801682	0.831868	-1.200025
C	-0.575291	1.090877	-1.077660
C	-1.082533	2.325713	-0.666105
C	-2.458201	2.490112	-0.547380
C	-3.349094	1.467219	-0.853660
C	-2.829436	0.261719	-1.310246
C	-1.458093	0.068587	-1.431150
C	-2.982445	3.791732	-0.007109
F	-4.237223	4.028586	-0.413519
C	-3.755335	-0.885201	-1.593366
F	-4.986276	-0.472401	-1.909161
C	5.303134	-2.680574	-0.454274
F	-2.993703	3.791237	1.333573
F	-2.225976	4.828067	-0.394301
F	-3.308778	-1.652068	-2.599211
F	-3.877810	-1.693384	-0.518734
H	3.064306	0.068661	-1.491293
H	1.009599	0.045029	-1.807933
H	5.142985	2.219579	-1.477212
H	4.230678	3.065609	-0.217544
H	5.995953	2.553535	1.449862
H	6.713079	3.383086	0.071672
H	8.090131	1.398511	0.774816
H	7.486222	1.221725	-0.870033
H	6.261533	-0.045107	1.634506
H	7.178940	-0.892273	0.386959
H	4.022554	0.986713	1.073592
H	5.477227	-0.238889	-1.313282
H	6.131622	-2.915564	0.233742
H	4.654229	-3.561040	-0.510102
H	5.723160	-2.498270	-1.448420
H	4.755009	-1.747835	2.084819
H	3.448578	-2.683127	1.332888
H	3.257235	-0.937730	1.545258
H	-0.412605	3.141939	-0.431704
H	-4.418595	1.608487	-0.746888
H	-1.071313	-0.884546	-1.782715
C	-1.841422	-2.726201	1.238733
O	-1.400582	-2.539240	2.581022
C	-2.111269	-1.491317	2.015523
N	-3.548503	-1.445279	2.493069
O	-3.992151	-2.433587	3.038683
O	-4.170202	-0.429875	2.247163
C	-1.475168	-0.138974	1.928677
H	-0.510065	-0.208597	1.425682
H	-1.309794	0.241457	2.941067
H	-2.113354	0.561819	1.392356
C	-0.845327	-2.815230	0.141265
C	0.910435	-2.944115	-2.025570
C	-1.264582	-3.363596	-1.074775
C	0.469118	-2.364533	0.279876
C	1.345480	-2.428324	-0.803367
C	-0.393640	-3.421234	-2.157824
H	-2.283601	-3.725895	-1.176112
H	0.809592	-1.984811	1.239635
H	2.372241	-2.080116	-0.691596
H	-0.732699	-3.838459	-3.100785
H	1.595172	-2.996407	-2.867198
H	-2.684558	-3.411683	1.159109

SR epoxide:Catalyst, binary complex 72; Energy = -2449.838418; 6-31G(d) basis set.

N	-0.930271	2.333052	0.105318

C	-0.142551	3.402511	0.305193
S	-0.703793	4.979205	0.473401
C	-2.391677	2.344406	0.221992
C	-2.972861	1.123442	-0.546362
C	-4.227039	0.613061	0.165454
C	-3.872850	0.040460	1.546467
C	-2.773278	0.877073	2.233807
C	-2.786023	2.314414	1.712144
N	-3.199365	1.312573	-1.977753
C	-4.300880	2.208500	-2.297972
N	1.208152	3.152868	0.344724
C	1.845701	1.916019	0.559284
C	1.327355	0.980888	1.458734
C	1.946581	-0.256437	1.599529
C	3.105203	-0.568375	0.899081
C	3.641424	0.392692	0.047581
C	3.020907	1.621761	-0.134972
C	1.341834	-1.240761	2.563070
F	1.458975	-0.815371	3.829168
C	4.905577	0.096146	-0.712435
F	4.887061	0.644135	-1.933080
C	-1.996826	1.707330	-2.695958
F	0.019934	-1.397368	2.338482
F	1.906572	-2.447242	2.487439
F	5.981358	0.591605	-0.078348
F	5.102001	-1.219738	-0.852557
H	-0.483471	1.478995	-0.218013
H	1.784864	3.982513	0.285482
H	-2.098314	2.958026	2.269509
H	-3.785953	2.746889	1.833517
H	-2.896892	0.856666	3.320437
H	-1.788472	0.431840	2.033577
H	-4.774637	0.023385	2.167141
H	-3.541207	-0.999692	1.441339
H	-4.944068	1.434629	0.277994
H	-4.706248	-0.146090	-0.460966
H	-2.745273	3.275675	-0.233860
H	-2.227648	0.314896	-0.471838
H	-1.185941	1.004691	-2.474500
H	-2.196591	1.671188	-3.771483
H	-1.650108	2.725685	-2.447843
H	-4.420671	2.236624	-3.384881
H	-4.139718	3.244896	-1.953229
H	-5.234850	1.839233	-1.869185
H	0.440581	1.218953	2.039074
H	3.564708	-1.544989	0.995871
H	3.416218	2.334024	-0.852251
C	-0.451578	-1.790415	-0.449657
O	0.779579	-2.476147	-0.168654
C	0.538642	-2.080493	-1.485562
N	1.430933	-0.921075	-1.870991
O	0.994815	0.211649	-1.755577
O	2.538999	-1.207006	-2.270949
C	0.452658	-3.116155	-2.561933
H	-0.215676	-3.909070	-2.222357
H	1.444035	-3.529033	-2.757182
H	0.053748	-2.678873	-3.480924
C	-1.716696	-2.566385	-0.324566
C	-4.107837	-3.956711	-0.022523
C	-1.809500	-3.590167	0.617285
C	-2.815985	-2.238451	-1.122173
C	-4.010267	-2.936812	-0.967622
C	-3.007520	-4.283755	0.767630
H	-0.943157	-3.830811	1.226076
H	-2.749499	-1.429690	-1.849379
H	-4.865235	-2.682362	-1.586547
H	-3.082700	-5.078457	1.503130
H	-5.041557	-4.497401	0.096617
H	-0.457072	-0.776416	-0.050417

SR epoxide:Catalyst, binary complex 73; Energy = -2449.842215; 6-31G(d) basis set.

N	3.186399	-0.462755	1.063855
C	3.466197	0.836548	1.251872
S	4.815593	1.346273	2.107710
C	2.401777	-1.135676	0.019414

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C          3.294524       -1.482618       -1.209136
C          2.582517       -2.475284       -2.142824
C          2.127953       -3.736917       -1.417512
C          1.150346       -3.361100       -0.310252
C          1.794583       -2.388595        0.674840
N          3.791746       -0.359077       -1.985073
C          2.811579        0.554750       -2.533361
N          2.620064        1.767744        0.677859
C          1.212913        1.803585        0.754289
C          0.554723        2.785878        0.011979
C         -0.821108        2.942170        0.128331
C         -1.569516        2.119774        0.959300
C         -0.904455        1.131233        1.679462
C          0.472377        0.962113        1.590777
C         -1.471946        4.072965       -0.619004
F         -1.211870        5.250444       -0.029578
C         -1.682209        0.281462        2.648472
F         -1.684171        0.815183        3.877179
C          4.990074        0.323826       -1.532225
F         -1.009188        4.164746       -1.876730
F         -2.801946        3.944647       -0.679822
F         -2.959500        0.152921        2.267332
F         -1.160652       -0.952028        2.758332
H          3.838533       -1.070194        1.550044
H          3.044452        2.688987        0.682814
H          2.605100       -2.920563        1.194325
H          1.079299       -2.085203        1.450173
H          0.265054       -2.900336       -0.774279
H          0.800760       -4.245751        0.230584
H          1.659499       -4.432316       -2.121144
H          2.995448       -4.253853       -0.984850
H          1.699207       -2.002256       -2.594267
H          3.271576       -2.702045       -2.961565
H          1.604615       -0.457785       -0.305778
H          4.180064       -1.999799       -0.810481
H          4.799762        1.182698       -0.870967
H          5.639488       -0.374598       -0.996860
H          5.540646        0.699729       -2.403737
H          2.388757        1.253923       -1.789588
H          1.988230        0.007730       -3.002167
H          3.289242        1.155326       -3.315362
H          1.125770        3.433717       -0.647732
H         -2.644457        2.234738        1.034261
H          0.971642        0.207049        2.190468
C         -2.022057       -1.628522       -0.038144
O         -3.147555       -2.090264        0.698162
C         -2.620132       -2.969466       -0.235238
N         -1.818428       -4.063873        0.424459
O         -1.359899       -3.837263        1.524737
O         -1.641475       -5.078204       -0.223016
C         -3.437644       -3.424609       -1.402704
H         -4.171137       -4.168730       -1.083283
H         -2.797932       -3.864874       -2.168039
H         -3.957601       -2.558936       -1.816038
C         -2.217480       -0.511121       -0.997635
C         -2.503319        1.654564       -2.725934
C         -1.123148       -0.055382       -1.735428
C         -3.454191        0.121893       -1.119741
C         -3.593852        1.202635       -1.986388
C         -1.265616        1.025213       -2.598843
H         -0.158202       -0.548279       -1.629578
H         -4.288572       -0.223570       -0.516284
H         -4.552418        1.704658       -2.072783
H         -0.408802        1.387618       -3.159746
H         -2.611108        2.510005       -3.384885
H         -1.104838       -1.605001        0.550037

SR epoxide:Catalyst, binary complex 74; Energy = -2449.845157; 6-31G(d) basis set.
N         -2.567307       -0.041625        0.586903
C         -1.472728       -0.187243        1.355499
S         -1.388764       -1.226989        2.672755
C         -3.873805       -0.618695        0.859580
C         -4.911602        0.164289        0.035500
C         -6.316411       -0.324194        0.417776
C         -6.452823       -1.823055        0.124121
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C         -5.362370       -2.634590        0.828519
C         -3.965294       -2.104046        0.497281
N         -4.660169        1.607401        0.096161
C         -4.800222        2.184947        1.426652
N         -0.446129        0.638996        0.960248
C          0.932790        0.535910        1.205447
C          1.696797        1.693231        1.046394
C          3.084147        1.626609        1.074664
C          3.743433        0.422364        1.281364
C          2.968809       -0.713443        1.482829
C          1.581350       -0.672454        1.466385
C          3.852284        2.886481        0.802444
F          3.378463        3.919433        1.515397
C          3.611491       -2.066339        1.579374
F          4.932065       -1.992312        1.777628
C         -5.438830        2.352781       -0.879377
F          5.152942        2.759841        1.081664
F          3.754421        3.243842       -0.493683
F          3.088488       -2.803498        2.566937
F          3.417674       -2.759354        0.437978
H         -2.610801        0.757279       -0.044924
H         -0.681158        1.352509        0.273541
H         -3.758571       -2.215183       -0.576337
H         -3.198676       -2.658698        1.043231
H         -5.513265       -2.580180        1.915115
H         -5.436756       -3.691353        0.552626
H         -7.445171       -2.175149        0.424315
H         -6.375196       -1.980480       -0.960569
H         -6.493070       -0.140557        1.485885
H         -7.075291        0.238269       -0.137467
H         -4.084894       -0.515420        1.933872
H         -4.745931       -0.109088       -1.020043
H         -6.517658        2.377691       -0.654322
H         -5.082823        3.387680       -0.910284
H         -5.306821        1.912379       -1.873539
H         -4.149112        1.666495        2.136471
H         -5.834050        2.153211        1.807324
H         -4.488230        3.233022        1.389803
H          1.202174        2.646016        0.878394
H          4.825436        0.369465        1.281820
H          1.008432       -1.578057        1.620271
C          1.467083       -0.125378       -2.696115
O          2.319096       -0.421396       -1.584905
C          1.552002       -1.464411       -2.082912
N          2.400124       -2.436374       -2.877511
O          3.414368       -2.007035       -3.384106
O          1.985133       -3.574809       -2.968308
C          0.516439       -2.139135       -1.235403
H         -0.156665       -2.730873       -1.857611
H         -0.055653       -1.375248       -0.704477
H          1.001822       -2.802986       -0.516877
C          0.321359        0.794837       -2.424367
C         -1.776504        2.558814       -1.879430
C         -0.998382        0.406026       -2.654491
C          0.592319        2.078204       -1.941782
C         -0.454322        2.956061       -1.665219
C         -2.044301        1.287930       -2.385910
H         -1.209411       -0.590068       -3.034533
H          1.621796        2.377526       -1.762738
H         -0.240064        3.950080       -1.283678
H         -3.071240        0.977623       -2.559519
H         -2.595772        3.235145       -1.654718
H          2.019704        0.023350       -3.623404

SR epoxide:Catalyst, binary complex 75; Energy = -2449.843770; 6-31G(d) basis set.
N          1.913911       -1.714438       -0.755501
C          0.792004       -1.066478       -1.146383
S          0.803342        0.261382       -2.167848
C          3.253433       -1.374428       -1.216483
C          4.249166       -1.828811       -0.140545
C          5.668152       -1.420848       -0.562402
C          6.024005       -2.034590       -1.920781
C          5.004512       -1.640508       -2.991836
C          3.584128       -2.015828       -2.565473
N          3.795234       -1.379856        1.179745
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C	4.582511	-1.933544	2.269059
N	-0.333497	-1.654322	-0.614261
C	-1.675094	-1.249410	-0.561370
C	-2.136985	0.040741	-0.833518
C	-3.489157	0.331473	-0.656598
C	-4.402394	-0.621492	-0.236591
C	-3.931323	-1.907315	0.018400
C	-2.592702	-2.222757	-0.135921
C	-3.929095	1.751224	-0.893813
F	-3.432153	2.567222	0.051007
C	-4.892032	-2.947928	0.522117
F	-4.424275	-4.191425	0.344310
C	3.674922	0.067990	1.298312
F	-3.507589	2.208826	-2.075347
F	-5.263578	1.872974	-0.859466
F	-5.129933	-2.800214	1.834648
F	-6.074969	-2.864938	-0.100218
H	1.911313	-2.114306	0.182781
H	-0.175271	-2.584737	-0.243066
H	3.492006	-3.106118	-2.469718
H	2.852080	-1.684968	-3.308806
H	5.053698	-0.556107	-3.159437
H	5.247305	-2.119374	-3.945845
H	7.031209	-1.725739	-2.219126
H	6.042793	-3.129177	-1.825924
H	5.733835	-0.327168	-0.630358
H	6.389257	-1.742124	0.197263
H	3.315926	-0.284234	-1.334595
H	4.217830	-2.930620	-0.108204
H	2.900391	0.439067	0.619544
H	3.360432	0.313278	2.315688
H	4.617142	0.603417	1.092292
H	5.596162	-1.505849	2.341039
H	4.675544	-3.016920	2.142263
H	4.067245	-1.737321	3.215068
H	-1.466077	0.810716	-1.193017
H	-5.451371	-0.376530	-0.116037
H	-2.253507	-3.234099	0.069227
C	0.020820	2.418963	1.007176
O	0.187342	3.835313	1.024251
C	0.864734	3.137287	0.027155
N	0.207064	3.355067	-1.319906
O	-1.007076	3.362082	-1.353005
O	0.941972	3.516165	-2.272233
C	2.358889	3.172084	-0.030037
H	2.753180	2.954810	0.964567
H	2.699568	4.159949	-0.347843
H	2.721553	2.426760	-0.740914
C	0.591439	1.642055	2.142580
C	1.568631	0.137435	4.281507
C	0.355088	0.267216	2.200635
C	1.313285	2.263846	3.161955
C	1.796624	1.511576	4.230381
C	0.849936	-0.484893	3.261018
H	-0.230022	-0.207049	1.417101
H	1.468334	3.338060	3.123073
H	2.344878	2.002140	5.028650
H	0.665114	-1.554239	3.299175
H	1.941958	-0.445812	5.117874
H	-0.961368	2.108201	0.654579

SR epoxide:Catalyst, binary complex 76; Energy = -2449.833507; 6-31G(d) basis set.

N	-1.724780	1.909158	-0.658637
C	-2.779656	2.451487	-1.287097
S	-2.799020	3.966393	-2.021459
C	-0.423690	2.547790	-0.478646
C	0.057552	2.315815	0.972210
C	0.303064	0.812180	1.182501
C	1.348869	0.281044	0.198885
C	0.919004	0.538554	-1.248889
C	0.602830	2.018389	-1.485655
N	1.277581	3.093120	1.217097
C	1.053965	4.524757	1.056351
N	-3.913113	1.674693	-1.328913
C	-4.179163	0.474380	-0.645106

C	-4.892007	-0.535182	-1.300197
C	-5.189535	-1.715963	-0.633805
C	-4.773814	-1.931539	0.677062
C	-4.072635	-0.920726	1.319881
C	-3.790214	0.283811	0.683678
C	-5.899525	-2.817154	-1.374128
F	-6.754208	-2.329736	-2.282937
C	-3.634508	-1.082034	2.749693
F	-4.367255	-0.325302	3.577842
C	1.837329	2.823540	2.533878
F	-5.030080	-3.599451	-2.030029
F	-6.589283	-3.604760	-0.540117
F	-3.736546	-2.349380	3.163692
F	-2.356040	-0.701306	2.907222
H	-1.774827	0.920320	-0.444896
H	-4.624644	2.025399	-1.957374
H	0.225072	2.187168	-2.500159
H	1.520100	2.605534	-1.359971
H	1.705314	0.213293	-1.938574
H	0.034772	-0.072851	-1.484533
H	2.302564	0.789332	0.384319
H	1.510641	-0.790615	0.360832
H	0.589953	0.609859	2.218187
H	-0.645836	0.272021	1.054136
H	-0.610104	3.605936	-0.656298
H	-0.749691	2.651532	1.656113
H	2.651288	3.528431	2.722785
H	1.094421	2.933263	3.345345
H	2.261133	1.816775	2.579014
H	1.954962	5.061964	1.363795
H	0.207175	4.895402	1.662437
H	0.866591	4.780497	0.011066
H	-5.205671	-0.393141	-2.330004
H	-4.995563	-2.863192	1.184441
H	-3.280672	1.076421	1.223697
C	5.327941	-1.578944	0.035503
O	5.180299	-2.414975	-1.108757
C	6.477662	-2.195967	-0.667530
N	7.032689	-3.410408	0.040970
O	6.238185	-4.175366	0.545895
O	8.243225	-3.517588	0.075317
C	7.472919	-1.503718	-1.544993
H	6.997390	-0.628851	-1.989964
H	7.806488	-2.176956	-2.338291
H	8.339506	-1.189947	-0.962816
C	4.991176	-0.136953	-0.109781
C	4.327267	2.565134	-0.322811
C	5.075504	0.696060	1.008486
C	4.576717	0.386073	-1.334725
C	4.246058	1.735331	-1.438734
C	4.751817	2.044259	0.899014
H	5.391907	0.285633	1.964364
H	4.496521	-0.273212	-2.194386
H	3.909888	2.134772	-2.391132
H	4.819239	2.686962	1.771056
H	4.049667	3.611889	-0.399602
H	5.027569	-2.061542	0.965155

SR epoxide:Catalyst, binary complex 77; Energy = -2449.838509; 6-31G(d) basis set.

N	1.374111	2.634871	0.945661
C	0.446628	3.594727	0.729537
S	0.722618	5.208490	1.080302
C	1.598511	1.457872	0.095532
C	2.414118	1.803715	-1.190308
C	3.905265	1.471894	-0.992678
C	4.366223	1.762820	0.435778
C	3.666747	0.817194	1.432625
C	2.298367	0.369530	0.897978
N	1.846650	1.063414	-2.328806
C	0.540833	1.596102	-2.710125
N	-0.757913	3.198756	0.187988
C	-1.494958	2.025976	0.446016
C	-2.610233	1.771836	-0.357809
C	-3.385167	0.642031	-0.134834
C	-3.067851	-0.268672	0.865494

C	-1.951504	-0.010982	1.649534
C	-1.175329	1.128901	1.468480
C	-4.555154	0.405751	-1.047989
F	-5.440584	1.409205	-0.982631
C	-1.569005	-0.957495	2.753037
F	-2.212383	-2.125526	2.665269
C	2.709681	1.102800	-3.508763
F	-4.160114	0.327186	-2.332798
F	-5.201887	-0.729582	-0.760352
F	-0.246692	-1.223066	2.728847
F	-1.830434	-0.439793	3.959781
H	2.204310	3.008957	1.391969
H	-1.316713	3.991606	-0.105848
H	1.652215	0.006114	1.703386
H	2.429771	-0.452496	0.188672
H	4.281309	-0.074180	1.598591
H	3.553076	1.300781	2.409027
H	5.451105	1.647939	0.506905
H	4.161674	2.815973	0.673492
H	4.065604	0.405235	-1.197562
H	4.509020	2.035149	-1.710070
H	0.626652	1.074797	-0.207423
H	2.319675	2.894335	-1.365886
H	2.213650	0.568947	-4.323422
H	2.909062	2.135820	-3.845648
H	3.662434	0.609154	-3.316346
H	0.595374	2.662893	-2.991543
H	-0.189621	1.496093	-1.902178
H	0.163881	1.031996	-3.568527
H	-2.862491	2.456323	-1.163968
H	-3.658366	-1.164461	1.012321
H	-0.323269	1.318224	2.113307
C	1.151996	-2.788700	0.319633
O	1.811480	-4.053583	0.161649
C	2.424391	-2.948041	-0.407014
N	3.630430	-2.495821	0.392479
O	4.514418	-1.925912	-0.221272
O	3.619736	-2.688684	1.589348
C	2.627892	-2.860085	-1.889348
H	1.755513	-3.297361	-2.376493
H	3.524295	-3.410125	-2.182997
H	2.729767	-1.815695	-2.198661
C	-0.139061	-2.586967	-0.402824
C	-2.564941	-2.279951	-1.743921
C	-1.200858	-3.453325	-0.136917
C	-0.298555	-1.549221	-1.325995
C	-1.514192	-1.397817	-1.990707
C	-2.409152	-3.303650	-0.811558
H	-1.070194	-4.252694	0.587161
H	0.532042	-0.876497	-1.544555
H	-1.642768	-0.591159	-2.706592
H	-3.227571	-3.988629	-0.612150
H	-3.507170	-2.161671	-2.269521
H	1.218546	-2.417597	1.340509

SR epoxide:Catalyst, binary complex 78; Energy = -2449.845756; 6-31G(d) basis set.

N	2.961714	-1.555896	-0.158881
C	2.964229	-2.016283	1.112262
S	4.247014	-2.892623	1.748924
C	2.380082	-0.277338	-0.607111
C	3.461145	0.854001	-0.631755
C	3.883141	1.180007	-2.072288
C	4.076433	-0.116057	-2.862006
C	2.736767	-0.859054	-3.047745
C	1.722176	-0.443621	-1.974382
N	2.944863	2.017351	0.105839
C	3.002910	1.750053	1.542348
N	1.868839	-1.730474	1.891556
C	0.517681	-1.638792	1.485065
C	-0.366613	-0.915146	2.288782
C	-1.709451	-0.844738	1.942993
C	-2.192448	-1.452696	0.787568
C	-1.300280	-2.164213	-0.003558
C	0.042285	-2.283770	0.343675
C	-2.658860	-0.090209	2.831106

F	-2.054379	0.942864	3.435442
C	-1.771660	-2.848521	-1.257046
F	-1.492255	-4.158885	-1.231372
C	3.692729	3.243557	-0.158972
F	-3.692412	0.408545	2.130142
F	-3.174340	-0.865994	3.793430
F	-3.087855	-2.713306	-1.445147
F	-1.161149	-2.352906	-2.353115
H	3.795116	-1.849095	-0.658091
H	2.016515	-1.960693	2.867208
H	0.898400	-1.159382	-1.914397
H	1.275897	0.524001	-2.231734
H	2.318814	-0.641567	-4.035680
H	2.895848	-1.942454	-3.014103
H	4.535101	0.095351	-3.831879
H	4.798614	-0.745713	-2.323600
H	3.119946	1.799319	-2.562324
H	4.810043	1.760277	-2.064667
H	1.616442	0.010446	0.111534
H	4.363721	0.465977	-0.117281
H	3.600415	3.540383	-1.205723
H	3.269917	4.043669	0.453623
H	4.765394	3.144433	0.085877
H	4.039113	1.566687	1.877815
H	2.398107	0.876243	1.802687
H	2.602766	2.608087	2.088768
H	0.004219	-0.390663	3.164450
H	-3.234532	-1.361613	0.502311
H	0.717092	-2.872282	-0.270627
C	-1.587893	1.712015	0.024728
O	-0.333750	1.048832	-0.109776
C	-0.321972	2.425579	-0.276709
N	0.267946	3.097588	0.939756
O	0.154009	2.517121	2.000693
O	0.782181	4.187570	0.782709
C	0.084630	3.046979	-1.573073
H	-0.225363	4.092277	-1.606960
H	-0.394161	2.500798	-2.388155
H	1.171705	2.991378	-1.669856
C	-2.624018	1.388655	-0.989843
C	-4.616942	0.683423	-2.805571
C	-2.328350	0.538282	-2.056521
C	-3.922155	1.873829	-0.824578
C	-4.913119	1.530342	-1.738506
C	-3.325917	0.182248	-2.958792
H	-1.323440	0.137284	-2.153062
H	-4.157326	2.509375	0.025244
H	-5.920544	1.913320	-1.610414
H	-3.095346	-0.498647	-3.772292
H	-5.395307	0.404913	-3.509112
H	-1.928114	1.797649	1.055897

SR epoxide:Catalyst, binary complex 79; Energy = -2449.839643; 6-31G(d) basis set.

N	-0.694454	1.371545	1.355320
C	-1.693653	2.207814	1.667596
S	-1.555366	3.841006	2.056192
C	0.667803	1.707894	0.927514
C	0.668261	2.590618	-0.336178
C	2.115889	2.846502	-0.782315
C	2.954313	3.459513	0.340180
C	2.953162	2.542940	1.564686
C	1.524359	2.299344	2.053024
N	-0.203289	2.011398	-1.364887
C	0.393264	0.900053	-2.093967
N	-2.942408	1.625989	1.721929
C	-3.421460	0.545338	0.954219
C	-2.937680	0.281415	-0.331483
C	-3.503573	-0.757832	-1.064705
C	-4.543167	-1.529182	-0.561201
C	-5.016540	-1.246810	0.716350
C	-4.462915	-0.226710	1.477127
C	-2.962650	-1.038236	-2.439325
F	-2.745015	0.097935	-3.122646
C	-6.102699	-2.103974	1.305196
F	-6.813193	-1.440910	2.227407

C	-0.726705	3.008412	-2.285984
F	-1.788419	-1.685953	-2.383292
F	-3.799292	-1.791405	-3.162891
F	-6.953778	-2.535407	0.364944
F	-5.595828	-3.192346	1.904451
H	-0.961191	0.406915	1.199027
H	-3.640377	2.219683	2.153125
H	1.081498	3.241652	2.387912
H	1.512762	1.609957	2.904461
H	3.415613	1.581685	1.296102
H	3.552658	2.976079	2.372322
H	3.978450	3.639956	-0.007610
H	2.538137	4.437118	0.617862
H	2.571407	1.892075	-1.081425
H	2.120561	3.487517	-1.671883
H	1.112210	0.740827	0.660699
H	0.221554	3.551332	-0.054849
H	0.049955	3.463265	-2.925659
H	-1.463773	2.533231	-2.941330
H	-1.226377	3.801873	-1.722512
H	-0.375422	0.410566	-2.696893
H	0.798300	0.155700	-1.400931
H	1.203062	1.212096	-2.776240
H	-2.142751	0.900010	-0.756573
H	-4.985763	-2.320800	-1.154935
H	-4.838703	-0.019206	2.474138
C	3.966153	-1.765145	-0.365946
O	3.117547	-0.656932	-0.055598
C	4.105330	-0.442658	-1.015516
N	3.491270	-0.362714	-2.398101
O	3.924766	0.492870	-3.144040
O	2.604076	-1.147492	-2.663517
C	5.196066	0.555032	-0.782533
H	4.812880	1.574018	-0.873361
H	5.993789	0.415614	-1.514180
H	5.597035	0.404815	0.220923
C	4.915794	-2.230590	0.681092
C	6.718097	-3.155140	2.595248
C	5.726660	-3.332813	0.404242
C	4.999485	-1.598426	1.921875
C	5.900703	-2.062791	2.876499
C	6.629658	-3.790374	1.358008
H	5.648171	-3.831860	-0.558330
H	4.348735	-0.755449	2.137419
H	5.961186	-1.573047	3.843311
H	7.259558	-4.646138	1.137062
H	7.419008	-3.515993	3.341308
H	3.470713	-2.533059	-0.956584

SR epoxide:Catalyst, binary complex 80; Energy = -2449.838168; 6-31G(d) basis set.

N	-2.469540	-1.471551	1.346223
C	-2.027078	-2.755145	1.319243
S	-2.910180	-4.031686	1.943433
C	-2.319597	-0.566605	0.198334
C	-3.331119	-0.954811	-0.898529
C	-3.567793	0.252081	-1.819228
C	-4.306490	1.365789	-1.045123
C	-3.906794	1.404544	0.446472
C	-2.472047	0.905879	0.609501
N	-2.933627	-2.214134	-1.519136
C	-4.044969	-2.899653	-2.157495
N	-0.780446	-2.971109	0.776757
C	0.360837	-2.154513	0.818525
C	0.468029	-1.030528	1.650504
C	1.651493	-0.306266	1.672173
C	2.750318	-0.666165	0.894097
C	2.632475	-1.783228	0.081283
C	1.453075	-2.520268	0.029591
C	1.781494	0.862237	2.611406
F	0.582223	1.333929	2.990377
C	3.793224	-2.257234	-0.748403
F	4.772808	-1.349171	-0.821915
C	-1.793836	-2.116172	-2.414197
F	2.448117	0.532635	3.724125
F	2.450277	1.878361	2.041113

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F          4.325485       -3.378724       -0.239422
F          3.412281       -2.550288       -2.003855
H         -3.373305       -1.404757        1.805571
H         -0.601741       -3.952208        0.600610
H         -2.089795        1.057635        1.625295
H         -1.841977        1.500999       -0.062197
H         -3.988832        2.423753        0.834906
H         -4.585089        0.783022        1.044874
H         -4.084759        2.335082       -1.502989
H         -5.387654        1.214385       -1.130282
H         -2.603234        0.623179       -2.193586
H         -4.144416       -0.047596       -2.701009
H         -1.310008       -0.708480       -0.188842
H         -4.284853       -1.165834       -0.391929
H         -1.523038       -3.122430       -2.748534
H         -1.986167       -1.501281       -3.310981
H         -0.922840       -1.704807       -1.890842
H         -4.445498       -2.365495       -3.037205
H         -4.853251       -3.036192       -1.433621
H         -3.715292       -3.889211       -2.487426
H         -0.363949       -0.739095        2.280915
H          3.662908       -0.081210        0.911427
H          1.379399       -3.382630       -0.627811
C          0.517554        2.638218        0.005058
O          0.861493        3.969398        0.370402
C         -0.249433        3.816645       -0.448449
N         -1.548584        3.993792        0.297343
O         -2.529881        4.241312       -0.380206
O         -1.542603        3.822751        1.497459
C         -0.255663        4.381728       -1.834630
H          0.737499        4.238679       -2.263076
H         -0.491820        5.447909       -1.812367
H         -0.995182        3.868964       -2.451849
C          1.412104        1.900433       -0.927163
C          3.074187        0.429706       -2.608027
C          2.760710        2.234379       -1.034092
C          0.892294        0.837191       -1.668175
C          1.722635        0.102008       -2.507315
C          3.590199        1.495468       -1.874495
H          3.149305        3.062614       -0.449013
H         -0.167158        0.595583       -1.595489
H          1.319814       -0.730447       -3.077379
H          4.643641        1.746590       -1.950541
H          3.725891       -0.155669       -3.248404
H          0.082026        2.074270        0.828290

SR epoxide:Catalyst, binary complex 81; Energy = -2449.840828; 6-31G(d) basis set.
N          2.584557        0.273829       -0.448448
C          1.527286        0.256565       -1.282623
S          1.521536       -0.528101       -2.765253
C          3.855526       -0.399406       -0.675753
C          5.008111        0.435548       -0.085328
C          6.333088       -0.306979       -0.307930
C          6.306464       -1.720580        0.277529
C          5.152393       -2.535386       -0.307992
C          3.821929       -1.815751       -0.089757
N          5.100538        1.813111       -0.569425
C          4.314518        2.791649        0.156213
N          0.472573        0.991701       -0.790210
C         -0.901408        0.885409       -1.056223
C         -1.504944       -0.256986       -1.586047
C         -2.889155       -0.354886       -1.595858
C         -3.707279        0.670414       -1.137191
C         -3.093804        1.825128       -0.670641
C         -1.710020        1.942645       -0.634434
C         -3.474537       -1.689659       -1.954318
F         -2.904106       -2.214781       -3.045460
C         -3.904719        2.955035       -0.106738
F         -3.777366        3.016128        1.234378
C          4.936774        1.968651       -2.005113
F         -3.269811       -2.571522       -0.951593
F         -4.792979       -1.631512       -2.165574
F         -3.496732        4.142267       -0.578710
F         -5.207396        2.832717       -0.375835
H          2.431758        0.620857        0.495429
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H          0.684453        1.600745       -0.003296
H          3.610167       -1.743608        0.988320
H          2.992262       -2.363211       -0.551144
H          5.312804       -2.672858       -1.385589
H          5.117429       -3.534358        0.138325
H          7.262482       -2.220548        0.091386
H          6.187836       -1.658990        1.368443
H          6.535573       -0.368168       -1.385845
H          7.135613        0.290539        0.134140
H          3.981481       -0.470866       -1.760803
H          4.849375        0.498031        1.003557
H          3.896810        1.819584       -2.346037
H          5.244078        2.979824       -2.289852
H          5.577416        1.263152       -2.541060
H          4.673595        3.795921       -0.094334
H          4.449548        2.647357        1.233412
H          3.232730        2.763963       -0.070027
H         -0.900159       -1.078356       -1.946840
H         -4.785687        0.568488       -1.134914
H         -1.253461        2.851724       -0.251327
C         -1.438282       -0.874281        2.513196
O         -2.236280       -0.872322        1.327287
C         -1.428555       -1.980443        1.537354
N         -2.249535       -3.176448        1.969468
O         -1.781713       -4.272773        1.734388
O         -3.298265       -2.956922        2.536116
C         -0.317279       -2.332764        0.595555
H          0.380537       -3.021752        1.074514
H          0.210496       -1.417422        0.319833
H         -0.719258       -2.811737       -0.299386
C         -0.342243        0.140340        2.562389
C          1.646579        2.099623        2.670578
C          0.982334       -0.221004        2.810433
C         -0.672912        1.486009        2.379874
C          0.319817        2.462454        2.426963
C          1.975237        0.758435        2.871330
H          1.238488       -1.266800        2.960145
H         -1.706593        1.761787        2.189088
H          0.058433        3.507362        2.288444
H          3.003623        0.473721        3.078132
H          2.416627        2.862899        2.722320
H         -2.023907       -1.025233        3.419347

SR epoxide:Catalyst, binary complex 82; Energy = -2449.845785; 6-31G(d) basis set.
N         -1.803187       -1.018472        0.428171
C         -0.605773       -1.596734        0.195300
S         -0.416084       -2.954244       -0.772765
C         -3.094730       -1.528830       -0.012833
C         -4.144831       -1.318850        1.096428
C         -5.506056       -1.830696        0.607632
C         -5.935028       -1.157141       -0.697115
C         -4.887836       -1.367437       -1.791347
C         -3.516807       -0.872483       -1.332156
N         -3.813224       -1.902514        2.396175
C         -3.313378       -3.266052        2.345406
N          0.409782       -0.952454        0.866631
C          1.780448       -0.835975        0.582276
C          2.524676       -1.719362       -0.201681
C          3.871804       -1.446327       -0.439941
C          4.505290       -0.332402        0.085239
C          3.756499        0.528776        0.884723
C          2.419207        0.284819        1.140653
C          4.644051       -2.437113       -1.267488
F          3.986636       -2.755393       -2.391303
C          4.420003        1.765279        1.425791
F          5.602965        1.468357        1.988665
C         -2.993809       -1.086098        3.272143
F          5.847292       -1.966203       -1.621124
F          4.844166       -3.581926       -0.597115
F          4.665976        2.650403        0.452040
F          3.674253        2.375632        2.354354
H         -1.803754       -0.072958        0.804316
H          0.087630       -0.209734        1.478031
H         -3.549545        0.217552       -1.188726
H         -2.749713       -1.087092       -2.085796
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H	-4.824530	-2.436796	-2.034012
H	-5.180345	-0.847781	-2.710210
H	-6.908023	-1.543978	-1.018111
H	-6.059881	-0.079161	-0.523326
H	-5.451163	-2.916432	0.449284
H	-6.238598	-1.661012	1.402386
H	-2.962140	-2.602623	-0.180019
H	-4.244534	-0.233510	1.255847
H	-3.344031	-0.048869	3.248374
H	-3.094519	-1.450903	4.300615
H	-1.917753	-1.101590	3.023881
H	-3.314975	-3.682638	3.357859
H	-2.284341	-3.340482	1.950020
H	-3.963315	-3.891423	1.727524
H	2.063717	-2.602190	-0.622700
H	5.552161	-0.135963	-0.116640
H	1.855278	0.984887	1.751692
C	-0.907544	2.887130	-0.106728
O	-0.367177	1.769791	0.615291
C	0.122463	1.995278	-0.675097
N	1.522209	2.573803	-0.617533
O	2.258096	2.316299	-1.545849
O	1.802465	3.251323	0.350298
C	-0.067809	0.980551	-1.760360
H	-1.074097	0.564987	-1.678795
H	0.667526	0.176648	-1.672406
H	0.053971	1.450382	-2.737976
C	-2.343038	2.779525	-0.498720
C	-5.044580	2.628597	-1.168813
C	-2.744818	2.963187	-1.821564
C	-3.295958	2.524509	0.490737
C	-4.645161	2.451361	0.155242
C	-4.094793	2.883048	-2.155733
H	-2.002515	3.164951	-2.589342
H	-2.977272	2.392018	1.522589
H	-5.384442	2.255686	0.926447
H	-4.403738	3.019306	-3.187047
H	-6.096569	2.568111	-1.430151
H	-0.555816	3.839484	0.286994

SR epoxide:Catalyst, binary complex 83; Energy = -2449.834999; 6-31G(d) basis set.

N	-3.204073	-1.435354	0.629653
C	-3.240353	-2.011588	-0.598960
S	-4.589872	-2.820100	-1.176499
C	-2.625077	-0.104122	0.875745
C	-3.660886	0.957651	0.448253
C	-3.372767	2.278933	1.171672
C	-3.614694	2.122162	2.686574
C	-3.304295	0.693612	3.178807
C	-2.189260	0.061498	2.343514
N	-3.729633	0.993058	-1.009328
C	-5.034894	1.391591	-1.506342
N	-2.094203	-1.948165	-1.354107
C	-0.756727	-1.944426	-0.925606
C	0.240895	-1.712865	-1.877420
C	1.580241	-1.749558	-1.506595
C	1.964628	-1.983790	-0.191893
C	0.961378	-2.191599	0.747401
C	-0.382331	-2.199558	0.397414
C	2.612458	-1.522273	-2.576090
F	2.526888	-2.457320	-3.536674
C	1.306700	-2.323787	2.203684
F	0.448880	-3.129502	2.848292
C	-2.677886	1.781968	-1.629719
F	2.431724	-0.337721	-3.189838
F	3.858155	-1.546638	-2.099096
F	2.538095	-2.797986	2.395379
F	1.234076	-1.124229	2.818257
H	-4.075285	-1.594536	1.126952
H	-2.244327	-2.234555	-2.313712
H	-1.884242	-0.907404	2.753055
H	-1.301921	0.706617	2.377851
H	-3.027507	0.707198	4.236843
H	-4.204344	0.068887	3.108761
H	-2.991154	2.841807	3.228085

H	-4.654795	2.369081	2.924494
H	-2.331565	2.565038	0.979023
H	-3.998626	3.080384	0.762453
H	-1.751110	-0.002575	0.229955
H	-4.644740	0.603171	0.789134
H	-2.664554	1.580172	-2.705823
H	-2.813605	2.867984	-1.488167
H	-1.692805	1.518315	-1.226842
H	-5.300833	2.433454	-1.250842
H	-5.801818	0.723507	-1.104377
H	-5.046105	1.300904	-2.596700
H	-0.032842	-1.507464	-2.909187
H	3.007450	-1.962872	0.098884
H	-1.136114	-2.404676	1.147386
C	2.055153	1.296678	0.326933
O	3.061834	0.703651	-0.488101
C	3.500674	1.574465	0.499073
N	4.122892	0.834584	1.657716
O	4.871322	1.473935	2.369741
O	3.813418	-0.328371	1.816950
C	4.214608	2.838527	0.134292
H	5.252434	2.622374	-0.129328
H	4.201902	3.537623	0.971087
H	3.708776	3.284874	-0.722949
C	1.172739	2.310766	-0.315277
C	-0.372091	4.315970	-1.482866
C	0.381714	3.139119	0.484687
C	1.172517	2.471378	-1.701377
C	0.395910	3.471681	-2.281843
C	-0.383122	4.144667	-0.099379
H	0.381727	3.009579	1.564832
H	1.782940	1.812783	-2.311131
H	0.396901	3.595836	-3.360257
H	-0.987263	4.794971	0.526199
H	-0.967813	5.101746	-1.937129
H	1.609963	0.604781	1.044208

SR epoxide:Catalyst, binary complex 84; Energy = -2449.834525; 6-31G(d) basis set.

N	3.033869	-0.556288	-0.627956
C	1.732180	-0.863643	-0.454199
S	1.010838	-2.108468	-1.330383
C	3.875013	0.200483	0.295483
C	5.328638	-0.282243	0.132627
C	6.177660	0.268222	1.300686
C	5.685938	1.649240	1.773871
C	5.093190	2.433429	0.601995
C	3.839667	1.725323	0.046315
N	5.395039	-1.724524	-0.092379
C	4.885831	-2.543918	0.998862
N	1.086018	-0.066641	0.451404
C	-0.249250	-0.108378	0.890727
C	-0.964823	-1.293672	1.069273
C	-2.264152	-1.237003	1.566829
C	-2.866490	-0.031550	1.900072
C	-2.139496	1.142583	1.714051
C	-0.846418	1.114632	1.214974
C	-2.994904	-2.531353	1.806363
F	-2.665549	-3.048449	3.004455
C	-2.827321	2.454853	1.958506
F	-1.991543	3.495598	1.852861
C	6.724434	-2.155898	-0.494786
F	-4.320967	-2.360315	1.806266
F	-2.686798	-3.450235	0.887774
F	-3.818485	2.645878	1.069269
F	-3.386698	2.500495	3.174700
H	3.548234	-1.245600	-1.173901
H	1.563256	0.793673	0.692159
H	3.758275	1.884460	-1.033695
H	2.942780	2.171160	0.496725
H	4.840851	3.454146	0.902430
H	5.850584	2.519925	-0.186098
H	4.920803	1.531943	2.551266
H	6.509108	2.203604	2.233646
H	6.155543	-0.439030	2.137338
H	7.219935	0.336979	0.971138

H	3.543599	-0.016607	1.322351
H	5.695347	0.166708	-0.802680
H	7.467314	-2.081835	0.317117
H	6.680936	-3.199467	-0.819437
H	7.068876	-1.547016	-1.336332
H	5.504658	-2.500924	1.909793
H	4.852589	-3.584380	0.664123
H	3.864335	-2.247675	1.254999
H	-0.518985	-2.246947	0.817507
H	-3.886476	-0.003511	2.269016
H	-0.313288	2.044957	1.036112
C	-2.451361	0.525603	-1.668920
O	-3.505461	0.331946	-2.623389
C	-2.537353	-0.660245	-2.535473
N	-3.044951	-1.879056	-1.789565
O	-2.507467	-2.937885	-2.037618
O	-3.933365	-1.707393	-0.977451
C	-1.725057	-0.996946	-3.748369
H	-0.824554	-1.547435	-3.472988
H	-1.454377	-0.064583	-4.246089
H	-2.323494	-1.606901	-4.429811
C	-1.473333	1.636057	-1.855401
C	0.380593	3.722983	-1.896448
C	-0.138927	1.380690	-2.171447
C	-1.879128	2.941817	-1.564852
C	-0.954964	3.981319	-1.585737
C	0.784985	2.423798	-2.194550
H	0.182192	0.361203	-2.371397
H	-2.914688	3.135404	-1.299963
H	-1.274230	4.992304	-1.352618
H	1.820256	2.214791	-2.447475
H	1.101621	4.534894	-1.909344
H	-2.814445	0.389642	-0.651259

SR epoxide:Catalyst, binary complex 85; Energy = -2449.829936; 6-31G(d) basis set.

N	3.605709	0.496745	0.440964
C	3.514843	0.176382	1.754184
S	4.799094	0.332278	2.819213
C	2.561582	1.238576	-0.296769
C	2.587331	2.756533	0.109051
C	3.285380	3.609443	-0.959020
C	4.526105	2.886428	-1.485865
C	4.138041	1.600896	-2.251796
C	2.777101	1.045860	-1.794943
N	1.288245	3.311396	0.483391
C	0.266990	3.248919	-0.549127
N	2.295469	-0.278156	2.194067
C	1.376207	-1.087630	1.494282
C	1.726254	-1.819480	0.358297
C	0.779955	-2.632390	-0.254352
C	-0.509760	-2.760856	0.248006
C	-0.841158	-2.035234	1.387430
C	0.080258	-1.196726	2.004047
C	1.215820	-3.386850	-1.481300
F	1.638948	-2.555405	-2.444331
C	-2.200767	-2.157085	2.018341
F	-3.031035	-2.925538	1.312951
C	0.779455	2.754775	1.723874
F	2.249078	-4.199056	-1.197847
F	0.238685	-4.144716	-1.986747
F	-2.111184	-2.684948	3.250362
F	-2.780820	-0.950019	2.170614
H	4.551772	0.774771	0.201181
H	2.242028	-0.338998	3.204121
H	2.665349	-0.011377	-2.056419
H	1.964301	1.575784	-2.304913
H	4.088805	1.808820	-3.325208
H	4.916941	0.839916	-2.128191
H	5.108930	3.548500	-2.132430
H	5.181428	2.650754	-0.635355
H	2.612047	3.814740	-1.799306
H	3.542821	4.576554	-0.517758
H	1.592417	0.813270	-0.025683
H	3.203946	2.823327	1.016523
H	-0.090965	3.333665	2.049060

H	0.465266	1.696217	1.636723
H	1.548167	2.813971	2.500833
H	0.602224	3.748586	-1.461340
H	-0.620288	3.779236	-0.187875
H	-0.034134	2.216944	-0.809138
H	2.730218	-1.752373	-0.047126
H	-1.240100	-3.395246	-0.240506
H	-0.201374	-0.631748	2.889059
C	-2.531687	0.534154	-0.363164
O	-2.937247	-0.836796	-0.521282
C	-2.453131	-0.169371	-1.645481
N	-1.091368	-0.707803	-2.019099
O	-1.094089	-1.735340	-2.664365
O	-0.099014	-0.115920	-1.637775
C	-3.342460	0.004985	-2.836903
H	-4.307704	0.381710	-2.495318
H	-3.478649	-0.956553	-3.335297
H	-2.905258	0.719431	-3.539411
C	-3.615761	1.525930	-0.106027
C	-5.622742	3.391925	0.389746
C	-3.504280	2.822119	-0.611955
C	-4.735528	1.159882	0.639375
C	-5.737041	2.095545	0.886571
C	-4.506173	3.754629	-0.361863
H	-2.640108	3.093701	-1.213097
H	-4.812368	0.145768	1.018564
H	-6.608582	1.810753	1.467500
H	-4.419315	4.760616	-0.760057
H	-6.405474	4.118975	0.582220
H	-1.603484	0.641979	0.200505

SR epoxide:Catalyst, binary complex 86; Energy = -2449.830529; 6-31G(d) basis set.

N	-0.420530	3.335781	-0.119150
C	0.542163	3.729587	-0.984034
S	0.693653	5.318041	-1.497721
C	-1.142062	2.050501	-0.159492
C	-2.323768	2.168370	0.843928
C	-3.537315	2.694631	0.068860
C	-4.040004	1.660787	-0.953647
C	-2.877308	0.844802	-1.544339
C	-1.606368	1.694891	-1.589091
N	-2.602151	0.888729	1.502911
C	-3.789947	0.982500	2.342698
N	1.399634	2.765010	-1.456749
C	1.944288	1.658468	-0.774954
C	1.926062	1.537716	0.619330
C	2.549985	0.449248	1.221038
C	3.204779	-0.522569	0.472937
C	3.217936	-0.388646	-0.910098
C	2.598018	0.686283	-1.537128
C	2.568088	0.383328	2.726018
F	3.203780	1.450869	3.236893
C	3.874582	-1.434947	-1.768599
F	4.611670	-2.285947	-1.053481
C	-1.481854	0.439843	2.320844
F	1.330156	0.396154	3.242851
F	3.187207	-0.709038	3.177161
F	2.961258	-2.159739	-2.441034
F	4.668720	-0.874314	-2.692933
H	-0.977480	4.124345	0.193315
H	1.958500	3.099382	-2.233401
H	-1.798901	2.622222	-2.144868
H	-0.797878	1.177339	-2.117442
H	-2.703811	-0.032463	-0.910932
H	-3.128273	0.482701	-2.546622
H	-4.753307	0.976627	-0.483046
H	-4.578153	2.186612	-1.750187
H	-4.337275	3.008947	0.744201
H	-3.217685	3.605688	-0.453763
H	-0.467973	1.270158	0.192833
H	-2.032212	2.913439	1.613912
H	-1.772328	-0.463156	2.865779
H	-0.612850	0.169170	1.718444
H	-1.165346	1.198911	3.059544
H	-3.714495	1.792478	3.091965

H	-3.922462	0.039620	2.880598
H	-4.685040	1.148055	1.739821
H	1.444007	2.298615	1.226957
H	3.675873	-1.369884	0.955786
H	2.620105	0.774196	-2.620215
C	-1.449975	-3.212398	0.383492
O	-0.600067	-3.906416	-0.551669
C	-0.212445	-2.637662	-0.156830
N	0.990425	-2.665731	0.749238
O	0.917364	-2.046378	1.794673
O	1.971504	-3.243998	0.330390
C	-0.070461	-1.532524	-1.157941
H	0.146094	-0.595448	-0.634517
H	-1.001282	-1.424013	-1.717868
H	0.752020	-1.760272	-1.839739
C	-2.787596	-2.781375	-0.106808
C	-5.272383	-1.894433	-1.007703
C	-3.150177	-2.958473	-1.442934
C	-3.677341	-2.175393	0.780576
C	-4.916323	-1.731600	0.330078
C	-4.390492	-2.512753	-1.891294
H	-2.459836	-3.452905	-2.119926
H	-3.398159	-2.052862	1.824059
H	-5.606311	-1.261821	1.024988
H	-4.669767	-2.653634	-2.930787
H	-6.238889	-1.545968	-1.358594
H	-1.403001	-3.607889	1.397774

SR epoxide:Catalyst, binary complex 87; Energy = -2449.839403; 6-31G(d) basis set.

N	-1.283552	-1.027982	-1.059023
C	-0.689720	-1.365349	-2.215424
S	-1.513460	-1.861227	-3.601859
C	-2.737758	-0.980744	-0.891308
C	-3.137726	-1.267572	0.576067
C	-4.597152	-0.794361	0.810329
C	-5.425205	-0.703330	-0.473376
C	-4.829700	0.351776	-1.420239
C	-3.293252	0.381752	-1.324235
N	-2.972985	-2.641487	1.049104
C	-3.734400	-3.637501	0.316961
N	0.682345	-1.280560	-2.276668
C	1.629197	-1.114435	-1.249991
C	2.815123	-0.426932	-1.538312
C	3.778113	-0.267958	-0.553183
C	3.580910	-0.756039	0.738047
C	2.406790	-1.441043	1.006597
C	1.446846	-1.649268	0.022521
C	5.053792	0.472400	-0.851223
F	5.301014	1.405290	0.073953
C	2.091571	-1.934661	2.389479
F	3.170388	-1.958426	3.178360
C	-1.604840	-3.077046	1.242288
F	6.105117	-0.364790	-0.851028
F	5.022115	1.070957	-2.046818
F	1.173788	-1.152556	2.982006
F	1.573407	-3.173356	2.360066
H	-0.738432	-0.531592	-0.353759
H	1.042052	-1.429179	-3.211632
H	-2.974775	1.129751	-0.583356
H	-2.850448	0.657909	-2.287176
H	-5.135246	0.139227	-2.449782
H	-5.221028	1.343379	-1.166744
H	-5.448894	-1.677485	-0.976142
H	-6.464282	-0.456149	-0.233573
H	-5.054463	-1.468008	1.541276
H	-4.575438	0.200666	1.267752
H	-3.142533	-1.754567	-1.548916
H	-2.477807	-0.653693	1.209275
H	-1.096611	-3.353860	0.301415
H	-1.030438	-2.287015	1.739673
H	-1.593437	-3.958953	1.892557
H	-3.650421	-4.597016	0.837064
H	-3.382450	-3.788385	-0.719388
H	-4.793039	-3.366241	0.290152
H	2.970749	0.000496	-2.524096

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H          4.320500       -0.588124        1.513176
H          0.564158       -2.233114        0.248216
C         -0.133389        2.384441        1.146200
O          0.177220        1.026616        0.775083
C          0.640223        2.040877       -0.061435
N          2.132936        2.238626        0.104022
O          2.750738        2.606531       -0.876439
O          2.606623        2.015563        1.197113
C          0.180341        2.103622       -1.486796
H         -0.894242        1.914645       -1.515924
H          0.693096        1.345615       -2.083811
H          0.393119        3.082955       -1.918223
C         -1.564598        2.799408        1.094316
C         -4.253484        3.538600        1.064888
C         -2.458961        2.222961        1.999817
C         -2.015231        3.764044        0.193040
C         -3.360520        4.124960        0.171694
C         -3.799410        2.596786        1.987518
H         -2.101103        1.484792        2.713281
H         -1.316753        4.231618       -0.495013
H         -3.708924        4.866985       -0.539419
H         -4.490035        2.154880        2.699026
H         -5.301033        3.822851        1.050950
H          0.447829        2.701008        2.010483

SR epoxide:Catalyst, binary complex 88; Energy = -2449.829887; 6-31G(d) basis set.
N         -1.703267       -0.762387        0.226358
C         -1.490496       -0.441743        1.511136
S         -2.640027        0.114612        2.611033
C         -2.936730       -0.658431       -0.578971
C         -4.131322       -1.484438       -0.070017
C         -5.323010       -1.231517       -1.012984
C         -5.698057        0.241551       -1.149651
C         -4.503067        1.027762       -1.681103
C         -3.302811        0.822415       -0.763820
N         -3.929516       -2.946083       -0.015300
C         -2.585636       -3.483660        0.073496
N         -0.194936       -0.583771        1.963683
C          0.945298       -1.040977        1.277822
C          2.149565       -0.348512        1.421832
C          3.275450       -0.768879        0.721095
C          3.228721       -1.864877       -0.131991
C          2.034225       -2.571187       -0.235580
C          0.905556       -2.188338        0.476804
C          4.566053       -0.018055        0.911165
F          5.417053       -0.230788       -0.095400
C          1.979528       -3.765127       -1.149930
F          2.981706       -4.616289       -0.899326
C         -4.750786       -3.525692        1.037148
F          4.345949        1.302611        0.997329
F          5.179669       -0.385910        2.044910
F          0.828115       -4.438754       -1.025729
F          2.092569       -3.394365       -2.433407
H         -0.879245       -0.986709       -0.317341
H         -0.053014       -0.173843        2.878856
H         -3.522852        1.240171        0.223070
H         -2.422834        1.357735       -1.142809
H         -4.263946        0.684231       -2.697293
H         -4.726978        2.098142       -1.748982
H         -6.561887        0.348269       -1.814385
H         -5.993034        0.642534       -0.170504
H         -5.056204       -1.639334       -1.997755
H         -6.178622       -1.815629       -0.659152
H         -2.649467       -1.070888       -1.555923
H         -4.377386       -1.100622        0.930861
H         -5.783552       -3.178581        0.949592
H         -4.753934       -4.616078        0.942420
H         -4.385490       -3.263154        2.046326
H         -2.651497       -4.572012       -0.028851
H         -2.078421       -3.270069        1.033106
H         -1.960687       -3.124086       -0.749296
H          2.191013        0.542613        2.040439
H          4.104405       -2.164144       -0.697906
H          0.004145       -2.788969        0.428741
C          1.187224        3.531179       -0.185718
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O          1.698897        2.515590        0.677948
C          1.727324        2.253068       -0.690918
N          3.148894        2.307271       -1.204055
O          3.826164        3.257504       -0.879343
O          3.521086        1.370286       -1.884751
C          0.904398        1.157473       -1.293410
H          0.702650        1.381983       -2.344245
H         -0.041903        1.119523       -0.748387
H          1.419258        0.196687       -1.235386
C         -0.282530        3.780323       -0.136413
C         -3.012829        4.331087       -0.029804
C         -0.874988        4.570492       -1.123899
C         -1.059205        3.258901        0.898202
C         -2.420681        3.546348        0.956732
C         -2.239839        4.836173       -1.074805
H         -0.266605        4.979458       -1.926828
H         -0.596660        2.636087        1.658927
H         -3.015032        3.137335        1.768455
H         -2.698489        5.446085       -1.846924
H         -4.075533        4.549738        0.014113
H          1.841164        4.396924       -0.269009

SR epoxide:Catalyst, binary complex 89; Energy = -2449.839201; 6-31G(d) basis set.
N          1.800871        0.178895        1.061670
C          1.293515        0.331311        2.301183
S          2.031656        1.195864        3.543117
C          2.983484        0.898529        0.585971
C          3.833186        0.100731       -0.424351
C          5.167147        0.859398       -0.615248
C          5.028505        2.385781       -0.478339
C          3.645788        2.831635       -0.953567
C          2.555847        2.240153       -0.042486
N          4.101744       -1.303033       -0.126010
C          3.145051       -2.224823       -0.699584
N          0.077947       -0.257447        2.548752
C         -0.670837       -1.079189        1.683032
C         -2.016295       -0.791930        1.439022
C         -2.741635       -1.600478        0.575486
C         -2.149685       -2.686990       -0.066362
C         -0.814945       -2.970818        0.195918
C         -0.080629       -2.193201        1.086662
C         -4.166454       -1.259273        0.232091
F         -4.963967       -2.329639        0.363761
C         -0.130284       -4.110110       -0.509340
F         -0.996083       -5.053122       -0.890156
C          4.402414       -1.592483        1.265796
F         -4.653443       -0.288049        1.008273
F         -4.262945       -0.857581       -1.042832
F          0.501200       -3.683132       -1.621580
F          0.799366       -4.683811        0.263250
H          1.182366       -0.172096        0.332998
H         -0.328846        0.004977        3.437745
H          1.638666        2.071777       -0.623020
H          2.303645        2.929757        0.771610
H          3.566341        3.922735       -0.976609
H          3.495365        2.483250       -1.984037
H          5.157395        2.686568        0.568941
H          5.819290        2.887321       -1.044532
H          5.890589        0.480730        0.115071
H          5.559381        0.596507       -1.603150
H          3.587212        1.083658        1.478438
H          3.291408        0.110754       -1.379924
H          3.525361       -1.541345        1.933158
H          4.829639       -2.597596        1.338685
H          5.147832       -0.886533        1.643559
H          3.114985       -2.103605       -1.788481
H          2.115819       -2.100312       -0.325079
H          3.449812       -3.254180       -0.483606
H         -2.484197        0.070174        1.902486
H         -2.723782       -3.303262       -0.750857
H          0.941418       -2.455576        1.339322
C         -2.130135        2.318797       -1.390474
O         -2.851496        1.585684       -0.403135
C         -2.159053        2.708700        0.036578
N         -3.093766        3.858086        0.331088
```

O	-4.147085	3.890185	-0.268872
O	-2.703707	4.682380	1.134359
C	-1.032353	2.573967	1.011803
H	-0.404727	3.466273	1.003507
H	-0.431677	1.710634	0.719050
H	-1.411700	2.425963	2.026414
C	-0.932636	1.667935	-1.991674
C	1.293410	0.458815	-3.160735
C	-0.092064	2.407724	-2.825064
C	-0.662393	0.319958	-1.750541
C	0.449195	-0.283958	-2.335012
C	1.020464	1.803945	-3.405513
H	-0.310649	3.453806	-3.023376
H	-1.351775	-0.253890	-1.139029
H	0.635127	-1.341576	-2.167901
H	1.669857	2.382852	-4.054663
H	2.153289	-0.014584	-3.626000
H	-2.771998	2.894745	-2.055843

SR epoxide:Catalyst, binary complex 90; Energy = -2449.842350; 6-31G(d) basis set.

N	1.852874	-0.681775	-1.223842
C	0.731326	-1.430915	-1.161944
S	0.668391	-3.082189	-0.880438
C	3.247888	-1.100642	-1.070004
C	3.552452	-1.791574	0.276275
C	5.066594	-2.033348	0.380754
C	5.567826	-2.890770	-0.783396
C	5.242201	-2.223750	-2.121023
C	3.742303	-1.947228	-2.248797
N	2.952048	-1.063386	1.394545
C	2.588219	-1.933265	2.499491
N	-0.385140	-0.660769	-1.428904
C	-1.700529	-0.734569	-0.956912
C	-2.203570	-1.725775	-0.109914
C	-3.508088	-1.615611	0.366982
C	-4.330543	-0.550111	0.034501
C	-3.819172	0.427502	-0.814955
C	-2.533083	0.338438	-1.318287
C	-4.040355	-2.723391	1.233855
F	-3.091961	-3.218569	2.041497
C	-4.683506	1.614405	-1.139612
F	-4.912968	2.358713	-0.050825
C	3.719986	0.079225	1.856962
F	-5.055034	-2.308268	2.004866
F	-4.498301	-3.745845	0.495894
F	-4.133812	2.405341	-2.068545
F	-5.884359	1.225258	-1.600836
H	1.703080	0.319820	-1.146641
H	-0.175469	0.242471	-1.838264
H	3.188840	-2.892304	-2.264823
H	3.521082	-1.422387	-3.184355
H	5.794557	-1.275839	-2.193273
H	5.575717	-2.849501	-2.955276
H	5.085857	-3.876678	-0.742826
H	6.646503	-3.058245	-0.693450
H	5.598025	-1.070877	0.371800
H	5.291623	-2.513306	1.341055
H	3.803382	-0.151498	-1.087123
H	3.061087	-2.767789	0.247073
H	4.645127	-0.197998	2.391969
H	3.990251	0.722398	1.013788
H	3.103973	0.673680	2.541419
H	2.032728	-1.353129	3.244874
H	3.460238	-2.384378	3.006601
H	1.938251	-2.733099	2.133312
H	-1.586357	-2.563777	0.182722
H	-5.337497	-0.474527	0.429955
H	-2.156008	1.126258	-1.964501
C	0.669918	3.071100	0.048558
O	0.176819	2.022457	-0.789712
C	-0.192023	1.984871	0.560837
N	-1.641951	2.396738	0.720696
O	-2.097962	3.159216	-0.107172
O	-2.238745	1.935019	1.669787
C	0.220394	0.854128	1.449321

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H          0.272247        1.199426        2.484984
H          1.197733        0.468018        1.143154
H         -0.510129        0.042556        1.395585
C          2.144061        3.092317        0.276232
C          4.905385        3.278132        0.619073
C          3.003989        2.746441       -0.768202
C          2.667842        3.528881        1.493477
C          4.046967        3.617596        1.663547
C          4.383474        2.841695       -0.597128
H          2.590069        2.429802       -1.723027
H          1.997772        3.801876        2.304765
H          4.451332        3.954687        2.612640
H          5.047798        2.580598       -1.415285
H          5.979748        3.353460        0.753632
H          0.176647        4.023725       -0.140749

SR epoxide:Catalyst, binary complex 91; Energy = -2449.839647; 6-31G(d) basis set.
N          3.782559       -0.103191        0.940283
C          2.515575       -0.537807        0.800287
S          2.103586       -1.914631       -0.071430
C          4.973593       -0.652946        0.304511
C          5.786925        0.483109       -0.357389
C          7.063101       -0.104058       -0.976117
C          7.899734       -0.869255        0.050683
C          7.081917       -1.992641        0.688473
C          5.808762       -1.435169        1.323706
N          5.064945        1.296493       -1.334161
C          4.349940        0.549939       -2.354797
N          1.614558        0.298394        1.419877
C          0.216006        0.217644        1.520466
C         -0.479274        1.431534        1.588689
C         -1.858116        1.438969        1.714298
C         -2.581102        0.249533        1.754878
C         -1.882338       -0.943097        1.651442
C         -0.492784       -0.981935        1.566313
C         -2.607533        2.739230        1.777456
F         -3.711401        2.694094        1.010955
C         -2.640371       -2.227215        1.479235
F         -2.752795       -2.519204        0.162989
C          4.232516        2.356075       -0.798068
F         -3.014639        3.019568        3.023327
F         -1.865277        3.771440        1.357401
F         -2.024494       -3.265530        2.052936
F         -3.881479       -2.155493        1.967745
H          3.951198        0.677766        1.566226
H          1.982941        1.199784        1.702774
H          6.077506       -0.763709        2.152634
H          5.188724       -2.235452        1.741961
H          6.809696       -2.727181       -0.081317
H          7.672728       -2.524369        1.441280
H          8.798672       -1.272905       -0.426525
H          8.239115       -0.178098        0.834662
H          6.792494       -0.789283       -1.790250
H          7.631993        0.716488       -1.423421
H          4.621207       -1.340603       -0.469979
H          6.104666        1.172606        0.441587
H          4.749399        2.860099        0.025018
H          4.049596        3.100372       -1.582108
H          3.244859        2.011940       -0.437504
H          4.020986        1.243462       -3.135898
H          3.457776        0.026444       -1.966810
H          5.003269       -0.191319       -2.822051
H          0.058270        2.371012        1.501947
H         -3.663368        0.253974        1.837401
H          0.022155       -1.930599        1.504401
C         -3.524465        0.318400       -1.358398
O         -4.476908        0.329541       -2.433189
C         -3.959756       -0.903848       -2.051139
N         -4.984503       -1.713331       -1.276421
O         -5.021458       -2.906883       -1.491484
O         -5.696289       -1.113763       -0.496029
C         -3.195565       -1.718948       -3.048536
H         -2.497431       -1.060820       -3.566960
H         -3.886202       -2.157351       -3.772206
H         -2.648512       -2.523276       -2.554150
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C	-2.194130	0.958804	-1.575480
C	0.270156	2.242573	-1.834414
C	-2.135039	2.352148	-1.682700
C	-1.014671	0.214891	-1.581102
C	0.215392	0.856454	-1.721666
C	-0.906954	2.991922	-1.807277
H	-3.054992	2.929699	-1.658785
H	-1.049240	-0.864508	-1.453163
H	1.125426	0.262914	-1.726214
H	-0.868267	4.073968	-1.886995
H	1.229910	2.739809	-1.946732
H	-4.005963	0.523803	-0.405670

SR epoxide:Catalyst, binary complex 92; Energy = -2449.840464; 6-31G(d) basis set.

N	-1.776457	-1.040349	0.323222
C	-0.542720	-1.416256	-0.068106
S	-0.268593	-2.411216	-1.393802
C	-3.012446	-1.606896	-0.197667
C	-4.106811	-1.465717	0.871587
C	-5.316679	-2.337123	0.467487
C	-5.474537	-2.422411	-1.063556
C	-4.998702	-1.125756	-1.723070
C	-3.489091	-0.911777	-1.487438
N	-3.576391	-1.670001	2.222041
C	-3.038639	-3.001847	2.468758
N	0.438208	-0.863099	0.724541
C	1.825640	-0.801740	0.507893
C	2.475361	0.370615	0.913276
C	3.845687	0.506006	0.740627
C	4.601817	-0.515922	0.177935
C	3.950378	-1.686233	-0.190908
C	2.578240	-1.850217	-0.026680
C	4.504214	1.805531	1.114549
F	4.485938	2.673928	0.094980
C	4.730911	-2.808110	-0.818596
F	4.293838	-4.006306	-0.405032
C	-4.535775	-1.294935	3.248119
F	3.887957	2.391669	2.149501
F	5.789315	1.625297	1.455881
F	4.624606	-2.793608	-2.155366
F	6.036573	-2.729608	-0.525600
H	-1.889221	-0.648242	1.257825
H	0.104189	-0.109887	1.318034
H	-3.275148	0.161148	-1.398417
H	-2.902038	-1.296884	-2.326355
H	-5.213594	-1.133270	-2.795733
H	-5.563498	-0.286096	-1.297297
H	-4.884952	-3.259817	-1.455823
H	-6.517707	-2.630491	-1.320129
H	-5.204620	-3.344406	0.884132
H	-6.222668	-1.909430	0.911652
H	-2.827349	-2.668355	-0.406818
H	-4.421054	-0.413086	0.850378
H	-5.405642	-1.971455	3.297198
H	-4.044520	-1.305695	4.225949
H	-4.899754	-0.279842	3.056012
H	-2.291304	-3.255334	1.710762
H	-3.807236	-3.791499	2.479913
H	-2.543851	-3.004441	3.444680
H	1.909241	1.178018	1.372535
H	5.672862	-0.409386	0.049915
H	2.100502	-2.779928	-0.303114
C	-0.988260	3.024298	0.118125
O	-0.310624	1.922689	0.733413
C	0.099925	2.283381	-0.549873
N	1.425456	3.013648	-0.518597
O	2.066212	3.015922	-1.547953
O	1.736691	3.564535	0.518543
C	-0.042039	1.331386	-1.696488
H	-0.031650	1.875110	-2.642625
H	-0.989362	0.798486	-1.589796
H	0.778398	0.608484	-1.702211
C	-2.415364	2.817729	-0.263386
C	-5.106951	2.538172	-0.933063
C	-3.316582	2.306188	0.671635

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C         -2.861410        3.181219       -1.534561
C         -4.204401        3.033336       -1.871606
C         -4.662424        2.177289        0.337936
H         -2.963585        2.017303        1.658688
H         -2.156610        3.579097       -2.260052
H         -4.545322        3.310299       -2.863881
H         -5.367458        1.796171        1.071415
H         -6.156326        2.433417       -1.190836
H         -0.717263        3.979293        0.567511

SR epoxide:Catalyst, binary complex 93; Energy = -2449.833003; 6-31G(d) basis set.
N         -3.366024       -0.655340        0.677276
C         -3.358463       -1.990751        0.528571
S         -4.707558       -2.931820        0.861991
C         -2.534036        0.364062        0.025553
C         -3.300623        1.018235       -1.164876
C         -2.726322        2.421724       -1.397524
C         -3.087409        3.352027       -0.227622
C         -3.075630        2.594874        1.115169
C         -2.093748        1.423321        1.062793
N         -3.353715        0.246417       -2.397261
C         -2.071491       -0.099495       -2.975302
N         -2.213700       -2.586242        0.031976
C         -0.873591       -2.324225        0.376492
C         -0.515583       -1.538025        1.473572
C          0.827685       -1.329988        1.764465
C          1.838320       -1.917520        1.011988
C          1.466778       -2.729889       -0.054513
C          0.130781       -2.927690       -0.385961
C          1.151026       -0.489041        2.968900
F          0.555220        0.717996        2.891712
C          2.518397       -3.350648       -0.933114
F          3.701687       -3.429229       -0.321997
C         -4.253419       -0.895574       -2.400548
F          0.688307       -1.061499        4.091011
F          2.458746       -0.291159        3.124285
F          2.167172       -4.587002       -1.315569
F          2.687046       -2.630772       -2.055077
H         -4.239009       -0.316523        1.069423
H         -2.391648       -3.543909       -0.249295
H         -1.991054        0.956043        2.046154
H         -1.100604        1.802347        0.795593
H         -2.814807        3.268973        1.936757
H         -4.080315        2.215962        1.345055
H         -2.373455        4.181369       -0.195650
H         -4.077541        3.789251       -0.394525
H         -1.634154        2.369529       -1.499412
H         -3.114296        2.807280       -2.344291
H         -1.653046       -0.137519       -0.377863
H         -4.346871        1.147849       -0.850617
H         -5.165056       -0.657959       -1.844932
H         -4.532018       -1.127475       -3.434742
H         -3.814487       -1.807733       -1.965637
H         -2.228761       -0.472761       -3.992252
H         -1.533311       -0.890597       -2.416337
H         -1.427277        0.781821       -3.040038
H         -1.283770       -1.107808        2.107524
H          2.882065       -1.737592        1.242372
H         -0.134701       -3.553644       -1.233282
C          2.902552        2.087430       -0.170127
O          2.522961        0.941014        0.596284
C          2.379221        0.845750       -0.776357
N          3.439296       -0.001949       -1.426008
O          3.399571       -0.048582       -2.639219
O          4.260744       -0.541379       -0.715155
C          1.025028        0.660595       -1.390931
H          1.035568        0.977985       -2.434663
H          0.309873        1.265564       -0.829552
H          0.728606       -0.392398       -1.341592
C          2.043407        3.300171       -0.072049
C          0.405031        5.550938        0.050563
C          1.071159        3.399098        0.922400
C          2.205639        4.332593       -0.997856
C          1.384154        5.453822       -0.937590
C          0.253783        4.525892        0.982020
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H	0.968814	2.595738	1.644629
H	2.969009	4.254694	-1.767656
H	1.507684	6.252313	-1.662058
H	-0.498441	4.604070	1.761956
H	-0.234039	6.427171	0.097486
H	3.981299	2.237333	-0.219573

SR epoxide:Catalyst, binary complex 94; Energy = -2449.837276; 6-31G(d) basis set.

N	-3.213600	1.307832	-0.297974
C	-3.221071	1.828375	0.940247
S	-4.501362	2.745819	1.522247
C	-2.485758	0.131158	-0.794025
C	-3.469690	-1.071607	-0.953690
C	-2.929392	-1.998251	-2.047063
C	-3.004966	-1.319704	-3.423641
C	-2.689805	0.186207	-3.321528
C	-1.775475	0.455308	-2.125759
N	-3.785795	-1.812265	0.259605
C	-2.650246	-2.445852	0.902909
N	-2.147828	1.535000	1.758948
C	-0.784072	1.565851	1.392966
C	-0.335427	2.266652	0.273887
C	1.021732	2.282419	-0.031115
C	1.955125	1.657011	0.785216
C	1.495556	0.990881	1.917976
C	0.140618	0.917758	2.215246
C	1.450465	3.007093	-1.276649
F	0.967085	4.256718	-1.304510
C	2.482592	0.354878	2.856950
F	2.831457	1.181181	3.850624
C	-4.594148	-1.097725	1.234344
F	2.779053	3.078292	-1.394800
F	0.982969	2.395117	-2.383994
F	1.980362	-0.754145	3.422754
F	3.612021	0.000670	2.220676
H	-4.025032	1.585696	-0.840478
H	-2.333545	1.783192	2.724298
H	-1.428232	1.491286	-2.118941
H	-0.881518	-0.175819	-2.201862
H	-2.228612	0.547635	-4.245114
H	-3.618472	0.760400	-3.203067
H	-2.296844	-1.804297	-4.104401
H	-4.002224	-1.462253	-3.853201
H	-1.885686	-2.246125	-1.819491
H	-3.494848	-2.934549	-2.032438
H	-1.735139	-0.136535	-0.048205
H	-4.428288	-0.667589	-1.314559
H	-5.375402	-0.522414	0.728293
H	-5.077301	-1.824405	1.896996
H	-4.014979	-0.408096	1.869925
H	-2.125168	-3.098324	0.196311
H	-3.011665	-3.079468	1.719161
H	-1.924942	-1.732708	1.333380
H	-1.041949	2.810474	-0.345745
H	3.010575	1.674629	0.537248
H	-0.203742	0.355170	3.077941
C	1.764818	-1.691809	0.155354
O	0.382817	-1.408136	-0.071039
C	0.788552	-2.729444	-0.241928
N	0.341054	-3.594715	0.913412
O	0.163363	-4.773021	0.674317
O	0.211084	-3.061821	1.996191
C	0.698714	-3.402282	-1.575792
H	1.409038	-4.229269	-1.628421
H	0.939348	-2.669813	-2.348348
H	-0.305084	-3.798441	-1.744257
C	2.761186	-1.119241	-0.788431
C	4.673409	0.021600	-2.464891
C	2.363048	-0.316469	-1.857435
C	4.118965	-1.341794	-0.552511
C	5.072002	-0.779112	-1.395810
C	3.319026	0.257224	-2.690496
H	1.307589	-0.110502	-2.008056
H	4.427039	-1.942852	0.298953
H	6.126669	-0.956022	-1.210586

H	3.003521	0.902793	-3.503858
H	5.418487	0.470149	-3.114363
H	2.032238	-1.697434	1.210520

SR epoxide:Catalyst, binary complex 95; Energy = -2449.840328; 6-31G(d) basis set.

N	-3.046981	-1.476570	0.364742
C	-1.857477	-0.972973	0.746990
S	-1.694004	0.501289	1.539808
C	-4.347559	-0.838835	0.530143
C	-5.173547	-0.979038	-0.765819
C	-6.549512	-0.330111	-0.560430
C	-7.286969	-0.913859	0.646226
C	-6.453101	-0.765672	1.919248
C	-5.082139	-1.417479	1.743565
N	-4.537718	-0.462768	-1.978199
C	-3.938462	0.853979	-1.845005
N	-0.806758	-1.780532	0.378726
C	0.574493	-1.621963	0.603946
C	1.102830	-1.072335	1.772549
C	2.482385	-0.983574	1.914956
C	3.355257	-1.467252	0.948938
C	2.815726	-2.044631	-0.193197
C	1.440474	-2.109492	-0.379846
C	3.024424	-0.270860	3.120930
F	2.291113	-0.519139	4.216191
C	3.720965	-2.681028	-1.210663
F	3.899190	-3.986912	-0.937779
C	-3.636082	-1.369430	-2.662401
F	4.287595	-0.629892	3.389001
F	3.018530	1.058292	2.939968
F	3.206856	-2.612577	-2.445358
F	4.931873	-2.117251	-1.227985
H	-3.069797	-2.421174	-0.006297
H	-1.027649	-2.518731	-0.280689
H	-5.205005	-2.501255	1.601525
H	-4.456779	-1.273856	2.631515
H	-6.318775	0.300779	2.144546
H	-6.970920	-1.209526	2.775630
H	-7.489171	-1.979299	0.468209
H	-8.258508	-0.423023	0.764468
H	-6.421998	0.750636	-0.411593
H	-7.125884	-0.460332	-1.481125
H	-4.147819	0.221412	0.711982
H	-5.345651	-2.053459	-0.938742
H	-2.639766	-1.452777	-2.189780
H	-4.081595	-2.367692	-2.720288
H	-3.477774	-1.013013	-3.686248
H	-3.698380	1.237215	-2.842364
H	-3.008155	0.851916	-1.248362
H	-4.639658	1.552476	-1.380570
H	0.447884	-0.711818	2.553962
H	4.428878	-1.392469	1.078191
H	1.041080	-2.540354	-1.294957
C	2.188695	2.281446	-1.044086
O	2.045470	1.092584	-0.273499
C	1.486787	1.073763	-1.542948
N	2.315396	0.223736	-2.478371
O	1.725030	-0.339901	-3.379575
O	3.510092	0.163466	-2.269461
C	0.010825	0.930141	-1.742843
H	-0.273206	1.286721	-2.734929
H	-0.501880	1.512915	-0.976045
H	-0.289879	-0.116468	-1.648564
C	1.435484	3.479764	-0.583916
C	0.020316	5.731514	0.243861
C	0.615555	3.410563	0.543482
C	1.557791	4.678774	-1.287732
C	0.847642	5.801918	-0.875635
C	-0.091562	4.537450	0.953066
H	0.540456	2.474302	1.090823
H	2.208319	4.731302	-2.157203
H	0.941763	6.732844	-1.426034
H	-0.729143	4.481974	1.830007
H	-0.532797	6.608821	0.564859
H	3.197724	2.437673	-1.423473

SR epoxide:Catalyst, binary complex 96; Energy = -2449.827522; 6-31G(d) basis set.

N	2.912520	0.243278	-0.416418
C	2.292349	-0.948289	-0.447501
S	2.949154	-2.401521	-0.989740
C	4.325894	0.527906	-0.701056
C	5.257203	-0.055474	0.374138
C	6.700151	0.303745	-0.009180
C	7.132053	-0.380644	-1.326081
C	5.930656	-0.837989	-2.168583
C	4.781987	0.172591	-2.139830
N	4.818829	0.373080	1.706263
C	5.218012	1.723577	2.072120
N	0.999265	-0.958548	0.014779
C	0.121120	0.096991	0.300073
C	0.151157	1.322288	-0.379875
C	-0.790362	2.296108	-0.072178
C	-1.777831	2.083252	0.884339
C	-1.814419	0.854071	1.531398
C	-0.877086	-0.132003	1.253785
C	-0.817568	3.585482	-0.845060
F	0.302020	3.775439	-1.553314
C	-2.821427	0.625586	2.625859
F	-3.149856	-0.667509	2.743765
C	5.211587	-0.568241	2.741904
F	-1.846548	3.606470	-1.709640
F	-0.972952	4.639575	-0.033623
F	-2.322205	1.007304	3.814271
F	-3.941544	1.325472	2.427801
H	2.507663	0.909173	0.233216
H	0.615011	-1.892295	0.117038
H	3.930563	-0.210877	-2.708164
H	5.104563	1.096314	-2.634638
H	6.242899	-1.002844	-3.205194
H	5.556816	-1.795874	-1.796833
H	7.750637	0.313581	-1.905357
H	7.762645	-1.248779	-1.108161
H	6.766264	1.394338	-0.120463
H	7.381141	0.036616	0.806641
H	4.374744	1.618287	-0.603146
H	5.141548	-1.144839	0.350614
H	6.305817	-0.634727	2.880263
H	4.773841	-0.258922	3.696460
H	4.831395	-1.564109	2.496802
H	4.699821	2.008918	2.992904
H	4.931053	2.438812	1.294807
H	6.302468	1.828494	2.247676
H	0.880120	1.501435	-1.161430
H	-2.510221	2.851748	1.108812
H	-0.917777	-1.087417	1.770039
C	-4.176603	-1.708892	-0.494481
O	-4.301411	-0.454242	0.191979
C	-4.186965	-0.407798	-1.189164
N	-5.518249	-0.093543	-1.844324
O	-5.476340	0.424130	-2.943026
O	-6.524509	-0.398147	-1.240593
C	-3.034508	0.312020	-1.818926
H	-3.177166	1.392617	-1.741226
H	-2.939229	0.047012	-2.872676
H	-2.125835	0.031523	-1.284532
C	-2.935643	-2.503999	-0.254003
C	-0.664330	-4.041703	0.275762
C	-2.766812	-3.100410	0.999413
C	-1.975845	-2.701413	-1.247044
C	-0.841750	-3.469510	-0.983666
C	-1.632547	-3.860491	1.265751
H	-3.520900	-2.954219	1.766786
H	-2.114428	-2.262437	-2.230863
H	-0.086060	-3.606283	-1.751260
H	-1.503915	-4.315998	2.242615
H	0.226076	-4.628661	0.480728
H	-5.115544	-2.261349	-0.505415

SR epoxide:Catalyst, binary complex 97; Energy = -2449.836189; 6-31G(d) basis set.

N	2.500064	0.241214	-0.602389

C	1.443694	0.293540	-1.429977
S	1.396788	-0.449776	-2.933247
C	3.767295	-0.430156	-0.864949
C	4.919342	0.350189	-0.213646
C	6.208692	-0.486974	-0.291122
C	6.069041	-1.885842	0.304026
C	4.959600	-2.648011	-0.415671
C	3.655492	-1.863861	-0.320286
N	5.193948	1.663489	-0.814705
C	5.820179	2.550914	0.149020
N	0.431121	1.076377	-0.920208
C	-0.956322	0.977693	-1.099154
C	-1.728648	2.025045	-0.595156
C	-3.112057	1.911499	-0.534837
C	-3.761115	0.770926	-0.984975
C	-2.980622	-0.244135	-1.526818
C	-1.599432	-0.148948	-1.616840
C	-3.869454	3.035607	0.108874
F	-3.536647	3.151935	1.410013
C	-3.600954	-1.571991	-1.848404
F	-3.423600	-2.427870	-0.816049
C	4.122903	2.369141	-1.499814
F	-3.582516	4.215699	-0.460502
F	-5.192550	2.862839	0.048297
F	-4.917268	-1.485118	-2.063210
F	-3.042857	-2.147574	-2.919722
H	2.386175	0.598789	0.343105
H	0.686963	1.657515	-0.126435
H	3.346586	-1.799157	0.734550
H	2.843679	-2.360176	-0.863525
H	5.233023	-2.781432	-1.470599
H	4.825332	-3.647722	0.009864
H	7.022454	-2.418453	0.227115
H	5.828869	-1.814006	1.374392
H	6.477826	-0.562477	-1.352470
H	7.022544	0.056480	0.198236
H	3.907795	-0.460242	-1.950703
H	4.642601	0.472758	0.857149
H	3.324656	2.734131	-0.825837
H	4.563112	3.242432	-1.991620
H	3.667857	1.748542	-2.274802
H	5.116703	2.870444	0.942950
H	6.186058	3.448032	-0.359067
H	6.672615	2.066135	0.630351
H	-1.242295	2.922143	-0.218849
H	-4.836546	0.668114	-0.903371
H	-1.024131	-0.961495	-2.041307
C	-1.341299	-0.917512	2.484556
O	-2.192012	-0.789076	1.344206
C	-1.463400	-1.965458	1.453215
N	-2.354012	-3.118644	1.859940
O	-3.354601	-2.853896	2.490621
O	-1.985138	-4.231293	1.540843
C	-0.420261	-2.345202	0.446090
H	0.253752	-3.094366	0.866219
H	0.154765	-1.454999	0.180857
H	-0.890059	-2.763441	-0.446281
C	-0.160801	-0.001901	2.522459
C	2.006124	1.761209	2.598485
C	-0.365263	1.367481	2.333298
C	1.125393	-0.483937	2.765783
C	2.206592	0.396677	2.810164
C	0.716458	2.245889	2.364532
H	-1.371829	1.736437	2.153317
H	1.284376	-1.548211	2.920527
H	3.204814	0.015082	3.006701
H	0.553225	3.310457	2.222009
H	2.848580	2.445944	2.630272
H	-1.890071	-1.074264	3.412816

SR epoxide:Catalyst, binary complex 98; Energy = -2449.835443; 6-31G(d) basis set.

N	-3.321323	-1.106714	-0.515558
C	-2.267120	-1.317646	0.294582
S	-2.377737	-1.380946	1.968951
C	-4.712480	-0.926927	-0.117322

C	-5.323732	0.265322	-0.886394
C	-6.808487	0.402655	-0.521710
C	-7.586981	-0.889973	-0.770460
C	-6.975156	-2.049592	0.015420
C	-5.500940	-2.221387	-0.346943
N	-4.636740	1.545222	-0.721648
C	-4.350446	1.911086	0.654347
N	-1.097497	-1.485652	-0.413422
C	0.222354	-1.648051	0.040042
C	1.079526	-2.413062	-0.755263
C	2.425052	-2.521016	-0.427724
C	2.945882	-1.886636	0.693164
C	2.080132	-1.138794	1.483249
C	0.731205	-1.008158	1.173883
C	3.344372	-3.251688	-1.363853
F	2.720589	-4.259791	-1.989023
C	2.602554	-0.485959	2.734778
F	2.433476	-1.282851	3.801017
C	-3.474969	1.766624	-1.564028
F	3.807924	-2.427185	-2.321344
F	4.408272	-3.755851	-0.730694
F	3.908343	-0.214985	2.647460
F	1.959184	0.661101	3.002011
H	-3.154672	-1.074286	-1.516077
H	-1.206926	-1.668109	-1.404256
H	-5.415751	-2.502073	-1.407170
H	-5.035724	-3.021552	0.239134
H	-7.063188	-1.847484	1.091354
H	-7.517961	-2.980239	-0.179188
H	-8.637917	-0.751423	-0.496173
H	-7.567091	-1.128677	-1.843029
H	-6.900490	0.670812	0.539229
H	-7.221955	1.235100	-1.098888
H	-4.702564	-0.698566	0.952845
H	-5.277096	0.026282	-1.961344
H	-2.554954	1.272564	-1.203923
H	-3.684480	1.425538	-2.583488
H	-3.262660	2.841315	-1.607167
H	-4.040674	2.961804	0.683932
H	-3.547500	1.303426	1.108472
H	-5.244649	1.812905	1.275590
H	0.696225	-2.922405	-1.635138
H	3.998228	-1.967485	0.941673
H	0.080992	-0.410335	1.798655
C	2.883405	2.824904	-0.122203
O	3.178705	1.566113	0.480070
C	3.216718	1.614098	-0.906491
N	4.631907	1.602177	-1.430433
O	5.504982	2.021862	-0.700655
O	4.786719	1.196409	-2.566193
C	2.263089	0.806026	-1.730063
H	2.639473	-0.210341	-1.859799
H	2.135829	1.260349	-2.714255
H	1.302231	0.780125	-1.212482
C	1.482378	3.321534	-0.038366
C	-1.135751	4.266449	0.090867
C	0.524089	2.622640	0.694740
C	1.132435	4.499625	-0.700136
C	-0.176402	4.967914	-0.638295
C	-0.783803	3.095188	0.759030
H	0.823722	1.728823	1.230794
H	1.884576	5.050039	-1.259789
H	-0.446227	5.883944	-1.154263
H	-1.523021	2.551623	1.340290
H	-2.153598	4.641488	0.147168
H	3.682279	3.556689	-0.008199

SR epoxide:Catalyst, binary complex 99; Energy = -2449.836809; 6-31G(d) basis set.

N	-1.710178	-0.396081	-0.176419
C	-1.440930	0.055297	1.058345
S	-2.572844	0.648409	2.152652
C	-2.988920	-0.890155	-0.699038
C	-3.462776	-2.133542	0.073446
C	-4.814337	-2.564449	-0.513215
C	-5.911634	-1.507575	-0.253807

C	-5.326872	-0.114067	0.028541
C	-4.100527	0.184260	-0.835275
N	-2.409140	-3.156320	0.086019
C	-2.310491	-3.939456	-1.138798
N	-0.109542	0.081632	1.401957
C	0.952952	-0.681311	0.891619
C	2.250712	-0.157294	0.974102
C	3.324843	-0.902165	0.508173
C	3.144080	-2.167238	-0.046231
C	1.855250	-2.678359	-0.103136
C	0.757509	-1.964011	0.368474
C	4.706868	-0.305601	0.548492
F	5.643667	-1.256081	0.685261
C	1.595983	-4.037981	-0.689068
F	0.960926	-3.946192	-1.869972
C	-2.502830	-4.033825	1.244119
F	4.980233	0.356965	-0.583316
F	4.846396	0.554453	1.562588
F	2.721936	-4.728305	-0.892615
F	0.805603	-4.773000	0.112073
H	-0.906459	-0.673801	-0.725731
H	0.101507	0.704642	2.172107
H	-3.684206	1.163402	-0.579795
H	-4.405593	0.230032	-1.887530
H	-6.089192	0.652992	-0.143294
H	-5.035889	-0.036617	1.079720
H	-6.578522	-1.465717	-1.121769
H	-6.529439	-1.811355	0.597476
H	-4.691038	-2.711354	-1.594566
H	-5.109943	-3.536217	-0.102086
H	-2.727508	-1.223488	-1.708900
H	-3.608828	-1.833570	1.117932
H	-3.408732	-4.664570	1.240074
H	-1.630339	-4.693899	1.261398
H	-2.499143	-3.434146	2.158833
H	-3.178642	-4.599361	-1.302607
H	-1.414678	-4.563162	-1.088740
H	-2.209526	-3.285381	-2.010626
H	2.413913	0.826940	1.406035
H	3.990062	-2.742773	-0.403472
H	-0.239161	-2.413158	0.349660
C	0.994588	3.916877	0.095687
O	1.097629	2.688717	0.813518
C	1.383903	2.636274	-0.543726
N	2.865985	2.508656	-0.795715
O	3.196059	2.156785	-1.910429
O	3.617118	2.794925	0.114404
C	0.547125	1.829537	-1.488627
H	0.630461	2.231412	-2.499473
H	-0.493536	1.873064	-1.162505
H	0.890713	0.791111	-1.499734
C	-0.368413	4.485386	-0.091079
C	-2.914327	5.546692	-0.487945
C	-0.522454	5.687788	-0.782659
C	-1.487555	3.821461	0.412067
C	-2.758285	4.352807	0.213339
C	-1.795217	6.213813	-0.983671
H	0.351586	6.210680	-1.162880
H	-1.365122	2.897991	0.971421
H	-3.621198	3.830555	0.616691
H	-1.912635	7.148596	-1.522762
H	-3.905124	5.962721	-0.641881
H	1.807096	4.611727	0.306773

SR epoxide:Catalyst, binary complex 100; Energy = -2449.838486; 6-31G(d) basis set.

N	2.015702	-0.673951	-0.803176
C	0.888981	-1.411267	-0.906183
S	0.829671	-3.085797	-0.903268
C	3.415716	-1.111880	-0.806861
C	3.827015	-1.937871	0.437241
C	5.342297	-2.182904	0.374248
C	5.762054	-2.868039	-0.927169
C	5.332388	-2.043135	-2.140702
C	3.822926	-1.798600	-2.116166
N	3.457897	-1.361367	1.728756

C	3.729129	0.050265	1.884871
N	-0.216714	-0.598060	-1.038975
C	-1.564297	-0.795238	-0.722551
C	-2.064537	-1.876523	0.009406
C	-3.415658	-1.905103	0.342303
C	-4.287642	-0.884068	-0.011626
C	-3.775256	0.190793	-0.730465
C	-2.438752	0.238509	-1.095745
C	-3.949168	-3.105645	1.075417
F	-3.028187	-3.640452	1.888785
C	-4.674414	1.351711	-1.056736
F	-4.763019	2.199355	-0.021980
C	2.145190	-1.719932	2.232523
F	-5.018732	-2.793463	1.821734
F	-4.331413	-4.070783	0.226325
F	-4.230810	2.050116	-2.108685
F	-5.920970	0.941776	-1.334155
H	1.889081	0.329064	-0.697775
H	-0.013720	0.354922	-1.323905
H	3.292333	-2.751664	-2.206001
H	3.512510	-1.170011	-2.958616
H	5.861650	-1.079161	-2.129266
H	5.612055	-2.548453	-3.070886
H	5.293639	-3.859838	-0.983416
H	6.845713	-3.026638	-0.935762
H	5.874274	-1.224060	0.459642
H	5.623803	-2.781843	1.245353
H	3.971544	-0.164815	-0.752302
H	3.327114	-2.909720	0.372014
H	1.309719	-1.194371	1.737252
H	1.980801	-2.792985	2.107533
H	2.099454	-1.484803	3.302298
H	3.628372	0.324283	2.940931
H	3.048928	0.708559	1.308470
H	4.751630	0.286500	1.575230
H	-1.410431	-2.680491	0.317874
H	-5.334728	-0.920179	0.267236
H	-2.069111	1.084977	-1.669691
C	0.530890	3.380439	-0.177118
O	-0.046177	2.262896	-0.861091
C	-0.458928	2.482876	0.454701
N	-1.860828	3.044936	0.494308
O	-2.275324	3.580471	-0.512184
O	-2.451886	2.935877	1.547882
C	-0.179943	1.474038	1.525706
H	-0.223875	1.947183	2.507997
H	0.820037	1.063613	1.369870
H	-0.914997	0.665008	1.491384
C	1.986303	3.267425	0.133119
C	4.720088	3.102603	0.651522
C	2.852756	2.756455	-0.837295
C	2.488769	3.691900	1.363286
C	3.854639	3.605644	1.621345
C	4.219284	2.677570	-0.577492
H	2.456611	2.440014	-1.799810
H	1.812443	4.086869	2.116861
H	4.242884	3.932716	2.580515
H	4.892115	2.290605	-1.336950
H	5.784508	3.040089	0.854760
H	0.154815	4.333436	-0.547490

SR epoxide:Catalyst, binary complex 101; Energy = -2449.829440; 6-31G(d) basis set.

N	3.033513	-0.586443	-0.807493
C	1.727099	-0.856789	-0.628556
S	0.937250	-1.960689	-1.627705
C	3.965014	0.115333	0.071913
C	5.239159	-0.733952	0.285712
C	6.155995	-0.035556	1.320433
C	5.944057	1.482636	1.413042
C	5.647114	2.054664	0.028419
C	4.309098	1.507965	-0.500146
N	5.026991	-2.123638	0.674650
C	4.812832	-3.079645	-0.400496
N	1.138247	-0.152641	0.388385
C	-0.185688	-0.205858	0.858670

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C         -0.724534        0.985896        1.355740
C         -2.012147        1.003634        1.867951
C         -2.791816       -0.151228        1.900279
C         -2.242728       -1.327491        1.408259
C         -0.948586       -1.374520        0.895561
C         -2.632720        2.299143        2.305863
F         -3.657535        2.632733        1.501049
C         -3.032015       -2.608440        1.473127
F         -2.775137       -3.399943        0.428392
C          4.067698       -2.323090        1.746294
F         -3.127783        2.218060        3.547489
F         -1.760201        3.315313        2.279678
F         -2.718588       -3.305696        2.580978
F         -4.348385       -2.378716        1.515849
H          3.435864       -1.064466       -1.605468
H          1.625615        0.692046        0.663809
H          4.338520        1.426525       -1.592832
H          3.489319        2.198596       -0.263698
H          5.623064        3.148105        0.046113
H          6.460241        1.770105       -0.650698
H          5.106003        1.710825        2.084956
H          6.827887        1.956071        1.850844
H          5.998496       -0.497253        2.299675
H          7.192992       -0.252631        1.045120
H          3.482940        0.214923        1.050866
H          5.763094       -0.760280       -0.680635
H          3.018535       -2.185570        1.427660
H          4.165723       -3.344408        2.127037
H          4.266351       -1.638738        2.576652
H          3.780194       -3.098097       -0.788641
H          5.038064       -4.085943       -0.030007
H          5.498721       -2.867130       -1.226539
H         -0.152336        1.908088        1.300929
H         -3.809376       -0.126479        2.275796
H         -0.547012       -2.305053        0.516882
C         -2.315878        0.839944       -1.583696
O         -3.391251        0.850243       -2.534695
C         -2.495398       -0.208830       -2.599564
N         -3.082238       -1.478467       -2.012340
O         -3.946104       -1.354181       -1.166221
O         -2.628909       -2.529774       -2.413038
C         -1.726748       -0.438354       -3.864951
H         -0.860148       -1.075238       -3.682057
H         -1.404667        0.530548       -4.249174
H         -2.374623       -0.918024       -4.603020
C         -1.275372        1.907642       -1.633570
C          0.680880        3.891937       -1.443174
C          0.024016        1.653597       -2.071957
C         -1.592268        3.160086       -1.098236
C         -0.618870        4.148998       -1.004982
C          0.998776        2.646479       -1.979565
H          0.280768        0.672508       -2.462660
H         -2.597937        3.345287       -0.729993
H         -0.870768        5.116516       -0.582020
H          2.007165        2.441329       -2.327497
H          1.441914        4.662835       -1.366787
H         -2.679254        0.593064       -0.587245

SR epoxide:Catalyst, binary complex 102; Energy = -2449.836853; 6-31G(d) basis set.
N         -2.668732        0.188404       -0.532849
C         -1.585518        0.363183       -1.308888
S         -1.523107        1.432914       -2.602976
C         -3.996610        0.721327       -0.799486
C         -4.995104       -0.024708        0.102236
C         -6.433327        0.297295       -0.357368
C         -6.551905        1.733533       -0.902517
C         -5.557603        2.653293       -0.191475
C         -4.109654        2.235146       -0.515472
N         -4.666093       -1.448323        0.232898
C         -4.689961       -2.198455       -1.016218
N         -0.544779       -0.461868       -0.951331
C          0.821728       -0.340959       -1.252363
C          1.581878       -1.508206       -1.304282
C          2.968198       -1.435582       -1.390224
C          3.621548       -0.213773       -1.448722
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C	2.846035	0.941775	-1.439204
C	1.462218	0.895493	-1.362011
C	3.744982	-2.717598	-1.330004
F	3.207867	-3.662821	-2.116130
C	3.511215	2.281437	-1.320613
F	3.613635	2.638260	-0.021701
C	-5.479400	-2.103300	1.245719
F	5.020607	-2.558295	-1.694947
F	3.748425	-3.222128	-0.079600
F	4.750260	2.283601	-1.824471
F	2.814872	3.248473	-1.929918
H	-2.667172	-0.569473	0.150082
H	-0.765797	-1.237166	-0.330601
H	-3.443059	2.475544	0.320844
H	-3.739098	2.778764	-1.386619
H	-5.715212	3.695530	-0.483768
H	-5.739300	2.603387	0.889637
H	-6.339949	1.746313	-1.978592
H	-7.577080	2.096198	-0.782871
H	-6.745069	-0.419475	-1.125842
H	-7.111302	0.164736	0.493131
H	-4.232972	0.535586	-1.856653
H	-4.858770	0.386485	1.114834
H	-6.535779	-2.212105	0.949173
H	-5.082245	-3.105069	1.441184
H	-5.442537	-1.529000	2.177400
H	-4.041532	-1.723135	-1.757930
H	-5.697854	-2.304978	-1.447811
H	-4.302260	-3.204664	-0.825959
H	1.088477	-2.474810	-1.253850
H	4.703094	-0.159365	-1.491125
H	0.883490	1.810603	-1.347891
C	1.693326	-0.315613	2.631872
O	2.479933	0.108846	1.513659
C	1.828536	1.098631	2.233945
N	2.803913	1.873851	3.096708
O	3.819915	1.306306	3.436184
O	2.482155	3.004208	3.405168
C	0.784034	1.967128	1.599932
H	1.261577	2.719240	0.968022
H	0.201248	2.478352	2.367686
H	0.123609	1.342482	0.994669
C	0.475533	-1.118234	2.307404
C	-1.749479	-2.666512	1.631118
C	-0.805808	-0.695619	2.663320
C	0.643473	-2.329890	1.632290
C	-0.466261	-3.103157	1.295121
C	-1.916248	-1.467659	2.324083
H	-0.937429	0.243114	3.194420
H	1.643447	-2.648404	1.348987
H	-0.330519	-4.042589	0.767502
H	-2.915292	-1.129430	2.584809
H	-2.619042	-3.255276	1.355023
H	2.301899	-0.644999	3.473432

SR epoxide:Catalyst, binary complex 103; Energy = -2449.831790; 6-31G(d) basis set.

N	0.998538	0.854589	-0.234189
C	-0.194923	0.602008	0.332226
S	-0.375601	0.619356	2.008953
C	1.291817	1.066940	-1.653092
C	2.457513	2.098099	-1.754497
C	3.344467	1.764567	-2.954854
C	4.034317	0.403687	-2.756986
C	3.101856	-0.613614	-2.068422
C	1.639476	-0.265666	-2.346740
N	2.042969	3.497624	-1.740572
C	1.379028	3.949532	-2.951464
N	-1.201184	0.325190	-0.555201
C	-2.561625	0.087818	-0.269818
C	-3.277631	0.881310	0.631085
C	-4.629225	0.636022	0.826685
C	-5.298634	-0.365734	0.127474
C	-4.580263	-1.127414	-0.781546
C	-3.219032	-0.912882	-0.980351
C	-5.382252	1.461210	1.833791

F	-4.893049	2.706071	1.917617
C	-5.246274	-2.227386	-1.559042
F	-4.953352	-2.142179	-2.866595
C	1.262088	3.853139	-0.565711
F	-6.681878	1.556465	1.517807
F	-5.314564	0.926658	3.060841
F	-4.834176	-3.436912	-1.150785
F	-6.578066	-2.193819	-1.438006
H	1.737130	1.050508	0.436244
H	-0.919888	0.073982	-1.495120
H	0.969180	-1.055514	-1.985822
H	1.472755	-0.176755	-3.426716
H	3.330797	-1.636306	-2.383791
H	3.259214	-0.579877	-0.981481
H	4.358052	0.020675	-3.729892
H	4.938316	0.536746	-2.152338
H	2.741352	1.742671	-3.870065
H	4.083116	2.562193	-3.080590
H	0.401602	1.516666	-2.114062
H	3.081067	1.960749	-0.856944
H	1.770617	3.505557	0.339835
H	1.170529	4.942436	-0.513485
H	0.241548	3.428281	-0.566532
H	1.161526	5.016781	-2.850468
H	0.420558	3.435660	-3.153399
H	2.029338	3.823737	-3.819881
H	-2.780970	1.683754	1.161240
H	-6.358423	-0.534709	0.277913
H	-2.671262	-1.527403	-1.690135
C	4.459607	-1.728464	1.421952
O	3.829406	-2.539567	2.408925
C	3.324842	-2.639868	1.123469
N	3.780515	-3.911619	0.437018
O	4.755949	-4.473924	0.886316
O	3.152489	-4.253854	-0.547161
C	1.890436	-2.306918	0.856345
H	1.701271	-2.255064	-0.215360
H	1.639005	-1.351919	1.320436
H	1.252899	-3.082302	1.290235
C	4.334935	-0.249839	1.518342
C	4.193691	2.537793	1.642061
C	5.229918	0.536262	0.785156
C	3.375612	0.365697	2.324792
C	3.301913	1.757775	2.377685
C	5.161239	1.924451	0.846316
H	5.989724	0.054726	0.173835
H	2.698747	-0.237473	2.922335
H	2.543325	2.225665	2.997646
H	5.860119	2.526520	0.273924
H	4.137183	3.620956	1.691012
H	5.440958	-2.100073	1.127097

SR epoxide:Catalyst, binary complex 104; Energy = -2449.834235; 6-31G(d) basis set.

N	0.195175	-0.915112	0.653235
C	1.290505	-0.375363	0.085604
S	1.233953	0.597997	-1.283424
C	-1.169080	-0.745459	0.155085
C	-1.496746	-1.834737	-0.896459
C	-1.631411	-3.188554	-0.187747
C	-2.683449	-3.174530	0.923094
C	-2.331552	-2.121429	1.973571
C	-2.157103	-0.746665	1.323823
N	-2.705799	-1.431698	-1.632557
C	-3.366262	-2.527757	-2.330896
N	2.453307	-0.719864	0.737530
C	3.769156	-0.320060	0.432713
C	4.094240	1.008747	0.146568
C	5.416624	1.344885	-0.108603
C	6.433365	0.395028	-0.065573
C	6.099155	-0.915429	0.245789
C	4.778590	-1.280116	0.486361
C	5.776369	2.781882	-0.367895
F	6.785757	2.884378	-1.244114
C	7.179971	-1.952739	0.364554
F	8.223163	-1.675251	-0.427288

C	-2.383367	-0.401180	-2.616775
F	4.742252	3.479760	-0.850195
F	6.175399	3.394309	0.759011
F	7.648189	-2.030884	1.620521
F	6.732255	-3.174247	0.039537
H	0.303166	-1.414591	1.528794
H	2.396090	-1.519199	1.358194
H	-1.841782	0.003843	2.057216
H	-3.120472	-0.410810	0.923558
H	-3.106650	-2.066551	2.745434
H	-1.410179	-2.426792	2.493484
H	-3.668127	-2.940107	0.498912
H	-2.758920	-4.165610	1.382843
H	-1.825525	-3.983984	-0.912722
H	-0.652162	-3.420025	0.253342
H	-1.193170	0.238831	-0.312586
H	-0.639615	-1.896649	-1.593191
H	-1.742508	-0.794217	-3.425749
H	-3.309494	-0.022810	-3.061700
H	-1.854697	0.433811	-2.155191
H	-2.696025	-3.046289	-3.039710
H	-4.205506	-2.117390	-2.900680
H	-3.769449	-3.262020	-1.630207
H	3.319418	1.763684	0.114493
H	7.460711	0.670475	-0.277522
H	4.533832	-2.317202	0.696431
C	-6.302122	1.553555	0.260628
O	-6.681286	1.199398	-1.066306
C	-6.679270	0.175405	-0.129625
N	-8.083539	-0.196394	0.288759
O	-8.950591	0.641321	0.155293
O	-8.235026	-1.306925	0.760578
C	-5.764059	-0.998065	-0.277090
H	-5.634526	-1.494894	0.687063
H	-4.789131	-0.665471	-0.646199
H	-6.185733	-1.718628	-0.983363
C	-4.888058	1.951726	0.501711
C	-2.266460	2.762916	1.000696
C	-3.966517	2.013423	-0.544217
C	-4.496127	2.300246	1.796364
C	-3.186554	2.697540	2.046089
C	-2.660660	2.428353	-0.293103
H	-4.285540	1.756254	-1.549923
H	-5.220131	2.265498	2.606767
H	-2.886884	2.964463	3.054819
H	-1.945396	2.497444	-1.108203
H	-1.244828	3.078853	1.189517
H	-7.067002	2.120915	0.790346

SR epoxide:Catalyst, binary complex 105; Energy = -2449.827465; 6-31G(d) basis set.

N	2.827783	-1.211764	-1.503361
C	1.552793	-1.620314	-1.751434
S	1.200673	-3.093309	-2.456030
C	3.235539	-0.553884	-0.245628
C	3.573720	-1.632390	0.849693
C	5.080564	-1.696317	1.123616
C	5.843059	-1.694234	-0.203390
C	5.666436	-0.354745	-0.954737
C	4.404507	0.394347	-0.498780
N	2.792105	-1.525517	2.078109
C	1.399865	-1.893368	1.885043
N	0.614509	-0.675268	-1.414656
C	-0.755900	-0.844964	-1.163699
C	-1.598850	0.240983	-1.396773
C	-2.929540	0.191034	-0.994166
C	-3.453164	-0.940317	-0.385447
C	-2.608495	-2.029282	-0.190742
C	-1.270937	-1.994814	-0.558848
C	-3.785639	1.399329	-1.238710
F	-3.135823	2.529505	-0.874366
C	-3.142675	-3.285932	0.440755
F	-3.476528	-4.194047	-0.488307
C	2.885289	-0.245989	2.757051
F	-4.083065	1.543424	-2.537870
F	-4.932642	1.359746	-0.562350

F	-2.231969	-3.860386	1.238458
F	-4.237784	-3.048321	1.173238
H	3.499924	-1.891225	-1.846833
H	0.942597	0.286337	-1.425583
H	4.113990	1.155686	-1.230190
H	4.605528	0.920515	0.443213
H	6.535699	0.288612	-0.786238
H	5.622357	-0.532365	-2.034825
H	6.904327	-1.897758	-0.036178
H	5.471633	-2.527311	-0.816775
H	5.411002	-0.847600	1.734043
H	5.288172	-2.601800	1.700471
H	2.378458	0.032025	0.100533
H	3.298936	-2.604241	0.416053
H	3.929136	0.035373	2.917566
H	2.377267	0.572866	2.214741
H	2.401570	-0.324254	3.735123
H	1.339203	-2.881623	1.416729
H	0.836921	-1.176783	1.257086
H	0.892739	-1.933505	2.853527
H	-1.205750	1.131010	-1.881353
H	-4.482436	-0.964223	-0.048199
H	-0.625970	-2.840653	-0.354336
C	0.079001	1.817603	0.996832
O	0.100132	1.963213	2.416457
C	-1.107133	2.218222	1.771930
N	-2.093658	1.086627	1.952803
O	-3.272303	1.371808	1.863209
O	-1.644814	-0.026504	2.130527
C	-1.713959	3.583897	1.854823
H	-2.165138	3.730345	2.839015
H	-2.481108	3.710738	1.091717
H	-0.920619	4.318590	1.708949
C	0.855540	2.777749	0.161012
C	2.351407	4.457197	-1.489472
C	0.255430	3.394870	-0.940414
C	2.202449	3.016769	0.442066
C	2.947487	3.854865	-0.383003
C	1.004343	4.231701	-1.764343
H	-0.803179	3.239828	-1.133750
H	2.659823	2.556700	1.314004
H	3.994026	4.038666	-0.160202
H	0.532390	4.713390	-2.614520
H	2.934956	5.109280	-2.131432
H	0.106966	0.768251	0.703702

SR epoxide:Catalyst, binary complex 106; Energy = -2449.827800; 6-31G(d) basis set.

N	-2.289124	-2.477812	0.533921
C	-1.623264	-3.542978	0.030940
S	-2.323176	-5.063246	-0.077098
C	-2.196202	-1.091203	0.033226
C	-3.061513	-0.962066	-1.243074
C	-4.585847	-0.896204	-0.933370
C	-4.932803	-0.667553	0.546971
C	-4.001692	0.362231	1.184005
C	-2.540112	-0.120766	1.184700
N	-2.537263	0.094888	-2.121601
C	-2.985891	-0.091409	-3.493948
N	-0.333354	-3.350444	-0.407788
C	0.665060	-2.487738	0.080158
C	1.849749	-2.383823	-0.654722
C	2.868903	-1.544910	-0.218497
C	2.739962	-0.786199	0.939591
C	1.565142	-0.916139	1.670623
C	0.540289	-1.764552	1.269944
C	4.083784	-1.390212	-1.090709
F	5.121822	-0.883489	-0.423083
C	1.372316	-0.163226	2.958070
F	0.205824	0.511885	2.955364
C	-2.780402	1.467025	-1.705167
F	4.462256	-2.564383	-1.616505
F	3.824933	-0.568334	-2.123126
F	1.314510	-1.003821	4.003499
F	2.350390	0.709841	3.196176
H	-3.205940	-2.745605	0.875466

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H          0.012503       -4.151036       -0.923874
H         -2.325255       -0.637003        2.127049
H         -1.858856        0.735464        1.153975
H         -4.088584        1.304222        0.629775
H         -4.312922        0.579308        2.210834
H         -5.973825       -0.338130        0.625789
H         -4.882423       -1.608755        1.111345
H         -5.020346       -0.075983       -1.517627
H         -5.074232       -1.809118       -1.288107
H         -1.168868       -0.932297       -0.289700
H         -2.866097       -1.885881       -1.800119
H         -2.371892        1.660850       -0.709707
H         -2.263680        2.137458       -2.400067
H         -3.847625        1.752693       -1.702560
H         -4.072658        0.058045       -3.622921
H         -2.735051       -1.100438       -3.833398
H         -2.471207        0.626281       -4.140185
H          1.968485       -2.947461       -1.576102
H          3.520504       -0.102592        1.253051
H         -0.353707       -1.860668        1.877142
C          1.264287        3.173116        0.090778
O          1.636567        1.956561        0.745172
C          1.592248        1.934080       -0.639307
N          2.955022        1.938810       -1.274922
O          3.930245        1.897156       -0.554822
O          2.962816        2.008486       -2.487764
C          0.607890        1.062816       -1.357989
H          0.365659        1.477032       -2.338299
H         -0.302201        1.013185       -0.760144
H          1.011934        0.055351       -1.490207
C         -0.157901        3.606264        0.214746
C         -2.827801        4.384504        0.412555
C         -0.725303        4.411399       -0.774499
C         -0.923460        3.196679        1.305592
C         -2.257637        3.588461        1.403835
C         -2.058968        4.797430       -0.675310
H         -0.125884        4.726219       -1.625199
H         -0.470905        2.565674        2.064143
H         -2.851217        3.268940        2.255623
H         -2.499914        5.417604       -1.449534
H         -3.868159        4.685703        0.487526
H          2.036567        3.941690        0.135876

SR epoxide:Catalyst, binary complex 107; Energy = -2449.832709; 6-31G(d) basis set.
N          0.164922       -2.537043        0.163454
C         -0.245205       -2.205847       -1.075501
S         -0.884708       -3.335050       -2.141142
C          0.173049       -1.757517        1.418532
C          1.544058       -1.186391        1.841543
C          1.422194       -0.668250        3.287743
C          0.321246        0.388911        3.401749
C         -1.021260       -0.182264        2.949196
C         -0.928051       -0.691471        1.508624
N          2.628899       -2.135554        1.594180
C          3.935573       -1.560600        1.872635
N         -0.118015       -0.883566       -1.446232
C          1.086108       -0.156226       -1.223711
C          2.332474       -0.781269       -1.320709
C          3.481743       -0.028073       -1.127139
C          3.415479        1.331265       -0.822389
C          2.168572        1.933796       -0.732902
C          1.002995        1.201003       -0.941297
C          4.833164       -0.662642       -1.311457
F          4.783200       -1.993744       -1.188170
C          2.040244        3.373638       -0.327936
F          3.186142        4.045627       -0.470136
C          2.502498       -3.413116        2.277997
F          5.334514       -0.391055       -2.525029
F          5.719084       -0.200565       -0.414437
F          1.101026        4.006432       -1.051989
F          1.668594        3.485082        0.960230
H          0.138596       -3.539580        0.298720
H         -0.551753       -0.704763       -2.346640
H         -0.718288        0.153898        0.841977
H         -1.879654       -1.128720        1.186122
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H         -1.308440       -1.009799        3.612563
H         -1.807849        0.573618        3.022122
H          0.256235        0.758221        4.430602
H          0.577550        1.249965        2.766349
H          1.196008       -1.502518        3.966319
H          2.381720       -0.247252        3.606086
H         -0.089749       -2.512672        2.171479
H          1.764357       -0.312120        1.215526
H          1.577731       -3.925701        1.999316
H          3.333923       -4.054510        1.971318
H          2.532604       -3.329330        3.378002
H          3.999418       -0.557121        1.441238
H          4.711243       -2.181028        1.413685
H          4.157463       -1.480816        2.950609
H          2.398054       -1.843627       -1.531392
H          4.322142        1.903904       -0.657696
H          0.026925        1.669872       -0.857147
C         -5.003725        0.834457       -0.112123
O         -5.402806        0.574472       -1.453957
C         -4.915647       -0.508176       -0.736427
N         -6.037700       -1.432611       -0.311843
O         -7.149657       -0.955282       -0.224820
O         -5.737408       -2.582323       -0.057988
C         -3.679183       -1.219927       -1.186637
H         -2.873509       -0.491269       -1.301569
H         -3.854171       -1.719907       -2.142710
H         -3.380145       -1.973995       -0.458630
C         -3.814708        1.705889        0.093221
C         -1.639064        3.403018        0.522044
C         -3.106450        2.222230       -0.993562
C         -3.436864        2.048384        1.392466
C         -2.345733        2.886441        1.605979
C         -2.027846        3.075920       -0.777045
H         -3.426413        1.973590       -2.001115
H         -4.002881        1.663421        2.237660
H         -2.054795        3.146484        2.619499
H         -1.488166        3.492171       -1.623200
H         -0.796184        4.065676        0.686619
H         -5.841437        0.986121        0.568188

SR epoxide:Catalyst, binary complex 108; Energy = -2449.836798; 6-31G(d) basis set.
N         -2.581417        0.061501       -0.601592
C         -1.484431        0.196020       -1.365895
S         -1.396512        1.211160       -2.701454
C         -3.892405        0.619480       -0.895451
C         -4.923312       -0.095060       -0.005556
C         -6.345162        0.259186       -0.491838
C         -6.418427        1.691606       -1.055035
C         -5.415403        2.596193       -0.336483
C         -3.971734        2.137171       -0.623657
N         -4.630163       -1.524639        0.139639
C         -4.642059       -2.280768       -1.106152
N         -0.456245       -0.620679       -0.953521
C          0.921264       -0.515965       -1.204598
C          1.566483        0.699271       -1.443086
C          2.953305        0.743530       -1.467148
C          3.731293       -0.395493       -1.294164
C          3.075532       -1.604493       -1.109180
C          1.687801       -1.674367       -1.074550
C          3.593626        2.098936       -1.540699
F          3.063139        2.853825       -2.510829
C          3.840460       -2.878819       -0.902933
F          5.162814       -2.693939       -0.950364
C         -5.482555       -2.156325        1.134931
F          3.406480        2.770283       -0.385258
F          4.913024        2.030640       -1.748803
F          3.552447       -3.427840        0.294428
F          3.524080       -3.801312       -1.824036
H         -2.603240       -0.674195        0.104720
H         -0.694544       -1.345689       -0.280497
H         -3.319341        2.364292        0.227822
H         -3.565149        2.665003       -1.488592
H         -5.540736        3.637717       -0.646289
H         -5.620281        2.566184        0.741166
H         -6.187475        1.686889       -2.127234
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H	-7.436314	2.080474	-0.957530
H	-6.663277	-0.458373	-1.257004
H	-7.039747	0.154079	0.349008
H	-4.114117	0.431280	-1.955021
H	-4.794695	0.320285	1.006764
H	-6.533191	-2.244276	0.812014
H	-5.111456	-3.164958	1.345299
H	-5.458475	-1.577485	2.064434
H	-3.966142	-1.825007	-1.835239
H	-5.642165	-2.366407	-1.560266
H	-4.282034	-3.294152	-0.901061
H	0.989988	1.606643	-1.573322
H	4.813019	-0.339878	-1.297604
H	1.196581	-2.631355	-0.920396
C	1.480944	0.093845	2.717650
O	2.331074	0.413419	1.611530
C	1.558703	1.443674	2.127410
N	2.402302	2.406624	2.937676
O	3.418292	1.973663	3.437603
O	1.982532	3.541738	3.046285
C	0.519126	2.127255	1.291951
H	1.000925	2.802531	0.581767
H	-0.153566	2.708377	1.924646
H	-0.052279	1.369511	0.751311
C	0.340730	-0.827213	2.427245
C	-1.745649	-2.586433	1.830064
C	0.619866	-2.096307	1.914489
C	-0.981832	-0.451424	2.664974
C	-2.022353	-1.330410	2.369164
C	-0.421301	-2.973150	1.613562
H	1.650875	-2.384420	1.727213
H	-1.197943	0.533653	3.070153
H	-3.052742	-1.031167	2.539659
H	-0.200134	-3.956102	1.207899
H	-2.561853	-3.258415	1.582097
H	2.034269	-0.068364	3.642240

SR epoxide:Catalyst, binary complex 109; Energy = -2449.826637; 6-31G(d) basis set.

N	2.971448	0.270174	-0.278221
C	2.342406	-0.905821	-0.423740
S	3.035301	-2.326821	-1.005166
C	4.391754	0.566185	-0.517878
C	5.340415	-0.137397	0.480321
C	6.764209	0.318505	0.130747
C	7.202050	-0.160715	-1.273276
C	6.009658	-0.585841	-2.142155
C	4.826148	0.371222	-1.995910
N	5.038248	0.084490	1.892371
C	4.021975	-0.777534	2.468334
N	1.026980	-0.937464	-0.032542
C	0.146449	0.111119	0.277495
C	-0.841679	-0.130046	1.239313
C	-1.780428	0.849009	1.530969
C	-1.751175	2.086686	0.895798
C	-0.770604	2.314207	-0.061824
C	0.170021	1.342149	-0.387981
C	-2.790981	0.607313	2.620172
F	-3.070787	-0.694440	2.763467
C	-0.798132	3.594804	-0.849762
F	0.418997	3.929858	-1.297249
C	4.851142	1.460462	2.298397
F	-2.323439	1.037721	3.804403
F	-3.933608	1.259204	2.390588
F	-1.595492	3.480416	-1.925301
F	-1.264026	4.615757	-0.121527
H	2.480282	0.974157	0.262350
H	0.635486	-1.873745	-0.002712
H	3.975459	0.003507	-2.575742
H	5.098133	1.348982	-2.410586
H	6.311332	-0.635599	-3.193560
H	5.680010	-1.590620	-1.861526
H	7.755569	0.641085	-1.774091
H	7.894145	-1.003915	-1.182129
H	6.804085	1.414955	0.172028
H	7.442319	-0.047691	0.905986

H	4.456866	1.636076	-0.291283
H	5.273100	-1.217948	0.322519
H	3.879063	1.890018	1.983290
H	4.887142	1.520748	3.391067
H	5.648014	2.095256	1.902223
H	4.150086	-0.807713	3.556622
H	4.131849	-1.792932	2.078673
H	2.986253	-0.446075	2.269567
H	-0.871926	-1.090044	1.746272
H	-2.484145	2.849793	1.133904
H	0.892036	1.529870	-1.175589
C	-4.110116	-1.737948	-0.530744
O	-4.236370	-0.506920	0.196019
C	-4.154178	-0.417461	-1.185727
N	-5.503929	-0.102966	-1.800375
O	-5.494407	0.444516	-2.885305
O	-6.491634	-0.436509	-1.181711
C	-3.026297	0.335273	-1.822313
H	-3.188787	1.411170	-1.724777
H	-2.945907	0.091223	-2.882319
H	-2.101235	0.064354	-1.311057
C	-2.850824	-2.519104	-0.345771
C	-0.542738	-4.035424	0.073762
C	-2.617657	-3.114531	0.897479
C	-1.934900	-2.701648	-1.382198
C	-0.782130	-3.458741	-1.173437
C	-1.464942	-3.864890	1.108423
H	-3.336458	-2.975598	1.699274
H	-2.122218	-2.258343	-2.355986
H	-0.061517	-3.585777	-1.975314
H	-1.286404	-4.320989	2.077045
H	0.361553	-4.614406	0.234801
H	-5.040434	-2.304657	-0.537349

SR epoxide:Catalyst, binary complex 110; Energy = -2449.830463; 6-31G(d) basis set.

N	-1.375152	-1.239284	0.014223
C	-1.226321	-0.606874	1.186854
S	-2.478663	-0.221212	2.245477
C	-2.630156	-1.684801	-0.611634
C	-3.338803	-2.828817	0.147083
C	-4.562317	-3.223247	-0.695059
C	-5.585279	-2.069178	-0.834966
C	-4.999581	-0.717734	-0.405169
C	-3.590702	-0.512469	-0.959960
N	-2.509490	-3.991650	0.448609
C	-1.684749	-4.490173	-0.630193
N	0.054766	-0.238343	1.531505
C	1.286497	-0.553217	0.939927
C	1.533367	-1.781597	0.321978
C	2.777718	-2.031447	-0.250925
C	3.805368	-1.104219	-0.185670
C	3.566743	0.096923	0.480981
C	2.327345	0.385674	1.031059
C	2.999902	-3.376159	-0.887823
F	3.189436	-4.329624	0.034217
C	4.684995	1.103846	0.570980
F	5.857995	0.490743	0.795950
C	-1.783435	-3.943219	1.703254
F	1.934762	-3.747366	-1.617964
F	4.066612	-3.377002	-1.693714
F	4.816163	1.792721	-0.567958
F	4.487345	1.979452	1.560891
H	-0.563690	-1.275696	-0.590879
H	0.076247	0.443441	2.280888
H	-3.177939	0.422490	-0.567539
H	-3.640262	-0.409104	-2.050551
H	-5.648124	0.098206	-0.742610
H	-4.955290	-0.656066	0.687206
H	-5.923344	-2.004295	-1.875195
H	-6.475177	-2.281812	-0.234125
H	-4.218688	-3.537070	-1.689646
H	-5.017342	-4.103000	-0.233008
H	-2.283790	-2.125962	-1.552712
H	-3.691475	-2.447155	1.108582
H	-2.428961	-3.546680	2.490959

H	-1.482683	-4.959662	1.981843
H	-0.868970	-3.324181	1.675154
H	-1.320382	-5.490039	-0.372531
H	-0.794863	-3.864978	-0.842206
H	-2.264747	-4.575669	-1.553700
H	0.779063	-2.562122	0.317244
H	4.774987	-1.312281	-0.623866
H	2.158666	1.336543	1.529984
C	-0.167059	3.795921	0.082951
O	0.294234	2.668330	0.827124
C	0.552093	2.657293	-0.537489
N	2.002411	2.944714	-0.833938
O	2.412299	2.593149	-1.921971
O	2.643753	3.525616	0.017842
C	-0.046585	1.613128	-1.429006
H	-0.138188	1.992360	-2.448106
H	-1.035919	1.356004	-1.045284
H	0.589835	0.723871	-1.446699
C	-1.637475	3.957730	-0.080088
C	-4.385996	4.250367	-0.435899
C	-2.133723	5.031110	-0.821689
C	-2.516976	3.041652	0.495719
C	-3.889485	3.187744	0.315702
C	-3.506382	5.173034	-1.001310
H	-1.447853	5.753366	-1.257346
H	-2.130203	2.220219	1.092649
H	-4.564741	2.467662	0.770097
H	-3.889929	6.006974	-1.580731
H	-5.456263	4.365856	-0.576388
H	0.423754	4.695416	0.253679

SR epoxide:Catalyst, binary complex 111; Energy = -2449.828599; 6-31G(d) basis set.

N	-1.820607	-0.990234	0.653332
C	-1.671263	-2.260029	1.057980
S	-2.896141	-3.281167	1.581161
C	-3.059084	-0.200107	0.618252
C	-4.074717	-0.677236	-0.446988
C	-5.272099	0.280126	-0.365287
C	-6.021600	0.161398	0.980995
C	-5.156728	-0.487371	2.071693
C	-3.706693	-0.004776	2.016251
N	-3.554281	-0.767009	-1.808762
C	-2.849633	0.399636	-2.295484
N	-0.383866	-2.750043	0.991747
C	0.828723	-2.040542	0.986391
C	0.989714	-0.821492	1.656626
C	2.223376	-0.180901	1.629224
C	3.317957	-0.733239	0.970515
C	3.148703	-1.952671	0.324252
C	1.921835	-2.604038	0.322792
C	2.378982	1.134750	2.344744
F	1.225224	1.822922	2.339534
C	4.263673	-2.527667	-0.505248
F	4.112439	-2.190649	-1.795632
C	-2.831509	-1.985003	-2.128484
F	2.741222	0.973157	3.620681
F	3.309512	1.897338	1.754819
F	5.460962	-2.082002	-0.111666
F	4.280215	-3.865713	-0.448212
H	-1.036482	-0.583672	0.150237
H	-0.328339	-3.752304	1.125774
H	-3.110751	-0.530799	2.767649
H	-3.670045	1.061055	2.270921
H	-5.575270	-0.272096	3.060345
H	-5.164928	-1.575348	1.957019
H	-6.343197	1.156975	1.305668
H	-6.933029	-0.431131	0.850798
H	-4.910312	1.309379	-0.491982
H	-5.935165	0.076008	-1.210269
H	-2.708366	0.779379	0.274630
H	-4.413595	-1.683905	-0.183201
H	-3.343885	-2.846196	-1.691044
H	-2.805457	-2.110605	-3.217883
H	-1.784512	-1.989614	-1.775844
H	-2.733367	0.323849	-3.381692

H	-1.829200	0.511570	-1.875239
H	-3.413998	1.312083	-2.079391
H	0.157805	-0.377724	2.193384
H	4.271876	-0.218174	0.945691
H	1.804174	-3.547125	-0.203255
C	1.277677	2.535945	-1.113619
O	1.171687	3.899215	-1.513588
C	0.291743	3.477978	-0.527854
N	0.692398	4.014177	0.828468
O	-0.192625	4.127057	1.654108
O	1.864442	4.266016	1.003745
C	-1.185979	3.504388	-0.767386
H	-1.395357	3.061986	-1.742237
H	-1.549678	4.534630	-0.751651
H	-1.706311	2.942002	0.009227
C	0.895036	1.499772	-2.112375
C	0.204178	-0.485917	-3.951208
C	1.128486	0.154919	-1.817918
C	0.337508	1.849507	-3.343534
C	-0.002407	0.857309	-4.259255
C	0.775984	-0.836018	-2.729416
H	1.610516	-0.112722	-0.883592
H	0.194753	2.898846	-3.584193
H	-0.429414	1.135474	-5.217944
H	0.969728	-1.878285	-2.491096
H	-0.065894	-1.256752	-4.666366
H	2.155065	2.327550	-0.500332

SR epoxide:Catalyst, binary complex 112; Energy = -2449.833281; 6-31G(d) basis set.

N	-2.500623	-0.331838	-0.602930
C	-1.439833	-0.516381	-1.408616
S	-1.399570	-0.048617	-3.017174
C	-3.790350	0.217514	-1.013711
C	-4.892275	-0.378814	-0.089147
C	-5.976617	0.668271	0.164857
C	-5.403285	1.858446	0.950892
C	-3.988369	2.242152	0.462287
C	-3.755034	1.756070	-0.967261
N	-5.444834	-1.658425	-0.527983
C	-6.272078	-1.582901	-1.722081
N	-0.413177	-1.176353	-0.767567
C	0.970717	-1.081426	-0.972413
C	1.582312	-0.014382	-1.634119
C	2.962379	0.119195	-1.579562
C	3.770392	-0.803177	-0.924720
C	3.152281	-1.892139	-0.326114
C	1.771166	-2.041820	-0.352690
C	3.545739	1.398850	-2.103892
F	3.240658	2.422209	-1.275728
C	3.947315	-2.924189	0.418760
F	3.543761	-3.005223	1.702663
C	-4.430336	-2.689320	-0.676835
F	4.877925	1.352236	-2.199674
F	3.056424	1.723249	-3.306575
F	3.786606	-4.148937	-0.104174
F	5.255554	-2.654207	0.426554
H	-2.386083	-0.533784	0.387336
H	-0.662458	-1.646359	0.098724
H	-2.791246	2.094786	-1.360365
H	-4.526889	2.157868	-1.633771
H	-3.835777	3.323030	0.535562
H	-3.226327	1.782074	1.107325
H	-6.080984	2.711812	0.848186
H	-5.374425	1.611887	2.018897
H	-6.379997	1.022128	-0.790711
H	-6.803997	0.201503	0.708250
H	-3.953511	-0.110131	-2.045707
H	-4.422108	-0.584111	0.888752
H	-3.822694	-2.743296	0.234092
H	-4.921240	-3.657039	-0.819267
H	-3.751664	-2.522235	-1.532377
H	-6.688184	-2.575249	-1.919407
H	-5.720493	-1.267562	-2.625626
H	-7.107585	-0.897003	-1.566966
H	0.982802	0.727970	-2.145773

H	4.843843	-0.669015	-0.872165
H	1.307432	-2.894270	0.138020
C	1.279103	1.137776	2.418333
O	2.121616	0.930390	1.283584
C	1.335000	2.073730	1.278799
N	2.166824	3.308989	1.544165
O	1.733825	4.359680	1.114570
O	3.188025	3.167753	2.181949
C	0.263594	2.285626	0.251989
H	-0.454200	3.030923	0.601206
H	-0.252748	1.337205	0.089132
H	0.701868	2.635702	-0.684503
C	0.144201	0.177166	2.567168
C	-1.947729	-1.659610	2.814639
C	-1.160405	0.625593	2.773530
C	0.405788	-1.194155	2.508151
C	-0.638594	-2.109919	2.625458
C	-2.204915	-0.290903	2.901058
H	-1.361753	1.692379	2.833474
H	1.426228	-1.538455	2.361578
H	-0.431156	-3.175378	2.584263
H	-3.217689	0.065361	3.070115
H	-2.760206	-2.373178	2.914863
H	1.829940	1.419630	3.314905

SR epoxide:Catalyst, binary complex 113; Energy = -2449.828034; 6-31G(d) basis set.

N	3.642415	0.341751	0.756091
C	3.325696	0.151431	2.059438
S	4.425660	0.392187	3.302055
C	2.793157	1.038253	-0.232402
C	2.889845	2.593742	-0.006340
C	3.709307	3.270873	-1.117379
C	3.351295	2.912432	-2.576780
C	2.695155	1.529621	-2.701756
C	3.223254	0.580130	-1.630563
N	1.629051	3.276820	0.279924
C	0.647587	3.339172	-0.786046
N	2.043708	-0.247882	2.345443
C	1.184220	-1.073732	1.596735
C	1.610791	-1.836416	0.507468
C	0.703390	-2.655432	-0.154689
C	-0.619470	-2.766753	0.256041
C	-1.025015	-2.021447	1.358196
C	-0.144944	-1.173525	2.019709
C	1.213653	-3.435810	-1.336299
F	1.692411	-2.626324	-2.292465
C	-2.430863	-2.121689	1.885471
F	-3.013900	-0.911790	1.962598
C	1.007899	2.827664	1.510068
F	2.228275	-4.239439	-0.973582
F	0.267959	-4.204478	-1.883393
F	-3.204067	-2.903475	1.130510
F	-2.440421	-2.624845	3.130800
H	4.627030	0.571531	0.654921
H	1.842937	-0.210968	3.337899
H	4.321536	0.548899	-1.681165
H	2.861109	-0.438226	-1.801122
H	1.607825	1.604410	-2.594354
H	2.878086	1.111117	-3.696105
H	2.706067	3.675555	-3.023251
H	4.276745	2.924746	-3.163224
H	3.670698	4.352759	-0.957185
H	4.750710	2.974526	-0.942505
H	1.755982	0.727700	-0.074221
H	3.470277	2.724998	0.916399
H	0.524542	1.833151	1.424494
H	1.753855	2.769719	2.310052
H	0.236458	3.546413	1.809899
H	1.096346	3.726451	-1.702068
H	-0.144996	4.035919	-0.490262
H	0.173430	2.363641	-1.007078
H	2.643581	-1.791828	0.179084
H	-1.319210	-3.401112	-0.274730
H	-0.487089	-0.589458	2.871019
C	-2.371338	0.510452	-0.388072

O	-2.891587	-0.779227	-0.757333
C	-2.247607	-0.039380	-1.744249
N	-0.913818	-0.673351	-2.068472
O	-0.967253	-1.718277	-2.682025
O	0.104369	-0.121467	-1.693640
C	-2.979444	0.361953	-2.987212
H	-3.223143	-0.528357	-3.570813
H	-2.359414	1.031300	-3.589229
H	-3.897224	0.882146	-2.709269
C	-3.363410	1.558451	-0.026385
C	-5.184669	3.557748	0.650757
C	-4.732319	1.335629	-0.178790
C	-2.910070	2.773932	0.487452
C	-3.818217	3.774074	0.818811
C	-5.639289	2.336273	0.158683
H	-5.077604	0.372674	-0.542842
H	-1.844297	2.930822	0.632099
H	-3.459477	4.719008	1.214595
H	-6.703857	2.158450	0.043038
H	-5.894154	4.336338	0.912941
H	-1.474916	0.460365	0.231763

SR epoxide:Catalyst, binary complex 114; Energy = -2449.832116; 6-31G(d) basis set.

N	1.761522	-1.521604	1.147174
C	0.763218	-1.449578	0.251505
S	0.939812	-1.133759	-1.386187
C	3.208041	-1.444240	0.917721
C	3.733160	-2.510660	-0.062740
C	5.266714	-2.412200	-0.129439
C	5.703088	-1.016416	-0.581818
C	5.179294	0.044605	0.386506
C	3.657040	-0.031397	0.514715
N	3.189549	-3.830740	0.252888
C	3.172159	-4.714558	-0.899349
N	-0.476048	-1.650288	0.836473
C	-1.726181	-1.296420	0.299394
C	-1.914014	-0.070566	-0.349990
C	-3.174129	0.274536	-0.811404
C	-4.271884	-0.564095	-0.627361
C	-4.075933	-1.766348	0.035167
C	-2.814355	-2.142397	0.491988
C	-3.365067	1.618398	-1.460604
F	-2.277747	1.999158	-2.145935
C	-5.214363	-2.725891	0.235825
F	-5.281794	-3.143197	1.510482
C	3.804255	-4.481166	1.396156
F	-4.399152	1.607006	-2.315753
F	-3.617309	2.571464	-0.553905
F	-6.395121	-2.178699	-0.074409
F	-5.069340	-3.824999	-0.519852
H	1.486042	-1.642270	2.113682
H	-0.505598	-2.244641	1.656625
H	3.189901	0.234538	-0.439951
H	3.300707	0.687653	1.261954
H	5.642030	-0.109048	1.371828
H	5.463525	1.048791	0.053438
H	6.794669	-0.963570	-0.654678
H	5.302403	-0.818664	-1.585692
H	5.700660	-2.617779	0.859549
H	5.651120	-3.178722	-0.812755
H	3.641636	-1.656725	1.903898
H	3.343376	-2.250475	-1.051410
H	3.812785	-3.811013	2.261908
H	3.215218	-5.364002	1.664636
H	4.840921	-4.813114	1.210919
H	2.633238	-5.632065	-0.641487
H	4.179382	-5.005679	-1.248565
H	2.642699	-4.227721	-1.723292
H	-1.080860	0.607604	-0.492188
H	-5.253017	-0.283862	-0.992284
H	-2.680103	-3.098979	0.989710
C	0.418950	3.757672	0.356023
O	-0.817350	3.062071	0.207639
C	-0.127446	2.858269	1.396057
N	-0.780374	3.574705	2.550637

O	-0.585482	3.113247	3.659492
O	-1.428382	4.567888	2.299434
C	0.405127	1.502639	1.734081
H	-0.403492	0.838110	2.051330
H	1.144064	1.572552	2.534540
H	0.881065	1.096291	0.837801
C	1.559947	3.323724	-0.498539
C	3.717422	2.520171	-2.068224
C	2.847347	3.779278	-0.202218
C	1.352990	2.469319	-1.579611
C	2.433817	2.070313	-2.364137
C	3.923554	3.375720	-0.984975
H	3.003811	4.450366	0.638842
H	0.348045	2.125036	-1.807182
H	2.267944	1.397081	-3.199248
H	4.923333	3.730230	-0.752729
H	4.559274	2.205667	-2.678003
H	0.293064	4.825528	0.531050

SR epoxide:Catalyst, binary complex 115; Energy = -2449.831835; 6-31G(d) basis set.

N	-2.685399	-0.559702	-0.426844
C	-1.575749	-0.715287	-1.175396
S	-1.530695	-0.496508	-2.839523
C	-4.001151	-0.171876	-0.938531
C	-5.075003	-0.827082	-0.025296
C	-5.178266	-0.087116	1.321864
C	-5.177348	1.448570	1.251418
C	-4.050357	1.987068	0.367450
C	-4.104931	1.354816	-1.021728
N	-6.377667	-1.068168	-0.642142
C	-6.300209	-1.819281	-1.880976
N	-0.496053	-1.111415	-0.423737
C	0.867169	-1.149405	-0.758573
C	1.662648	-2.083178	-0.096524
C	3.046266	-2.043527	-0.228677
C	3.664388	-1.092383	-1.026264
C	2.854908	-0.189051	-1.707378
C	1.472302	-0.217481	-1.604899
C	3.856024	-3.003085	0.592505
F	3.359557	-4.248137	0.534807
C	3.479507	0.978232	-2.413177
F	3.548669	2.040142	-1.578078
C	-7.337535	0.015209	-0.731044
F	5.133925	-3.053318	0.206862
F	3.844226	-2.650455	1.893659
F	4.725839	0.723857	-2.823269
F	2.765469	1.373395	-3.473586
H	-2.569652	-0.568054	0.583133
H	-0.695474	-1.442551	0.516917
H	-3.292931	1.722853	-1.658023
H	-5.047044	1.620342	-1.516257
H	-4.121230	3.076897	0.290759
H	-3.073462	1.771540	0.825062
H	-6.129074	1.818893	0.857083
H	-5.090574	1.849671	2.268414
H	-6.062528	-0.456452	1.853166
H	-4.316591	-0.395932	1.930852
H	-4.064546	-0.599003	-1.941765
H	-4.687656	-1.834003	0.189056
H	-7.049245	0.835155	-1.411485
H	-8.280316	-0.399239	-1.102716
H	-7.536280	0.433902	0.257490
H	-5.577229	-2.634354	-1.773112
H	-6.003294	-1.213527	-2.754531
H	-7.280141	-2.256790	-2.098347
H	1.199829	-2.831842	0.541451
H	4.744148	-1.043602	-1.104306
H	0.869154	0.501946	-2.143171
C	1.784053	1.391552	2.184335
O	2.497624	0.986649	1.013753
C	1.834646	2.204230	0.953812
N	2.811600	3.358332	1.030640
O	3.867450	3.158706	1.591265
O	2.451671	4.410924	0.542059
C	0.710631	2.445039	-0.009311

H	1.107987	2.643521	-1.007015
H	0.123685	3.309441	0.306396
H	0.070226	1.560202	-0.033952
C	0.580694	0.575028	2.527980
C	-1.634361	-1.006472	3.159302
C	0.733872	-0.801245	2.717547
C	-0.676967	1.159094	2.674411
C	-1.782330	0.370573	2.993921
C	-0.371814	-1.591353	3.025517
H	1.718156	-1.248322	2.605137
H	-0.794715	2.231300	2.539918
H	-2.755347	0.836828	3.124153
H	-0.248897	-2.660198	3.173965
H	-2.493678	-1.619923	3.415045
H	2.440822	1.692983	2.999748

SR epoxide:Catalyst, binary complex 116; Energy = -2449.827005; 6-31G(d) basis set.

N	-2.269612	-1.741241	-1.775957
C	-0.920212	-1.675051	-1.797475
S	-0.108441	-1.829110	-3.266997
C	-3.206969	-1.499906	-0.675727
C	-3.115225	-2.556918	0.478128
C	-2.952532	-1.848454	1.828183
C	-4.067961	-0.835304	2.098168
C	-4.300999	0.100128	0.886553
C	-3.208510	-0.045861	-0.177791
N	-4.322086	-3.393668	0.430713
C	-4.471574	-4.249496	1.602216
N	-0.339283	-1.479234	-0.577109
C	0.998865	-1.284386	-0.185084
C	1.177939	-0.779820	1.109826
C	2.450431	-0.533498	1.599458
C	3.575801	-0.764342	0.817464
C	3.386493	-1.277689	-0.458510
C	2.122609	-1.556975	-0.969463
C	2.600846	-0.008314	3.000103
F	1.567423	0.767994	3.351473
C	4.571089	-1.456755	-1.367332
F	4.424719	-2.521058	-2.169162
C	-4.295728	-4.239569	-0.758999
F	2.653186	-1.014218	3.891600
F	3.722227	0.704105	3.146973
F	4.742298	-0.389418	-2.158410
F	5.706813	-1.624434	-0.674148
H	-2.664171	-1.866510	-2.698796
H	-0.983524	-1.368871	0.195323
H	-2.231465	0.262281	0.217908
H	-3.411213	0.611396	-1.030864
H	-5.261169	-0.140253	0.415726
H	-4.370119	1.142173	1.215168
H	-4.994126	-1.369878	2.330672
H	-3.806302	-0.253609	2.986992
H	-2.875144	-2.577074	2.638749
H	-1.988211	-1.322074	1.837308
H	-4.192139	-1.646663	-1.125335
H	-2.223294	-3.192685	0.307625
H	-3.441553	-4.940308	-0.750431
H	-5.221163	-4.818584	-0.813218
H	-4.224215	-3.639699	-1.669404
H	-3.579290	-4.873205	1.792868
H	-5.321442	-4.916917	1.438083
H	-4.684476	-3.658852	2.495423
H	0.316454	-0.535871	1.725297
H	4.568262	-0.535001	1.187684
H	2.014763	-1.961378	-1.965433
C	-0.036746	3.263781	0.407272
O	-0.126761	1.883075	0.765648
C	0.634519	2.193570	-0.359641
N	2.114063	2.080425	-0.073482
O	2.827807	1.745213	-0.996562
O	2.490548	2.346491	1.051310
C	0.233408	1.716077	-1.720740
H	0.623793	2.392735	-2.484125
H	-0.857648	1.707691	-1.775113
H	0.618752	0.714549	-1.922612

C	-1.266654	3.917224	-0.122764
C	-3.556355	5.140574	-1.136426
C	-1.160305	5.107667	-0.843486
C	-2.518983	3.348030	0.099549
C	-3.662730	3.958155	-0.408097
C	-2.304433	5.715794	-1.350609
H	-0.183036	5.553625	-1.010328
H	-2.585254	2.432177	0.677810
H	-4.636845	3.510561	-0.232593
H	-2.219543	6.638882	-1.915248
H	-4.447159	5.615986	-1.534681
H	0.594710	3.840204	1.081579

SR epoxide:Catalyst, binary complex 117; Energy = -2449.831212; 6-31G(d) basis set.

N	-2.374843	-1.216151	-0.194841
C	-1.255995	-1.582299	-0.852828
S	-1.162160	-1.748640	-2.514860
C	-3.643890	-0.852250	-0.832411
C	-4.789973	-1.178158	0.165989
C	-4.928591	-0.090647	1.253754
C	-4.774581	1.370176	0.808315
C	-3.534130	1.558814	-0.064890
C	-3.585421	0.619729	-1.269402
N	-6.067688	-1.550302	-0.441480
C	-6.015044	-2.837314	-1.114647
N	-0.215936	-1.851002	0.018305
C	1.165099	-1.674648	-0.138005
C	1.976902	-2.065793	0.934372
C	3.336777	-1.791652	0.922028
C	3.929332	-1.123788	-0.144211
C	3.117117	-0.766372	-1.210081
C	1.757200	-1.050180	-1.236429
C	4.159146	-2.161201	2.124726
F	3.724993	-3.298443	2.689223
C	3.658682	0.035702	-2.358315
F	4.976196	0.232978	-2.270294
C	-6.714122	-0.565615	-1.291493
F	5.449874	-2.326959	1.813136
F	4.098416	-1.211441	3.071022
F	3.406984	-0.546299	-3.537263
F	3.070131	1.250963	-2.400316
H	-2.260330	-0.907248	0.767417
H	-0.497389	-2.062669	0.969035
H	-2.710123	0.747268	-1.916597
H	-4.466224	0.853485	-1.877454
H	-3.454966	2.599174	-0.399007
H	-2.631085	1.358843	0.531651
H	-5.656063	1.711338	0.254597
H	-4.708318	2.002833	1.701151
H	-5.884227	-0.250267	1.763827
H	-4.145232	-0.279116	2.002507
H	-3.733444	-1.494411	-1.712819
H	-4.474359	-2.092196	0.684997
H	-6.205301	-0.414367	-2.259753
H	-7.731917	-0.906405	-1.507604
H	-6.787837	0.395333	-0.780102
H	-5.579013	-3.588140	-0.449200
H	-5.433436	-2.827603	-2.053284
H	-7.033963	-3.150691	-1.362702
H	1.540354	-2.579502	1.787415
H	4.987106	-0.890495	-0.141335
H	1.162247	-0.769378	-2.094742
C	1.088353	2.520744	1.130314
O	1.874263	1.510794	0.503928
C	1.131810	2.330270	-0.335594
N	1.996839	3.340268	-1.045218
O	3.053561	3.633760	-0.528888
O	1.548194	3.809589	-2.072109
C	0.016455	1.784176	-1.173031
H	0.393961	1.414913	-2.127959
H	-0.726546	2.561366	-1.366904
H	-0.455920	0.966754	-0.621835
C	-0.093374	2.074821	1.921415
C	-2.297586	1.264062	3.428876
C	-0.253667	0.728999	2.253621

C	-1.034205	3.013779	2.347795
C	-2.135691	2.607945	3.096095
C	-1.353313	0.326104	3.010449
H	0.509052	0.021762	1.939308
H	-0.902082	4.062811	2.096262
H	-2.864998	3.341498	3.424818
H	-1.461581	-0.715505	3.304687
H	-3.150330	0.950156	4.023317
H	1.676689	3.346236	1.529196

SR epoxide:Catalyst, binary complex 118; Energy = -2449.839675; 6-31G(d) basis set.

N	2.326551	-0.753613	-0.379358
C	1.159062	-1.405600	-0.487272
S	1.006714	-3.077680	-0.454783
C	3.629767	-1.393707	-0.242436
C	4.726282	-0.500644	-0.855959
C	6.070789	-1.263589	-0.846705
C	6.190290	-2.278063	0.302131
C	5.439274	-1.769844	1.531477
C	3.931087	-1.715277	1.240041
N	4.464027	0.016108	-2.199975
C	3.963687	-0.962519	-3.148156
N	0.092120	-0.541923	-0.673132
C	-1.277486	-0.808914	-0.537101
C	-2.167836	-0.099106	-1.346188
C	-3.535994	-0.234216	-1.158978
C	-4.049631	-1.086612	-0.188234
C	-3.153924	-1.793845	0.604607
C	-1.779144	-1.658663	0.452252
C	-4.491761	0.530416	-2.029003
F	-5.493718	1.060724	-1.307485
C	-3.680269	-2.735053	1.651706
F	-3.807161	-3.983677	1.182109
C	3.706189	1.249783	-2.282884
F	-3.889381	1.536283	-2.680604
F	-5.060418	-0.255597	-2.954554
F	-2.867251	-2.796456	2.716755
F	-4.890878	-2.355711	2.090721
H	2.308411	0.252287	-0.216900
H	0.318034	0.355247	-1.091636
H	3.455007	-0.952817	1.865051
H	3.456148	-2.672053	1.480238
H	5.628949	-2.405414	2.402006
H	5.808082	-0.767958	1.786900
H	5.763029	-3.243326	0.000427
H	7.244824	-2.462241	0.530027
H	6.201116	-1.770280	-1.808329
H	6.872343	-0.520500	-0.780662
H	3.570538	-2.327396	-0.811824
H	4.827258	0.378050	-0.205908
H	3.999372	1.924690	-1.472390
H	3.922346	1.745239	-3.237020
H	2.611981	1.107805	-2.230968
H	4.026831	-0.545809	-4.159001
H	2.912740	-1.247594	-2.962144
H	4.571043	-1.871261	-3.124168
H	-1.789701	0.576057	-2.107288
H	-5.120046	-1.181061	-0.040203
H	-1.101032	-2.196187	1.103174
C	0.526457	1.943791	1.059447
O	1.331655	2.201853	-0.101603
C	1.567511	2.999860	1.013844
N	2.857660	2.592284	1.692338
O	3.312903	1.497815	1.412633
O	3.331109	3.372782	2.487431
C	1.371738	4.482224	0.960039
H	0.389175	4.700422	0.542834
H	2.142106	4.938684	0.333402
H	1.436391	4.901143	1.963892
C	-0.931769	2.200770	0.931526
C	-3.684847	2.578116	0.697964
C	-1.800869	1.601960	1.846144
C	-1.447184	2.962801	-0.119803
C	-2.821443	3.154943	-0.230795
C	-3.173550	1.793028	1.730019

H	-1.402248	0.974362	2.639267
H	-0.774176	3.377538	-0.865005
H	-3.219272	3.739616	-1.053921
H	-3.845410	1.318067	2.438041
H	-4.756264	2.718794	0.602698
H	0.807849	1.026870	1.580570

SR epoxide:Catalyst, binary complex 119; Energy = -2449.832178; 6-31G(d) basis set.

N	1.755483	-1.706499	1.040161
C	0.744123	-1.498498	0.174453
S	0.914432	-1.123043	-1.448928
C	3.203883	-1.640007	0.792501
C	3.709454	-2.712896	-0.200223
C	5.236299	-2.598109	-0.319847
C	5.673554	-1.189952	-0.726936
C	5.189157	-0.162261	0.294620
C	3.668387	-0.220284	0.435274
N	3.322210	-4.086750	0.118993
C	3.500996	-4.488852	1.497441
N	-0.491012	-1.652897	0.775841
C	-1.734391	-1.237798	0.262517
C	-2.847236	-2.055134	0.432006
C	-4.097481	-1.624901	-0.008002
C	-4.255868	-0.396131	-0.631029
C	-3.133141	0.413713	-0.790637
C	-1.883382	0.014454	-0.344051
C	-5.264357	-2.553993	0.171436
F	-5.361163	-2.972521	1.443845
C	-3.282141	1.783034	-1.396646
F	-2.188311	2.143737	-2.082691
C	2.036065	-4.523503	-0.392583
F	-6.425416	-1.975454	-0.154505
F	-5.135203	-3.654514	-0.584941
F	-4.324396	1.835764	-2.239709
F	-3.489298	2.716017	-0.458193
H	1.494567	-1.792947	2.015560
H	-0.532633	-2.246328	1.596611
H	3.199477	0.093566	-0.503161
H	3.329155	0.472055	1.215600
H	5.661763	-0.367420	1.265959
H	5.486566	0.850358	0.001273
H	6.763339	-1.148885	-0.828266
H	5.249018	-0.946634	-1.711006
H	5.706495	-2.850976	0.641331
H	5.572929	-3.344998	-1.044915
H	3.642160	-1.887197	1.768782
H	3.285508	-2.488322	-1.183691
H	1.897475	-4.158905	-1.413108
H	2.011337	-5.619406	-0.409152
H	1.175637	-4.181499	0.210629
H	3.435684	-5.579885	1.566066
H	2.735978	-4.071397	2.181209
H	4.487068	-4.190986	1.864806
H	-2.741016	-3.031358	0.897398
H	-5.227992	-0.073960	-0.985131
H	-1.029236	0.670523	-0.465251
C	0.581253	3.714203	0.423853
O	-0.680884	3.066366	0.277651
C	0.019124	2.807951	1.449518
N	-0.590836	3.516247	2.632027
O	-0.397635	3.018416	3.725326
O	-1.205293	4.538629	2.416296
C	0.506809	1.425102	1.743504
H	-0.320533	0.784429	2.061290
H	1.264282	1.446834	2.529167
H	0.947336	1.024814	0.826252
C	1.694119	3.263272	-0.458260
C	3.802529	2.427422	-2.076950
C	3.000428	3.665136	-0.166763
C	1.443819	2.446311	-1.559075
C	2.500282	2.031316	-2.368083
C	4.051933	3.245805	-0.974119
H	3.191312	4.306314	0.690372
H	0.424459	2.144602	-1.783356
H	2.300159	1.389486	-3.220300

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H          5.066491        3.558045       -0.745417
H          4.625099        2.100282       -2.706066
H          0.495572        4.780843        0.628245

SR epoxide:Catalyst, binary complex 120; Energy = -2449.830253; 6-31G(d) basis set.
N         -2.341829       -1.016431       -0.771924
C         -1.194987       -1.122218       -1.474200
S         -1.032469       -0.668116       -3.075220
C         -3.588982       -0.432052       -1.281363
C         -4.758897       -1.096384       -0.517191
C         -4.904867       -0.529089        0.915032
C         -4.780200        0.996180        1.034965
C         -3.523504        1.513893        0.331971
C         -3.508542        1.094887       -1.139093
N         -5.982232       -1.143569       -1.329158
C         -6.822508        0.043704       -1.311067
N         -0.188628       -1.696939       -0.719329
C          1.197984       -1.502565       -0.752778
C          1.962642       -2.265145        0.139048
C          3.322778       -2.029493        0.278157
C          3.962385       -1.036963       -0.455920
C          3.197485       -0.309930       -1.356315
C          1.839115       -0.540824       -1.535021
C          4.087093       -2.822146        1.301149
F          3.662104       -4.093951        1.356502
C          3.790687        0.837836       -2.121713
F          5.103554        0.967557       -1.915830
C         -6.791514       -2.308251       -1.002665
F          5.399111       -2.841326        1.040118
F          3.933952       -2.310096        2.532511
F          3.590420        0.717044       -3.439735
F          3.207237        1.998835       -1.752553
H         -2.264965       -1.077885        0.240249
H         -0.507230       -2.231459        0.080755
H         -2.595416        1.433947       -1.641328
H         -4.344750        1.559708       -1.671620
H         -3.461626        2.604453        0.415368
H         -2.631955        1.117524        0.841468
H         -5.659535        1.490329        0.608059
H         -4.754199        1.267595        2.096770
H         -5.854034       -0.874762        1.343183
H         -4.119271       -0.978453        1.540442
H         -3.666856       -0.718155       -2.331672
H         -4.463729       -2.147419       -0.418671
H         -7.204483       -2.281631        0.022496
H         -7.634518       -2.364201       -1.697639
H         -6.198703       -3.220174       -1.113741
H         -6.254262        0.932196       -1.588511
H         -7.300992        0.225400       -0.332010
H         -7.619294       -0.083657       -2.050127
H          1.489177       -3.042120        0.734628
H          5.019505       -0.838582       -0.328690
H          1.282233        0.036333       -2.260650
C          1.088893        1.915013        1.960926
O          1.890333        1.181048        1.039789
C          1.188507        2.264037        0.527321
N          2.088748        3.442429        0.258718
O          3.127681        3.506910        0.879950
O          1.683310        4.260305       -0.542929
C          0.100183        2.081044       -0.485498
H          0.507824        2.077126       -1.497583
H         -0.630619        2.889278       -0.405454
H         -0.396413        1.128177       -0.284108
C         -0.128332        1.240715        2.495017
C         -2.400658       -0.009029        3.524986
C         -0.303571       -0.133857        2.329178
C         -1.088576        1.987422        3.179788
C         -2.223546        1.363621        3.690348
C         -1.437928       -0.757686        2.847362
H          0.474577       -0.698973        1.823132
H         -0.946044        3.056439        3.314917
H         -2.968178        1.947934        4.221565
H         -1.560616       -1.834347        2.751974
H         -3.280956       -0.496403        3.933324
H          1.667573        2.528191        2.650708
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SR epoxide:Catalyst, binary complex 121; Energy = -2449.835933; 6-31G(d) basis set.

N	-1.810772	-0.893896	0.495218
C	-0.642901	-1.528362	0.264148
S	-0.521501	-2.906264	-0.684919
C	-3.123382	-1.344035	0.047396
C	-4.189589	-0.968299	1.109129
C	-5.586331	-0.890138	0.451846
C	-5.710966	-1.775819	-0.789279
C	-4.775040	-1.269229	-1.897287
C	-3.454368	-0.728196	-1.317340
N	-4.218149	-1.808895	2.307125
C	-4.634221	-3.183703	2.087017
N	0.403928	-0.926256	0.928061
C	1.774490	-0.862663	0.629638
C	2.473120	-1.766398	-0.172918
C	3.826370	-1.543235	-0.427803
C	4.509540	-0.459328	0.097835
C	3.805646	0.422781	0.915203
C	2.463853	0.227696	1.188556
C	4.549260	-2.556574	-1.272489
F	4.731352	-3.706755	-0.606206
C	4.524947	1.627045	1.457896
F	3.807955	2.269574	2.387531
C	-3.001821	-1.768266	3.102451
F	3.856933	-2.855371	-2.380605
F	5.757709	-2.121442	-1.653868
F	5.693351	1.276136	2.020175
F	4.811055	2.501047	0.485188
H	-1.765259	0.056893	0.855290
H	0.117239	-0.170219	1.540524
H	-3.512055	0.361662	-1.186008
H	-2.621702	-0.931387	-1.999082
H	-4.572255	-2.076585	-2.607790
H	-5.268970	-0.468047	-2.458789
H	-5.454425	-2.811315	-0.537477
H	-6.746396	-1.790319	-1.143944
H	-6.336413	-1.135819	1.210052
H	-5.774741	0.146936	0.146743
H	-3.059005	-2.432034	-0.052840
H	-3.935456	0.041590	1.467987
H	-2.691740	-0.728070	3.252494
H	-3.207354	-2.205836	4.085235
H	-2.156768	-2.319831	2.656506
H	-4.704847	-3.685483	3.057029
H	-3.933315	-3.766362	1.462477
H	-5.623889	-3.217786	1.625021
H	1.971682	-2.625257	-0.597507
H	5.560209	-0.300610	-0.117198
H	1.934840	0.944581	1.811061
C	-0.739421	2.952862	-0.092763
O	-0.243486	1.822508	0.641680
C	0.260274	2.019241	-0.647798
N	1.680669	2.544425	-0.586404
O	1.981578	3.215759	0.379460
O	2.410869	2.253305	-1.509296
C	0.037428	1.004889	-1.726922
H	0.741933	0.174580	-1.631829
H	0.180414	1.463917	-2.706884
H	-0.984302	0.629174	-1.647177
C	-2.177037	2.890404	-0.487684
C	-4.883077	2.804697	-1.154880
C	-3.137541	2.688144	0.506596
C	-2.573794	3.057833	-1.814128
C	-3.925908	3.009993	-2.146664
C	-4.488617	2.647534	0.173236
H	-2.823560	2.571731	1.541633
H	-1.826499	3.220481	-2.586152
H	-4.230880	3.132317	-3.180916
H	-5.232183	2.494690	0.949786
H	-5.936390	2.769297	-1.415504
H	-0.355977	3.895168	0.295342

SR epoxide:Catalyst, binary complex 122; Energy = -2449.828357; 6-31G(d) basis set.

N	-0.885806	-2.637627	-0.277206

C	-0.816858	-2.216562	-1.560613
S	-0.392418	-3.266405	-2.806506
C	-0.663275	-1.942705	1.013602
C	0.468598	-0.877157	0.987287
C	0.365022	-0.003329	2.262972
C	-0.227034	-0.728976	3.477395
C	-1.662097	-1.228569	3.201376
C	-1.920931	-1.379286	1.695734
N	1.834442	-1.389361	0.809528
C	2.265413	-2.363309	1.798346
N	-1.075849	-0.897306	-1.822306
C	-2.123476	-0.159555	-1.213643
C	-1.902047	1.153761	-0.809971
C	-2.921739	1.848436	-0.164862
C	-4.156514	1.257694	0.076583
C	-4.369223	-0.045562	-0.362775
C	-3.370801	-0.754258	-1.017891
C	-2.627997	3.246421	0.303685
F	-2.380952	4.067707	-0.725953
C	-5.661069	-0.745633	-0.050031
F	-6.071746	-1.508903	-1.070948
C	2.151364	-1.857920	-0.533573
F	-3.644697	3.766737	1.002431
F	-1.540807	3.270525	1.090128
F	-5.520356	-1.558780	1.011385
F	-6.642516	0.117086	0.239227
H	-0.753113	-3.639870	-0.227038
H	-0.800781	-0.606132	-2.753532
H	-2.165946	-0.397651	1.285586
H	-2.778661	-2.032491	1.506472
H	-1.821954	-2.188132	3.705682
H	-2.396353	-0.530421	3.614884
H	0.407254	-1.579551	3.747888
H	-0.217805	-0.059599	4.342871
H	1.367030	0.378539	2.487496
H	-0.254111	0.873133	2.034655
H	-0.326123	-2.761468	1.660441
H	0.289810	-0.222872	0.126622
H	1.719764	-1.177490	-1.274816
H	3.242767	-1.860554	-0.656014
H	1.779274	-2.871099	-0.755430
H	3.294965	-2.659514	1.574055
H	1.665312	-3.289778	1.804126
H	2.251762	-1.930279	2.802650
H	-0.926608	1.607344	-0.961180
H	-4.938025	1.799374	0.596391
H	-3.543012	-1.773852	-1.351879
C	3.882228	1.286028	0.126250
O	3.885372	2.526706	-0.579280
C	3.275301	1.454111	-1.215144
N	1.770430	1.593692	-1.174852
O	1.276767	2.161301	-0.222182
O	1.144936	1.109502	-2.101850
C	3.790093	0.942023	-2.524041
H	4.873045	0.837481	-2.455474
H	3.544086	1.640576	-3.327063
H	3.351668	-0.029914	-2.753948
C	5.184242	0.599777	0.328076
C	7.578251	-0.763132	0.749520
C	6.354593	1.041084	-0.290530
C	5.220754	-0.504210	1.180365
C	6.413530	-1.190187	1.384519
C	7.548184	0.356601	-0.079693
H	6.327994	1.927852	-0.916909
H	4.306213	-0.806511	1.682071
H	6.435533	-2.051955	2.044521
H	8.458859	0.702583	-0.558551
H	8.511208	-1.294217	0.910106
H	3.178113	1.250227	0.955685

SR epoxide:Catalyst, binary complex 123; Energy = -2449.832224; 6-31G(d) basis set.

N	3.155454	-0.808949	0.925818
C	1.994054	-1.069142	0.293501
S	1.934550	-1.601224	-1.300522
C	4.483139	-0.917338	0.332361

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C          5.453592        0.064205        1.033159
C          6.916559       -0.337345        0.706174
C          7.048903       -1.173162       -0.569413
C          6.293913       -2.506493       -0.429024
C          5.025670       -2.346865        0.429712
N          5.232583        1.487330        0.782320
C          5.327546        1.883110       -0.609767
N          0.902628       -0.809893        1.089193
C         -0.470246       -1.036538        0.915589
C         -1.036703       -1.843288       -0.076922
C         -2.419102       -1.998809       -0.124895
C         -3.267220       -1.403991        0.799619
C         -2.691799       -0.610020        1.784630
C         -1.318008       -0.419563        1.844450
C         -2.973077       -2.851367       -1.235180
F         -2.399052       -4.065199       -1.242520
C         -3.541302        0.084770        2.812759
F         -3.153903       -0.242464        4.057193
C          4.053816        2.055081        1.412891
F         -4.291919       -3.028624       -1.130504
F         -2.725396       -2.304946       -2.436685
F         -3.421904        1.422092        2.720113
F         -4.833349       -0.218470        2.696084
H          3.131780       -0.622521        1.922881
H          1.110116       -0.303220        1.942524
H          5.244815       -2.555179        1.485952
H          4.249500       -3.050178        0.115200
H          6.023147       -2.881385       -1.421201
H          6.946144       -3.258699        0.026688
H          6.650025       -0.613420       -1.423660
H          8.105230       -1.356188       -0.788904
H          7.512418        0.578670        0.651416
H          7.320263       -0.920210        1.542626
H          4.370958       -0.650168       -0.723006
H          5.309260       -0.065658        2.117300
H          4.023911        1.756619        2.467321
H          4.123998        3.148141        1.376567
H          3.101869        1.768337        0.935900
H          5.320277        2.976579       -0.668715
H          4.497915        1.508043       -1.236808
H          6.269631        1.534036       -1.041068
H         -0.410562       -2.340248       -0.804600
H         -4.342103       -1.525719        0.734746
H         -0.900997        0.215250        2.623216
C         -2.274295        2.198388       -0.455050
O         -3.291070        2.963532       -1.112762
C         -3.147126        1.639817       -1.505060
N         -4.272923        0.788744       -0.964422
O         -4.774573        1.121684        0.089797
O         -4.571690       -0.200341       -1.605379
C         -2.755188        1.294072       -2.907715
H         -1.945047        1.958477       -3.211059
H         -3.605933        1.425309       -3.580358
H         -2.421883        0.255990       -2.961307
C         -0.861532        2.587701       -0.738813
C          1.776451        3.363564       -1.200880
C          0.088322        1.639850       -1.120516
C         -0.489952        3.925803       -0.595811
C          0.827701        4.311927       -0.822831
C          1.405033        2.029504       -1.354739
H         -0.196620        0.598509       -1.255667
H         -1.239454        4.660591       -0.314965
H          1.111610        5.353871       -0.712047
H          2.129654        1.281697       -1.665716
H          2.804296        3.664590       -1.384057
H         -2.537741        1.953319        0.573056

SR epoxide:Catalyst, binary complex 124; Energy = -2449.854641; 6-31G(d) basis set.
N         -1.062602        2.947502       -1.570534
O         -1.770249        2.079524       -1.090909
O         -1.416414        3.774266       -2.381822
N         -2.948042       -0.429364        0.073274
C         -1.848705       -1.139284        0.373689
S         -1.827839       -2.820235        0.503773
C         -4.298399       -0.965613        0.000943
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N	-0.749767	-0.351313	0.604534
C	0.592729	-0.763311	0.732320
C	1.392716	-0.119897	1.675489
C	2.758667	-0.378966	1.718707
C	3.348585	-1.280225	0.842810
C	2.538032	-1.921406	-0.087019
C	1.172537	-1.673232	-0.154417
C	3.597881	0.348224	2.729410
F	3.485694	-0.187114	3.953912
C	3.138177	-2.859512	-1.096142
F	2.711979	-2.573878	-2.340640
F	3.228519	1.636367	2.837650
F	4.899052	0.331005	2.408304
F	2.800260	-4.133510	-0.859864
F	4.476866	-2.793260	-1.111314
H	-2.915045	0.580607	0.193262
H	-0.882428	0.658914	0.590126
H	0.949911	0.609036	2.347556
H	4.417874	-1.453445	0.861105
H	0.561063	-2.152194	-0.911485
C	0.388782	2.976499	-1.144063
C	1.024681	1.635976	-1.155229
H	0.380633	0.821223	-1.490287
O	0.559027	2.270664	0.040302
C	1.048892	4.301700	-1.357822
H	2.098768	4.221347	-1.074978
H	0.980194	4.588922	-2.407031
H	0.566388	5.067943	-0.746257
C	2.487485	1.395720	-1.266513
C	5.203110	0.786372	-1.419667
C	3.386964	1.983058	-0.373907
C	2.950270	0.498472	-2.229909
C	4.305892	0.193873	-2.305905
C	4.742631	1.679437	-0.453678
H	3.014560	2.632573	0.412803
H	2.244735	0.009449	-2.896741
H	4.655727	-0.523746	-3.041124
H	5.434569	2.120421	0.256678
H	6.259008	0.539737	-1.471576
C	-4.608591	-1.640072	-1.338326
H	-4.409153	-1.719379	0.792541
C	-6.036383	-2.191352	-1.327894
H	-4.491891	-0.898598	-2.140149
H	-3.882011	-2.437991	-1.512267
C	-7.054666	-1.092763	-1.011711
H	-6.265282	-2.658612	-2.291301
H	-6.107758	-2.981076	-0.567634
C	-6.709029	-0.372906	0.296274
H	-7.059501	-0.359992	-1.830444
H	-8.064866	-1.511930	-0.954963
C	-5.282516	0.193406	0.235085
H	-7.424969	0.435403	0.482891
H	-6.790024	-1.077530	1.134696
H	-5.222437	0.844576	-0.652128
N	-4.854146	1.033607	1.355352
C	-5.590543	2.284039	1.431233
C	-4.836853	0.357147	2.644019
H	-4.412497	1.035724	3.390142
H	-5.838948	0.056813	2.993246
H	-4.200694	-0.531754	2.600696
H	-5.102377	2.945806	2.153563
H	-5.580366	2.775743	0.453548
H	-6.640178	2.158322	1.747079

SR epoxide:Catalyst, binary complex 125; Energy = -2449.850374; 6-31G(d) basis set.

C	-2.005955	-1.923428	-0.701624
C	-1.373892	-0.743760	-1.094476
C	-2.125264	0.439541	-1.169106
C	-3.456615	0.447957	-0.794232
C	-4.086765	-0.712090	-0.347592
C	-3.346360	-1.882271	-0.318293
N	-0.015003	-0.632358	-1.441394
C	1.091077	-1.286781	-0.938522
S	1.000045	-2.722335	-0.060268
C	-4.256692	1.716397	-0.867409

C	-3.961760	-3.145204	0.213531
N	2.234804	-0.637941	-1.226883
C	3.615263	-1.018564	-0.902628
C	3.892026	-1.191421	0.606155
C	5.388461	-1.469860	0.818955
C	5.833783	-2.712640	0.045452
C	5.556847	-2.537376	-1.448076
C	4.076041	-2.246872	-1.698829
N	3.350429	-0.068809	1.383344
C	2.945914	-0.472119	2.722286
C	4.221402	1.097235	1.452776
H	4.202242	-0.157496	-1.247943
H	3.472895	-3.110640	-1.399776
H	3.888744	-2.068361	-2.763033
H	5.857172	-3.431551	-2.004128
H	6.164308	-1.704990	-1.830585
H	5.286207	-3.589631	0.415998
H	6.898405	-2.902971	0.218056
H	5.981814	-0.609315	0.479975
H	5.584390	-1.590297	1.891523
H	3.341947	-2.078407	0.929553
H	0.191279	0.244698	-1.909570
H	2.153090	0.298807	-1.614971
H	2.427826	0.361451	3.209917
H	2.253417	-1.316787	2.656263
H	3.798156	-0.760807	3.362334
H	3.646919	1.953458	1.828607
H	5.081130	0.953001	2.128072
H	4.602720	1.356580	0.461245
H	-5.124773	-0.697520	-0.033923
F	-5.102534	1.709082	-1.909647
F	-5.006761	1.885895	0.234134
F	-3.482036	2.803939	-0.997559
F	-3.584160	-4.219313	-0.492955
F	-3.591582	-3.365821	1.486145
F	-5.301708	-3.098263	0.196632
O	0.703515	2.171831	-1.131793
C	0.911838	1.918497	0.290213
C	1.366435	3.143794	-0.404657
N	2.857083	3.093803	-0.674904
C	0.858360	4.558816	-0.346813
O	3.526766	3.962511	-0.159769
O	3.285142	2.175948	-1.349749
H	0.980938	4.979181	0.652321
H	1.408474	5.181605	-1.055187
H	-0.194300	4.564510	-0.627352
C	-0.292999	1.729027	1.139671
H	1.691080	1.168008	0.464964
C	-1.338221	2.647835	1.266270
C	-2.492889	2.298325	1.957725
C	-2.621650	1.027067	2.515700
C	-1.578589	0.111157	2.406180
C	-0.415487	0.466038	1.729599
H	-1.275379	3.630092	0.814345
H	-3.307643	3.011060	2.033599
H	-3.537931	0.751029	3.028678
H	-1.643589	1.365185	-1.471179
H	-1.677198	-0.887750	2.820030
H	0.387440	-0.259332	1.608612
H	-1.461898	-2.856127	-0.677101

SR epoxide:Catalyst, binary complex 126; Energy = -2449.854780; 6-31G(d) basis set.

N	-2.488515	2.852699	-1.349782
O	-3.097429	2.028349	-0.692731
O	-2.987962	3.678411	-2.082870
N	-2.346853	-0.705207	0.418818
C	-1.181423	-1.325113	0.673897
S	-0.981209	-2.993889	0.621645
C	-3.631660	-1.376516	0.276942
C	-3.855597	-1.955571	-1.123470
C	-5.207907	-2.671389	-1.180686
C	-6.353757	-1.742407	-0.769656
C	-6.092380	-1.105152	0.599954
C	-4.746756	-0.363598	0.590647
N	-0.184314	-0.441665	1.020315

C	1.207308	-0.599201	1.007414
C	1.953585	0.290433	1.781982
C	3.341799	0.282626	1.710156
C	4.015220	-0.618618	0.899464
C	3.259045	-1.501241	0.132512
C	1.872521	-1.499970	0.166576
C	4.105893	1.366076	2.410324
F	3.532561	1.725258	3.566490
C	3.971249	-2.473045	-0.766688
F	3.213416	-2.848149	-1.805498
F	4.161504	2.475445	1.644624
F	5.368993	1.009849	2.671466
F	4.325599	-3.588633	-0.112189
F	5.100822	-1.940724	-1.264170
H	-2.429567	0.295043	0.607327
H	-0.488487	0.500220	1.246278
H	-4.769240	0.352127	-0.243424
N	-4.418616	0.436029	1.771090
H	-6.080157	-1.885938	1.372252
H	-6.900697	-0.410448	0.854838
H	-7.302007	-2.289991	-0.757034
H	-6.457105	-0.944973	-1.518121
H	-5.179234	-3.534668	-0.502128
H	-5.380552	-3.066923	-2.186885
H	-3.658283	-2.206161	0.996748
H	-3.829806	-1.129904	-1.848600
H	1.447558	1.008342	2.421472
H	5.097777	-0.613396	0.839162
H	1.308874	-2.168783	-0.469863
C	-0.978270	2.825972	-1.273551
C	-0.413239	1.455908	-1.357127
H	-1.145028	0.654362	-1.472260
O	-0.554344	2.171295	-0.123772
C	-0.336398	4.104640	-1.711127
H	0.746492	3.986187	-1.674571
H	-0.637903	4.345332	-2.730395
H	-0.635058	4.921816	-1.050192
C	0.967265	1.155925	-1.819043
C	3.537514	0.469063	-2.656308
C	2.081130	1.744771	-1.214171
C	1.145079	0.209446	-2.829246
C	2.428241	-0.130692	-3.248267
C	3.361549	1.403047	-1.636098
H	1.946126	2.436003	-0.386987
H	0.279436	-0.273467	-3.275347
H	2.561753	-0.876713	-4.024719
H	4.221023	1.848588	-1.144567
H	4.537727	0.189676	-2.970903
H	-3.041005	-2.642735	-1.366266
C	-5.241170	1.628677	1.883575
C	-4.402381	-0.315521	3.016556
H	-4.025529	0.330712	3.815152
H	-5.398453	-0.679956	3.319111
H	-3.728643	-1.173881	2.934138
H	-4.842954	2.264367	2.680785
H	-5.199717	2.187425	0.944268
H	-6.296821	1.413802	2.122445

SR epoxide:Catalyst, binary complex 127; Energy = -2449.862528; 6-31G(d) basis set.

N	2.125044	-0.344686	-1.105800
C	1.587504	-0.547227	-2.313189
S	2.451346	-0.543602	-3.765113
C	3.565341	-0.309150	-0.875888
C	4.114651	-1.736235	-0.758867
C	5.634739	-1.723544	-0.618367
C	6.048159	-0.867242	0.576575
C	5.462887	0.544256	0.481064
C	3.924022	0.517224	0.365878
H	3.807460	-2.299025	-1.646437
N	0.225672	-0.744987	-2.370864
C	-0.669937	-1.183860	-1.390217
C	-2.027270	-0.903943	-1.578313
C	-2.967323	-1.335617	-0.650653
C	-2.585379	-2.030902	0.490001
C	-1.230638	-2.300134	0.668167

C	-0.275238	-1.908672	-0.258621
C	-4.422173	-1.047343	-0.900337
F	-5.114692	-0.969580	0.245288
C	-0.789645	-2.924682	1.961570
F	-0.816456	-2.016576	2.952875
F	-4.992747	-2.011725	-1.638781
F	-4.590669	0.104817	-1.561079
F	0.455014	-3.407958	1.896179
F	-1.600756	-3.926029	2.331225
H	1.515516	-0.111776	-0.322188
H	-0.134562	-0.691105	-3.315479
H	3.532990	-0.008643	1.251877
N	3.266976	1.838933	0.369548
H	5.886581	1.060312	-0.392035
H	5.758932	1.114437	1.366066
H	7.139109	-0.811776	0.654881
H	5.686979	-1.339966	1.500343
H	6.076073	-1.312543	-1.536359
H	6.013685	-2.745160	-0.511848
H	4.019691	0.158308	-1.757063
H	3.658147	-2.217082	0.118139
H	-2.341278	-0.317449	-2.436670
H	-3.316930	-2.343581	1.227554
H	0.765328	-2.156807	-0.090428
N	0.938149	1.183976	2.032271
O	1.137231	0.009545	1.767406
O	1.339060	1.753884	3.023316
C	0.041224	1.967641	1.103714
C	-1.189552	1.214190	0.753621
H	-1.271638	0.226036	1.206712
O	-0.071686	1.347323	-0.128527
C	-2.463408	1.865383	0.355049
C	-4.889895	3.026440	-0.371040
C	-3.609617	1.622108	1.113589
C	-2.537646	2.671989	-0.781675
C	-3.750870	3.251818	-1.140741
C	-4.818965	2.207518	0.753898
H	-3.555607	0.964593	1.978202
H	-1.647688	2.823298	-1.386123
H	-3.807010	3.874990	-2.027747
H	-5.708998	2.009606	1.342724
H	-5.835644	3.476535	-0.656098
C	0.195742	3.451468	1.186815
H	0.181625	3.781694	2.225056
H	1.140280	3.743131	0.722729
H	-0.627642	3.919827	0.645148
C	3.743271	2.660129	1.477961
C	3.388326	2.573482	-0.886102
H	2.891215	3.542404	-0.772369
H	4.434334	2.771982	-1.174496
H	2.892727	2.037675	-1.700099
H	3.069278	3.509608	1.625402
H	3.744296	2.072054	2.400186
H	4.756367	3.060289	1.313872

SR epoxide:Catalyst, binary complex 128; Energy = -2449.857476; 6-31G(d) basis set.

N	2.449061	0.846636	-1.089014
C	1.255908	1.359364	-0.732410
S	1.083736	2.667223	0.317357
C	3.753019	1.280755	-0.606206
C	4.674373	1.527236	-1.807448
C	6.067801	1.978759	-1.369503
C	6.688559	0.970956	-0.402541
C	5.766612	0.744413	0.796814
C	4.379792	0.247423	0.354898
H	4.209904	2.271419	-2.462753
N	0.199624	0.695561	-1.317796
C	-1.180973	0.806037	-1.074458
C	-1.830766	1.984265	-0.706643
C	-3.190666	1.944137	-0.404322
C	-3.932489	0.777105	-0.494993
C	-3.284680	-0.378489	-0.924017
C	-1.932122	-0.368762	-1.216201
C	-3.838865	3.189355	0.130558
F	-3.319666	4.298224	-0.410933

C	-4.089728	-1.636753	-1.071876
F	-3.313260	-2.726954	-1.184106
F	-3.670963	3.286527	1.461548
F	-5.159705	3.202703	-0.097257
F	-4.869297	-1.598280	-2.163622
F	-4.903642	-1.825345	-0.023868
H	2.465270	0.097450	-1.777667
H	0.450970	-0.143083	-1.836571
H	4.522554	-0.674749	-0.227683
N	3.473019	-0.109938	1.450502
H	5.655190	1.689898	1.344840
H	6.210080	0.022416	1.492126
H	7.670065	1.319621	-0.064739
H	6.849716	0.017237	-0.923606
H	5.990469	2.955841	-0.874215
H	6.705610	2.116859	-2.248729
H	3.591104	2.224776	-0.078476
H	4.759621	0.593803	-2.384513
H	-1.285071	2.913131	-0.631478
H	-4.986537	0.762119	-0.239206
H	-1.437747	-1.287679	-1.515934
N	1.976238	-2.357222	-1.264669
O	1.636814	-1.779550	-2.297278
O	3.117921	-2.530780	-0.921558
C	0.850734	-2.792989	-0.357294
C	0.746589	-1.899995	0.832178
H	1.511145	-1.116464	0.909632
O	1.295796	-3.229597	0.867410
C	-0.545776	-1.626810	1.506983
C	-3.041883	-0.964776	2.556253
C	-0.854886	-0.295246	1.796386
C	-1.469453	-2.633800	1.798926
C	-2.717146	-2.299328	2.316889
C	-2.104060	0.036230	2.310925
H	-0.125202	0.487384	1.593621
H	-1.205022	-3.674433	1.634115
H	-3.439778	-3.081285	2.527819
H	-2.348697	1.077393	2.499934
H	-4.023849	-0.707382	2.941762
C	-0.207610	-3.566764	-1.091087
H	0.086117	-4.619831	-1.120618
H	-1.163170	-3.478214	-0.574691
H	-0.319186	-3.199099	-2.111485
C	3.823232	-1.383251	2.068338
C	3.345128	0.911740	2.484923
H	2.485093	0.664629	3.116423
H	4.236443	0.973616	3.132105
H	3.155039	1.890103	2.040033
H	3.038260	-1.658762	2.782004
H	3.879859	-2.167625	1.309953
H	4.777072	-1.347244	2.622230

SR epoxide:Catalyst, binary complex 1; Energy = -2450.618419; TZVP basis set.

N	-2.230342	-0.794379	-1.195591
C	-1.405335	-1.789598	-0.878849
S	-1.897503	-3.274796	-0.246175
C	-3.666014	-0.778918	-0.952996
C	-4.124469	0.676452	-0.812408
C	-5.617128	0.688426	-0.454526
C	-6.436675	-0.032785	-1.526825
C	-5.942661	-1.463000	-1.735772
C	-4.450068	-1.485588	-2.058650
N	-3.230573	1.425726	0.076363
C	-3.532054	2.849135	0.102649
N	-0.067081	-1.566461	-1.100031
C	0.608312	-0.337664	-1.127700
C	0.197302	0.744106	-0.347379
C	0.968632	1.896096	-0.322248
C	2.145976	2.000517	-1.045545
C	2.538541	0.917633	-1.822076
C	1.778499	-0.236119	-1.884623
C	0.505133	3.067115	0.502333
F	-0.262612	2.685736	1.529531
C	3.828700	1.024512	-2.593734
F	3.829764	2.107645	-3.386618

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C         -3.139274        0.885837        1.424662
F          1.533792        3.757691        1.006294
F         -0.220384        3.927625       -0.228886
F          4.878715        1.149781       -1.772901
F          4.046635       -0.036907       -3.369903
H         -1.841419        0.069339       -1.553173
H          0.504432       -2.403366       -1.122683
H         -4.262134       -0.973977       -3.008365
H         -4.083949       -2.508572       -2.150891
H         -6.118902       -2.045573       -0.825522
H         -6.504337       -1.947761       -2.535892
H         -7.493005       -0.030782       -1.252180
H         -6.352927        0.517955       -2.469857
H         -5.765579        0.194611        0.511039
H         -5.964088        1.717839       -0.349701
H         -3.841612       -1.317681       -0.018105
H         -4.019393        1.147237       -1.799799
H         -2.783195       -0.145735        1.396776
H         -2.410263        1.468008        1.989462
H         -4.093011        0.912444        1.971596
H         -4.469957        3.082496        0.626256
H         -3.602086        3.228625       -0.917996
H         -2.723842        3.377009        0.608917
H         -0.699871        0.684597        0.257138
H          2.747484        2.899535       -1.002006
H          2.096766       -1.071858       -2.494976
C          2.421011       -0.861062        1.585528
O          3.535037       -1.647959        2.033190
C          2.631918       -2.266499        1.197188
N          3.168937       -2.393241       -0.219932
O          2.521451       -3.092363       -0.979255
O          4.148617       -1.766858       -0.523341
C          1.878246       -3.476527        1.653007
H          1.609668       -3.330711        2.696828
H          2.512602       -4.358453        1.564465
H          0.973561       -3.627189        1.064374
C          1.400682       -0.465221        2.595437
C         -0.454032        0.322352        4.510068
C          1.769667        0.426356        3.599595
C          0.097613       -0.952174        2.542222
C         -0.824195       -0.563583        3.506563
C          0.842928        0.820379        4.553964
H          2.785534        0.801977        3.635748
H         -0.199601       -1.643049        1.758160
H         -1.831253       -0.959557        3.474689
H          1.133552        1.512152        5.333998
H         -1.174943        0.622472        5.259893
H          2.723675       -0.104611        0.863254

SR epoxide:Catalyst, binary complex 2; Energy = -2450.614118; TZVP basis set.
N         -2.882992       -0.835482        0.514602
C         -2.774909       -1.627321        1.588541
S         -4.059437       -2.094151        2.570294
C         -4.134455       -0.233772        0.067516
C         -3.795922        0.956722       -0.838953
C         -5.098761        1.670441       -1.218678
C         -6.041458        0.712088       -1.949580
C         -6.320775       -0.535167       -1.112553
C         -5.021991       -1.220378       -0.691259
N         -2.741580        1.789794       -0.252549
C         -3.116368        2.448496        0.992720
N         -1.508530       -2.052803        1.912414
C         -0.322552       -1.970136        1.172720
C         -0.297212       -2.071192       -0.219033
C          0.914167       -2.006176       -0.889801
C          2.117476       -1.853966       -0.216136
C          2.079495       -1.800129        1.169466
C          0.882731       -1.851286        1.864050
C          0.894033       -2.072804       -2.393797
F          0.608722       -0.874950       -2.934242
C          3.348278       -1.599676        1.954497
F          3.495663       -0.315323        2.321932
C         -2.193198        2.745064       -1.203674
F          2.066137       -2.464985       -2.898772
F         -0.038900       -2.922789       -2.840155
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F          3.351993       -2.322186        3.081538
F          4.435029       -1.938544        1.257662
H         -2.061146       -0.312999        0.220237
H         -1.456445       -2.490962        2.821103
H         -4.477765       -1.573555       -1.573605
H         -5.226541       -2.082027       -0.056527
H         -6.880884       -0.253198       -0.214975
H         -6.946318       -1.234812       -1.669229
H         -6.974277        1.221984       -2.196785
H         -5.581361        0.413683       -2.897569
H         -5.587753        2.042415       -0.312863
H         -4.878939        2.534860       -1.848108
H         -4.684021        0.111313        0.949407
H         -3.360429        0.544035       -1.758650
H         -2.895964        3.548709       -1.462428
H         -1.301958        3.212433       -0.780353
H         -1.900800        2.228088       -2.119033
H         -3.894835        3.211222        0.856471
H         -2.236211        2.939380        1.412648
H         -3.465086        1.716120        1.721527
H         -1.214758       -2.228590       -0.769631
H          3.055617       -1.790708       -0.752257
H          0.875158       -1.786832        2.945762
C          2.654007        2.835229       -0.172452
O          1.432183        3.302167       -0.737479
C          1.339353        2.636469        0.472106
N          1.064344        3.605240        1.612951
O          1.432184        4.746471        1.478472
O          0.503685        3.156120        2.587929
C          0.595702        1.349346        0.585509
H          0.889279        0.714959       -0.250624
H         -0.482630        1.515131        0.548061
H          0.850727        0.857038        1.520681
C          3.358326        1.731032       -0.877794
C          4.755707       -0.269693       -2.213445
C          4.517674        1.197410       -0.319749
C          2.894886        1.255498       -2.100804
C          3.598563        0.262024       -2.769272
C          5.210569        0.194788       -0.984073
H          4.879938        1.569137        0.631665
H          1.994946        1.677066       -2.530750
H          3.240813       -0.096911       -3.725439
H          6.107632       -0.220587       -0.543617
H          5.302382       -1.043843       -2.736969
H          3.271516        3.630069        0.235764

SR epoxide:Catalyst, binary complex 3; Energy = -2450.617614; TZVP basis set.
N         -1.579582        0.329512       -1.032752
C         -0.926701        0.639293       -2.152706
S         -1.601862        1.501927       -3.435683
C         -3.007494        0.518224       -0.820146
C         -3.499979       -0.529345        0.183689
C         -5.024997       -0.407270        0.305360
C         -5.405133        0.994169        0.789662
C         -4.848941        2.073206       -0.138013
C         -3.339267        1.923098       -0.316825
N         -2.961879       -1.859202       -0.118229
C         -3.349423       -2.382414       -1.421292
N          0.390110        0.259381       -2.223528
C          1.064008       -0.708839       -1.464196
C          0.428431       -1.858128       -0.992804
C          1.153476       -2.782329       -0.255093
C          2.501819       -2.605820        0.013945
C          3.126162       -1.475027       -0.494175
C          2.425523       -0.530411       -1.223212
C          0.445690       -3.999599        0.276641
F         -0.550375       -4.390537       -0.527598
C          4.575155       -1.217194       -0.175541
F          5.200992       -0.585170       -1.173116
C         -3.247651       -2.819409        0.937130
F          1.273925       -5.037260        0.422892
F         -0.101278       -3.768613        1.483751
F          4.701784       -0.448287        0.916653
F          5.242965       -2.350498        0.065532
H         -1.093763       -0.156990       -0.287861
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H          0.893209        0.681628       -2.990819
H         -2.824804        2.080620        0.639274
H         -2.956245        2.653854       -1.030753
H         -5.331167        1.992923       -1.117772
H         -5.082289        3.066510        0.249172
H         -6.490184        1.082477        0.868295
H         -4.999478        1.142705        1.796866
H         -5.490596       -0.598339       -0.666792
H         -5.405088       -1.157323        1.001204
H         -3.498643        0.374914       -1.786199
H         -3.073075       -0.259740        1.157140
H         -4.311157       -3.089893        1.000583
H         -2.679231       -3.731661        0.758627
H         -2.937325       -2.407228        1.899651
H         -3.030844       -1.704922       -2.215909
H         -4.431853       -2.548195       -1.516353
H         -2.849025       -3.339527       -1.576592
H         -0.621357       -2.037488       -1.193597
H          3.057456       -3.338654        0.583053
H          2.921324        0.361082       -1.583982
C          1.618574        2.560522        1.420332
O          2.127083        2.160199        0.148672
C          1.391045        3.333223        0.186428
N          2.286551        4.557436        0.067720
O          1.761403        5.579587       -0.311721
O          3.445884        4.436047        0.379218
C          0.106482        3.440591       -0.564300
H         -0.456743        4.313010       -0.240140
H         -0.475961        2.542892       -0.365919
H          0.290799        3.515037       -1.636299
C          0.535257        1.726591        2.010972
C         -1.449665        0.166408        3.174182
C         -0.467902        2.325701        2.766692
C          0.543870        0.345697        1.836597
C         -0.452074       -0.433518        2.413420
C         -1.459404        1.545364        3.347406
H         -0.473444        3.401791        2.898190
H          1.336018       -0.113876        1.256503
H         -0.442602       -1.507934        2.275293
H         -2.238802        2.013859        3.934712
H         -2.221175       -0.440900        3.631677
H          2.391219        2.928566        2.089900

SR epoxide:Catalyst, binary complex 4; Energy = -2450.617771; TZVP basis set.
N          1.307278       -0.410262        1.389413
C          0.667634       -0.435889        2.557913
S          1.434974       -0.381621        4.062118
C          2.745111       -0.575887        1.237315
C          3.040161       -1.359855       -0.045183
C          4.547707       -1.653040       -0.087609
C          5.355148       -0.352731       -0.056697
C          4.997497        0.508083        1.154140
C          3.491934        0.757249        1.227434
N          2.145481       -2.511655       -0.193882
C          2.219003       -3.481441        0.889910
N         -0.703668       -0.475183        2.518835
C         -1.544061       -0.744939        1.426042
C         -2.778383       -0.097197        1.364489
C         -3.631515       -0.341068        0.302009
C         -3.275375       -1.204326       -0.724466
C         -2.052851       -1.847935       -0.640223
C         -1.194757       -1.654452        0.430832
C         -4.990356        0.308473        0.278180
F         -5.007459        1.462519        0.949518
C         -1.590960       -2.756379       -1.746022
F         -1.061931       -3.892307       -1.267807
C          2.298558       -3.162785       -1.486046
F         -5.408705        0.551238       -0.966407
F         -5.913306       -0.486570        0.848468
F         -2.581907       -3.097087       -2.574539
F         -0.637627       -2.173433       -2.491604
H          0.772470       -0.340419        0.530205
H         -1.138038       -0.323979        3.418118
H          3.166942        1.343937        0.359076
H          3.230786        1.311258        2.131267
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H          5.317211        0.000957        2.070502
H          5.531673        1.459369        1.113283
H          6.423483       -0.577577       -0.059595
H          5.145452        0.215330       -0.968261
H          4.821835       -2.275844        0.770083
H          4.791683       -2.218046       -0.989221
H          3.085801       -1.146828        2.103792
H          2.808155       -0.697749       -0.889337
H          3.243054       -3.717582       -1.581056
H          1.478348       -3.864837       -1.635646
H          2.253167       -2.415403       -2.280198
H          1.999707       -3.006602        1.847977
H          3.196318       -3.979947        0.961400
H          1.463797       -4.250908        0.718931
H         -3.058053        0.603889        2.142632
H         -3.935190       -1.366840       -1.565450
H         -0.249830       -2.187567        0.464250
C         -0.138978        2.294764       -1.436265
O         -0.552828        1.116326       -0.730619
C         -0.729232        2.336078       -0.089307
N         -2.200961        2.735105       -0.084243
O         -2.882190        2.370893       -1.012141
O         -2.582021        3.396896        0.853372
C         -0.030164        2.627805        1.198643
H          1.000852        2.288503        1.118834
H         -0.516526        2.101063        2.019740
H         -0.051088        3.694779        1.410088
C          1.323270        2.455000       -1.665287
C          4.043785        2.712834       -2.172674
C          1.996794        1.464509       -2.375701
C          2.010283        3.578923       -1.219281
C          3.371320        3.704428       -1.469475
C          3.354543        1.595057       -2.629530
H          1.454010        0.591896       -2.722578
H          1.483534        4.352587       -0.673314
H          3.905472        4.576241       -1.114606
H          3.876065        0.822573       -3.181201
H          5.104550        2.810933       -2.365786
H         -0.804128        2.532858       -2.261078

SR epoxide:Catalyst, binary complex 5; Energy = -2450.614009; TZVP basis set.
N          1.524037       -1.645100       -0.363725
C          0.797679       -2.655699       -0.854264
S          1.416876       -4.138850       -1.344026
C          2.948731       -1.760932       -0.072449
C          3.596166       -0.375639       -0.048612
C          5.107327       -0.558553        0.165991
C          5.392279       -1.309915        1.467954
C          4.678159       -2.658343        1.502846
C          3.182925       -2.481811        1.256032
N          3.202166        0.422445       -1.216105
C          3.828443        1.735545       -1.207161
N         -0.559404       -2.425646       -0.984478
C         -1.417539       -1.705314       -0.152875
C         -2.757965       -1.617208       -0.531016
C         -3.677624       -0.985749        0.292144
C         -3.295997       -0.394886        1.484115
C         -1.956987       -0.478341        1.844496
C         -1.023931       -1.130986        1.060865
C         -5.105242       -0.884375       -0.176211
F         -5.943071       -0.592073        0.821837
C         -1.523932        0.192313        3.120786
F         -0.226884       -0.007841        3.388094
C          3.402610       -0.231111       -2.504158
F         -5.244071        0.078970       -1.102217
F         -5.527753       -2.022579       -0.737654
F         -1.707948        1.521173        3.054662
F         -2.220806       -0.240368        4.176967
H          1.162625       -0.702706       -0.496174
H         -1.006112       -3.127519       -1.558472
H          2.734713       -1.888064        2.060923
H          2.675849       -3.446903        1.230023
H          5.091330       -3.312162        0.727840
H          4.844168       -3.155034        2.460231
H          6.468553       -1.442818        1.592422
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H          5.048301       -0.700607        2.310828
H          5.530861       -1.111253       -0.679116
H          5.596051        0.416123        0.193648
H          3.405464       -2.357959       -0.867436
H          3.200883        0.166886        0.822689
H          4.456528       -0.468710       -2.709140
H          2.815289       -1.147000       -2.571155
H          3.051603        0.440095       -3.289491
H          3.333653        2.381505       -1.935152
H          4.896097        1.702453       -1.465396
H          3.719663        2.192310       -0.221167
H         -3.082095       -2.062416       -1.464493
H         -4.015189        0.110582        2.114691
H         -0.003068       -1.216860        1.400473
C          0.455852        2.030833       -1.524659
O         -0.064842        0.716812       -1.367700
C         -0.977030        1.707672       -1.697097
N         -1.404347        1.600794       -3.150175
O         -0.657246        1.040714       -3.914903
O         -2.460935        2.113054       -3.442283
C         -2.083628        2.075268       -0.766208
H         -2.909548        1.372686       -0.862928
H         -2.447661        3.075755       -0.990665
H         -1.700074        2.049880        0.252364
C          0.944418        2.727397       -0.307556
C          1.940103        4.040792        1.932466
C          0.973938        2.082388        0.923268
C          1.409533        4.034594       -0.415468
C          1.904072        4.689911        0.703287
C          1.472308        2.736942        2.041827
H          0.612312        1.063732        1.000865
H          1.398087        4.532985       -1.378285
H          2.266436        5.706015        0.615353
H          1.491777        2.227554        2.996865
H          2.330162        4.551469        2.803398
H          1.037160        2.155206       -2.433909

SR epoxide:Catalyst, binary complex 6; Energy = -2450.611582; TZVP basis set.
N         -2.885632       -1.836532        0.654633
C         -2.836327       -2.299333       -0.610942
S         -3.977423       -3.352505       -1.241459
C         -2.512101       -0.473232        1.045050
C         -3.646886        0.500867        0.676753
C         -3.298928        1.917204        1.154459
C         -3.015191        1.946979        2.654541
C         -1.884807        0.981117        3.003576
C         -2.212670       -0.436835        2.541044
N         -3.976052        0.381681       -0.737628
C         -5.363663        0.681967       -1.036277
N         -1.760170       -1.907808       -1.379534
C         -0.421946       -1.769883       -0.988076
C          0.049188       -2.152994        0.267977
C          1.399629       -2.042874        0.559104
C          2.315796       -1.574514       -0.368767
C          1.837475       -1.214014       -1.619533
C          0.488908       -1.289698       -1.930562
C          1.848980       -2.464265        1.932367
F          1.430763       -3.701733        2.230746
C          2.785713       -0.740014       -2.688184
F          2.713939       -1.505422       -3.785026
C         -3.075012        1.085372       -1.632641
F          3.177192       -2.450958        2.064025
F          1.348198       -1.657812        2.887526
F          2.503961        0.515338       -3.086482
F          4.056713       -0.744119       -2.281403
H         -3.687913       -2.201387        1.153975
H         -1.897424       -2.119296       -2.358191
H         -3.090327       -0.805162        3.085598
H         -1.386680       -1.115299        2.764508
H         -0.966188        1.309204        2.505035
H         -1.689649        0.985945        4.077220
H         -2.763367        2.961294        2.972717
H         -3.919081        1.661215        3.202730
H         -2.409202        2.260367        0.616038
H         -4.111584        2.599651        0.894131
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H         -1.613544       -0.183410        0.500538
H         -4.532909        0.167087        1.231618
H         -2.036051        0.877672       -1.375279
H         -3.242832        0.735267       -2.653109
H         -3.221766        2.176607       -1.623407
H         -5.625290        1.738698       -0.866111
H         -6.017640        0.055695       -0.428478
H         -5.560417        0.452882       -2.084504
H         -0.633771       -2.559703        1.001798
H          3.365937       -1.489296       -0.124807
H          0.137214       -0.991691       -2.912103
C          1.300170        1.968722       -0.456059
O          0.026367        1.513762        0.006392
C          0.240176        2.886593        0.010066
N         -0.524009        3.553901       -1.129904
O         -0.973373        4.656696       -0.917439
O         -0.625714        2.941575       -2.165506
C          0.205530        3.663862        1.283444
H         -0.818734        3.750950        1.646149
H          0.607442        4.662208        1.125510
H          0.810249        3.147736        2.025430
C          2.492272        1.620799        0.354762
C          4.767011        0.875801        1.769967
C          2.371424        1.060811        1.623844
C          3.752841        1.795419       -0.208808
C          4.888449        1.426382        0.500349
C          3.507151        0.692420        2.329713
H          1.386836        0.875735        2.036749
H          3.844108        2.202494       -1.209361
H          5.866251        1.558279        0.055528
H          3.407602        0.240903        3.308362
H          5.651344        0.579061        2.319034
H          1.412970        1.893808       -1.531989

SR epoxide:Catalyst, binary complex 7; Energy = -2450.612308; TZVP basis set.
N         -3.935018        0.602979       -0.143753
C         -2.898307        1.439141        0.004086
S         -3.131431        3.105535        0.154415
C         -3.898740       -0.848621       -0.244494
C         -5.326193       -1.380573       -0.044152
C         -5.281938       -2.913839       -0.017589
C         -4.707765       -3.458591       -1.327122
C         -3.327751       -2.868715       -1.615246
C         -3.363507       -1.342050       -1.592572
N         -5.987347       -0.722972        1.081356
C         -5.388883       -0.995200        2.378839
N         -1.671204        0.839874        0.052273
C         -0.434747        1.503137        0.175846
C          0.453570        1.099757        1.166415
C          1.687012        1.729215        1.278927
C          2.044705        2.757617        0.424249
C          1.153747        3.133913       -0.573334
C         -0.074923        2.514122       -0.714068
C          2.665860        1.324583        2.347623
F          2.187107        0.379739        3.156016
C          1.584300        4.197615       -1.546510
F          2.104369        5.261127       -0.920390
C         -7.421049       -0.960696        1.106700
F          3.810736        0.859385        1.815544
F          3.009915        2.369641        3.115246
F          2.540061        3.737636       -2.374158
F          0.579636        4.629855       -2.309071
H         -4.843882        1.003518        0.056196
H         -1.636677       -0.164679        0.182859
H         -4.025795       -0.965164       -2.377936
H         -2.370772       -0.936524       -1.786289
H         -2.614491       -3.216874       -0.860940
H         -2.959848       -3.214735       -2.582863
H         -4.655931       -4.548245       -1.288811
H         -5.386530       -3.201309       -2.146961
H         -4.661865       -3.247774        0.820536
H         -6.286836       -3.308159        0.146309
H         -3.267151       -1.260627        0.556521
H         -5.894600       -1.077884       -0.932717
H         -7.684823       -1.991098        1.387224
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H         -7.882731       -0.288039        1.830541
H         -7.846794       -0.749850        0.124910
H         -4.332076       -0.726883        2.375264
H         -5.486579       -2.046208        2.687278
H         -5.882032       -0.376470        3.128954
H          0.179259        0.306394        1.849704
H          3.001221        3.255961        0.527242
H         -0.761306        2.809763       -1.494029
C          2.396351       -2.608610        0.045376
O          2.107282       -1.439980        0.806910
C          1.918649       -1.343101       -0.557213
N          0.445813       -1.372397       -0.915739
O         -0.332774       -1.801097       -0.085963
O          0.139704       -0.978556       -2.014083
C          2.705949       -0.381609       -1.385746
H          2.253036        0.609600       -1.344884
H          2.740768       -0.710889       -2.421942
H          3.715630       -0.332936       -0.984120
C          3.814139       -3.034546       -0.071241
C          6.451459       -3.866683       -0.336281
C          4.833234       -2.316288        0.546068
C          4.113902       -4.175095       -0.811851
C          5.431804       -4.586665       -0.947867
C          6.150193       -2.735768        0.412290
H          4.587867       -1.440184        1.133323
H          3.316133       -4.740717       -1.279582
H          5.662752       -5.471567       -1.526699
H          6.941806       -2.179583        0.897624
H          7.479194       -4.190605       -0.438595
H          1.653686       -3.393252        0.161902

SR epoxide:Catalyst, binary complex 8; Energy = -2450.615500; TZVP basis set.
N          2.992165        0.743934       -0.691530
C          1.784815        1.182456       -0.312360
S          1.524712        2.005214        1.133979
C          4.226753        0.927586        0.060572
C          5.207801       -0.192251       -0.299719
C          6.480362       -0.027285        0.542770
C          7.119604        1.342235        0.308728
C          6.131511        2.467145        0.609042
C          4.851854        2.297729       -0.206165
N          4.558518       -1.504773       -0.234420
C          4.050006       -1.859321        1.084220
N          0.788678        0.869085       -1.210841
C         -0.587486        1.119938       -1.082371
C         -1.086188        2.346462       -0.649921
C         -2.457248        2.522065       -0.544460
C         -3.352507        1.516798       -0.880183
C         -2.839133        0.318928       -1.352128
C         -1.472110        0.112797       -1.456711
C         -2.970712        3.831603       -0.007200
F         -4.246663        4.046941       -0.345235
C         -3.770577       -0.817107       -1.668678
F         -5.000665       -0.396279       -1.969354
C          5.386637       -2.571079       -0.776145
F         -2.906174        3.872548        1.330968
F         -2.256662        4.869485       -0.461488
F         -3.334373       -1.553642       -2.699179
F         -3.892590       -1.657309       -0.621334
H          3.064765        0.147829       -1.506638
H          1.005518        0.119199       -1.856717
H          5.074563        2.380387       -1.275292
H          4.122638        3.069454        0.043307
H          5.880710        2.456580        1.674805
H          6.581614        3.438640        0.398568
H          8.015221        1.445279        0.923870
H          7.441141        1.414640       -0.735831
H          6.230989       -0.132453        1.603173
H          7.188953       -0.820215        0.295973
H          3.975334        0.869410        1.121965
H          5.488766       -0.053368       -1.353032
H          6.228341       -2.842125       -0.123447
H          4.773661       -3.463167       -0.918283
H          5.786206       -2.270591       -1.745971
H          4.838175       -1.948748        1.843874
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H          3.542899       -2.823441        1.016591
H          3.318383       -1.122651        1.422174
H         -0.409809        3.148209       -0.395510
H         -4.419189        1.666861       -0.786771
H         -1.087605       -0.836851       -1.811267
C         -1.777346       -2.792013        1.267244
O         -1.263138       -2.593799        2.580782
C         -2.060228       -1.584240        2.075832
N         -3.462492       -1.616756        2.677427
O         -3.829612       -2.646121        3.189755
O         -4.124337       -0.609306        2.570152
C         -1.517677       -0.201143        1.933137
H         -0.556237       -0.231529        1.427310
H         -1.374664        0.237062        2.921461
H         -2.201728        0.427445        1.369125
C         -0.834425       -2.818609        0.121726
C          0.845709       -2.901678       -2.098754
C         -1.282774       -3.364370       -1.080969
C          0.471077       -2.342270        0.216903
C          1.308695       -2.384769       -0.892552
C         -0.450207       -3.398827       -2.190039
H         -2.290505       -3.756536       -1.147889
H          0.839255       -1.962850        1.162994
H          2.330566       -2.025957       -0.811009
H         -0.810828       -3.817554       -3.120694
H          1.502224       -2.939554       -2.959479
H         -2.579237       -3.523829        1.228689

SR epoxide:Catalyst, binary complex 9; Energy = -2450.618228; TZVP basis set.
N         -1.097001        3.078371       -1.384820
O         -1.817070        2.247501       -0.874416
O         -1.445887        3.902021       -2.193033
N         -2.918634       -0.458898        0.073894
C         -1.820743       -1.153863        0.390741
S         -1.783073       -2.833583        0.536221
C         -4.265476       -1.002578       -0.004392
N         -0.728432       -0.358627        0.630517
C          0.613407       -0.766818        0.730263
C          1.424810       -0.159187        1.681019
C          2.784452       -0.434417        1.705977
C          3.356270       -1.320961        0.809470
C          2.531824       -1.926467       -0.128004
C          1.173858       -1.660538       -0.179748
C          3.633920        0.246294        2.742787
F          3.443808       -0.272195        3.964847
C          3.109865       -2.883919       -1.134102
F          2.637062       -2.650072       -2.369264
F          3.347851        1.555470        2.837641
F          4.940119        0.147722        2.473395
F          2.807423       -4.156738       -0.844941
F          4.443765       -2.803172       -1.201503
H         -2.887414        0.552544        0.156690
H         -0.876573        0.644968        0.687014
H          0.992701        0.546343        2.379971
H          4.418948       -1.517346        0.823400
H          0.549570       -2.120487       -0.933990
C          0.375996        3.064979       -0.998145
C          0.984928        1.719085       -1.098966
H          0.319058        0.929855       -1.441593
O          0.573156        2.304864        0.140156
C          1.046055        4.386414       -1.175549
H          2.098793        4.280928       -0.925942
H          0.952933        4.717646       -2.206697
H          0.590807        5.128011       -0.519469
C          2.435880        1.472816       -1.288791
C          5.131465        0.877370       -1.623734
C          3.380852        2.003261       -0.414435
C          2.842928        0.634613       -2.323420
C          4.188699        0.341460       -2.492872
C          4.726035        1.707234       -0.584958
H          3.056914        2.613058        0.419807
H          2.104532        0.190799       -2.981564
H          4.497541       -0.321770       -3.290532
H          5.455410        2.110672        0.105813
H          6.179892        0.639090       -1.749181
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C         -4.549809       -1.709659       -1.330483
H         -4.384089       -1.733737        0.802026
C         -5.972997       -2.265351       -1.331400
H         -4.424804       -0.988296       -2.144784
H         -3.821113       -2.506887       -1.472855
C         -6.998206       -1.164163       -1.064841
H         -6.180884       -2.755834       -2.283965
H         -6.054879       -3.033200       -0.554902
C         -6.679272       -0.412225        0.229067
H         -6.989290       -0.455246       -1.899652
H         -8.004746       -1.583991       -1.016061
C         -5.255539        0.156039        0.182559
H         -7.396879        0.396682        0.381225
H         -6.772560       -1.094970        1.079606
H         -5.176999        0.785097       -0.714162
N         -4.857834        1.020723        1.295184
C         -5.584524        2.278642        1.315831
C         -4.886344        0.374785        2.598442
H         -4.472579        1.059982        3.339392
H         -5.900914        0.100402        2.921838
H         -4.266951       -0.522877        2.592565
H         -5.113575        2.953609        2.032079
H         -5.541972        2.743506        0.329851
H         -6.640266        2.166508        1.604007

SR epoxide:Catalyst, binary complex 10; Energy = -2450.613956; TZVP basis set.
C         -2.022306       -1.909519       -0.675085
C         -1.386878       -0.731548       -1.052961
C         -2.132467        0.451883       -1.121378
C         -3.465066        0.457140       -0.766789
C         -4.102172       -0.702498       -0.339732
C         -3.364232       -1.869945       -0.310523
N         -0.032040       -0.626201       -1.405436
C          1.071345       -1.289988       -0.913190
S          0.973625       -2.719332       -0.024582
C         -4.268361        1.724106       -0.857482
C         -3.998502       -3.144074        0.177096
N          2.217070       -0.661055       -1.218516
C          3.595479       -1.053463       -0.902344
C          3.878689       -1.231966        0.601406
C          5.375902       -1.503715        0.799039
C          5.811283       -2.749652        0.029474
C          5.518740       -2.583565       -1.459902
C          4.039429       -2.286035       -1.696677
N          3.339263       -0.118456        1.390907
C          2.965902       -0.531348        2.735687
C          4.198658        1.056238        1.441389
H          4.187005       -0.200488       -1.249464
H          3.434661       -3.140867       -1.387471
H          3.844856       -2.110849       -2.756556
H          5.805725       -3.481566       -2.010005
H          6.124642       -1.760362       -1.854306
H          5.268070       -3.620411        0.410526
H          6.874484       -2.938720        0.190064
H          5.962219       -0.647809        0.448036
H          5.582619       -1.618378        1.866332
H          3.337217       -2.120504        0.921947
H          0.177847        0.248785       -1.870457
H          2.143651        0.262412       -1.631685
H          2.459910        0.294986        3.240150
H          2.275159       -1.374138        2.681186
H          3.832218       -0.821810        3.349637
H          3.628335        1.904861        1.830594
H          5.072889        0.918890        2.093380
H          4.555067        1.315411        0.444148
H         -5.144070       -0.690567       -0.048885
F         -5.123562        1.694079       -1.892257
F         -5.011231        1.923259        0.241393
F         -3.501602        2.809612       -1.020403
F         -3.630914       -4.201286       -0.556644
F         -3.646950       -3.413894        1.445262
F         -5.335614       -3.086080        0.150182
O          0.709361        2.187121       -1.137320
C          0.951530        1.947541        0.282189
C          1.381097        3.164368       -0.435381
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N          2.875568        3.113008       -0.741568
C          0.873662        4.575550       -0.380568
O          3.555697        3.980591       -0.250932
O          3.285816        2.198042       -1.420339
H          1.020270        5.004275        0.608321
H          1.403514        5.188743       -1.107767
H         -0.182591        4.574827       -0.634863
C         -0.231032        1.759753        1.158041
H          1.731995        1.201208        0.444711
C         -1.259023        2.686087        1.327290
C         -2.391893        2.340962        2.049296
C         -2.515652        1.069013        2.597608
C         -1.488663        0.146645        2.445889
C         -0.347277        0.495805        1.737653
H         -1.199138        3.671819        0.891000
H         -3.190711        3.061702        2.167215
H         -3.413518        0.799284        3.139268
H         -1.647320        1.372318       -1.422127
H         -1.578079       -0.849072        2.861719
H          0.446956       -0.230272        1.595455
H         -1.478199       -2.839364       -0.653857

SR epoxide:Catalyst, binary complex 11; Energy = -2450.618072; TZVP basis set.
N         -2.867381        3.145212       -0.294227
O         -3.459184        2.117562       -0.053023
O         -3.366344        4.160317       -0.716245
N         -2.253646       -0.781573        0.131137
C         -1.052287       -1.354292       -0.008854
S         -0.795909       -2.771311       -0.884044
C         -3.511435       -1.386393       -0.283040
C         -3.831770       -1.123617       -1.754639
C         -5.131851       -1.829170       -2.137956
C         -6.282974       -1.402827       -1.227208
C         -5.930800       -1.607224        0.248312
C         -4.644751       -0.846073        0.598301
N         -0.056932       -0.683180        0.662896
C          1.331940       -0.840321        0.579665
C          2.085019       -0.536186        1.707372
C          3.471946       -0.569121        1.648483
C          4.131649       -0.917296        0.485479
C          3.364377       -1.215855       -0.635519
C          1.984254       -1.173141       -0.610411
C          4.247641       -0.147315        2.864071
F          3.731624       -0.653903        3.991436
C          4.077127       -1.596011       -1.904902
F          3.285995       -1.524435       -2.978864
F          4.236123        1.191259        3.008067
F          5.528926       -0.520270        2.806505
F          4.553708       -2.848787       -1.849019
F          5.133380       -0.798819       -2.136143
H         -2.352382        0.024550        0.743012
H         -0.364151       -0.000527        1.344626
H         -4.796331        0.202037        0.320090
N         -4.256210       -0.821232        2.009003
H         -5.794136       -2.675089        0.447034
H         -6.750742       -1.260692        0.880877
H         -7.189672       -1.957058       -1.477313
H         -6.500429       -0.342839       -1.395978
H         -4.984096       -2.911051       -2.054207
H         -5.376210       -1.622593       -3.181451
H         -3.414815       -2.467190       -0.144527
H         -3.929431       -0.042157       -1.900673
H          1.586694       -0.267885        2.631757
H          5.212290       -0.944882        0.443769
H          1.412604       -1.378571       -1.501810
C         -1.361594        3.154106       -0.083967
C         -0.687481        1.986937       -0.697153
H         -1.338091        1.278886       -1.206770
O         -0.963707        2.087714        0.704112
C         -0.800345        4.520691        0.127689
H          0.278058        4.442837        0.239922
H         -1.028162        5.154936       -0.725294
H         -1.227605        4.965896        1.025987
C          0.734175        1.998771       -1.121700
C          3.383098        1.944056       -1.967165
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C	1.759756	2.281133	-0.222059
C	1.039874	1.667187	-2.438554
C	2.362486	1.646573	-2.861174
C	3.080440	2.253351	-0.645645
H	1.523390	2.495107	0.813505
H	0.243713	1.415867	-3.130048
H	2.596545	1.384020	-3.884618
H	3.874582	2.461205	0.060497
H	4.414341	1.915531	-2.294184
H	-3.001766	-1.477098	-2.367434
C	-5.177871	-0.051038	2.826304
C	-4.008463	-2.132646	2.587146
H	-3.625167	-2.004553	3.600404
H	-4.912276	-2.756774	2.645065
H	-3.252494	-2.667262	2.010198
H	-4.740968	0.102497	3.814366
H	-5.343590	0.925510	2.368833
H	-6.152861	-0.542104	2.963557

SR epoxide:Catalyst, binary complex 12, AS-SR1; Energy = -2450.622694; TZVP basis set.

N	2.134749	-0.321525	-1.096957
C	1.587604	-0.504809	-2.297370
S	2.441547	-0.498816	-3.755955
C	3.576215	-0.282126	-0.875272
C	4.133562	-1.705296	-0.783735
C	5.651474	-1.682760	-0.648462
C	6.060129	-0.849006	0.561054
C	5.464772	0.557745	0.494711
C	3.930026	0.522357	0.378232
H	3.828300	-2.252015	-1.677574
N	0.223215	-0.682262	-2.348058
C	-0.663094	-1.147934	-1.374182
C	-2.020293	-0.877841	-1.550955
C	-2.949876	-1.348565	-0.637926
C	-2.560949	-2.077731	0.474028
C	-1.206482	-2.340139	0.638980
C	-0.259756	-1.903727	-0.270174
C	-4.413015	-1.089235	-0.881354
F	-5.104278	-1.015695	0.262513
C	-0.774759	-3.085130	1.874171
F	-0.984376	-2.349278	2.977692
F	-4.968889	-2.073167	-1.606351
F	-4.617030	0.048246	-1.552027
F	0.519651	-3.407347	1.852060
F	-1.468894	-4.220319	2.034925
H	1.533877	-0.081244	-0.312545
H	-0.140382	-0.615571	-3.288160
H	3.540540	-0.018619	1.250928
N	3.271245	1.842762	0.400810
H	5.882294	1.092970	-0.365004
H	5.753121	1.109282	1.389408
H	7.147349	-0.786625	0.636882
H	5.705503	-1.341585	1.472767
H	6.084565	-1.249896	-1.556237
H	6.037043	-2.700191	-0.563700
H	4.024411	0.201245	-1.746679
H	3.685330	-2.201867	0.084281
H	-2.341988	-0.278803	-2.394099
H	-3.288413	-2.428423	1.194526
H	0.780808	-2.150141	-0.120392
N	0.891376	1.198879	2.071256
O	1.109863	0.040729	1.782223
O	1.261180	1.746106	3.080066
C	0.011839	2.002967	1.129531
C	-1.215717	1.264623	0.751341
H	-1.315867	0.270081	1.179231
O	-0.081933	1.398400	-0.107347
C	-2.473609	1.938564	0.348607
C	-4.867952	3.152506	-0.369469
C	-3.614899	1.741277	1.121455
C	-2.535414	2.730656	-0.794105
C	-3.733142	3.336208	-1.149840
C	-4.808265	2.352719	0.765115
H	-3.570071	1.100818	1.995482
H	-1.649091	2.856524	-1.404140

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H         -3.781647        3.947535       -2.041843
H         -5.694315        2.193715        1.365957
H         -5.800949        3.623146       -0.651496
C          0.176163        3.480596        1.234037
H          0.126898        3.800254        2.271509
H          1.136950        3.765220        0.808196
H         -0.621462        3.958313        0.668710
C          3.735449        2.644263        1.528240
C          3.394820        2.597532       -0.841753
H          2.903516        3.563439       -0.713018
H          4.439254        2.793316       -1.124768
H          2.898239        2.079190       -1.662084
H          3.060814        3.486157        1.687648
H          3.733789        2.040833        2.436870
H          4.745200        3.048912        1.376983

SR epoxide:Catalyst, binary complex 13, AA-SR2; Energy = -2450.619977; TZVP basis set.
N          2.367535        0.969112       -1.004508
C          1.165265        1.407871       -0.600991
S          0.955772        2.648238        0.522447
C          3.664568        1.423037       -0.523468
C          4.522811        1.828165       -1.725384
C          5.912211        2.293969       -1.299920
C          6.611157        1.222607       -0.468182
C          5.753154        0.843129        0.736373
C          4.370427        0.332604        0.305034
H          4.001101        2.610737       -2.279340
N          0.126342        0.728230       -1.196242
C         -1.253621        0.811200       -0.949258
C         -1.918149        1.986398       -0.619893
C         -3.281767        1.942872       -0.350760
C         -4.011176        0.772357       -0.436735
C         -3.343438       -0.384456       -0.821714
C         -1.987248       -0.372280       -1.075550
C         -3.953258        3.215855        0.089023
F         -3.556098        4.267338       -0.637886
C         -4.139424       -1.649422       -0.981356
F         -3.360674       -2.734763       -1.091260
F         -3.670313        3.502569        1.369615
F         -5.285813        3.143953       -0.008454
F         -4.907148       -1.612114       -2.082111
F         -4.965853       -1.854568        0.051745
H          2.399011        0.269383       -1.738497
H          0.396109       -0.081366       -1.745812
H          4.519979       -0.523478       -0.365364
N          3.530032       -0.161265        1.399987
H          5.628111        1.723528        1.375215
H          6.252635        0.079354        1.336178
H          7.589806        1.574961       -0.137107
H          6.782822        0.335705       -1.087230
H          5.818777        3.208597       -0.705598
H          6.503148        2.545827       -2.182237
H          3.480470        2.298567        0.098836
H          4.618911        0.963777       -2.394111
H         -1.379851        2.918415       -0.557265
H         -5.071017        0.756525       -0.220563
H         -1.477528       -1.289762       -1.339693
N          2.083656       -2.345357       -1.426898
O          1.737780       -1.644689       -2.370046
O          3.219745       -2.604741       -1.147790
C          0.956983       -2.840550       -0.534600
C          0.884851       -2.042962        0.716367
H          1.655888       -1.276593        0.837040
O          1.413871       -3.379043        0.639150
C         -0.381302       -1.797887        1.443648
C         -2.805627       -1.156754        2.646768
C         -0.634563       -0.492377        1.859465
C         -1.323074       -2.796161        1.685940
C         -2.534452       -2.471038        2.280202
C         -1.848110       -0.169527        2.449624
H          0.110725        0.280169        1.699772
H         -1.103753       -3.824134        1.425213
H         -3.270798       -3.244746        2.455782
H         -2.043021        0.853587        2.747141
H         -3.758512       -0.907921        3.096564
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C	-0.114917	-3.532208	-1.320669
H	0.196297	-4.560275	-1.509709
H	-1.041738	-3.542637	-0.753360
H	-0.284043	-3.031651	-2.271442
C	3.976943	-1.454504	1.903785
C	3.375906	0.771614	2.510836
H	2.572305	0.415642	3.158958
H	4.288651	0.857023	3.118188
H	3.091165	1.757127	2.148279
H	3.232876	-1.839208	2.605253
H	4.066483	-2.168192	1.085052
H	4.936710	-1.399087	2.437482

RS epoxide:Catalyst:Aniline, Transition State 1; Energy = -2737.313901; 6-31G(d) basis set.

N	-1.044615	2.470764	0.814840
C	0.288399	2.598869	0.687512
S	1.028867	3.906785	-0.080868
C	-2.041315	3.479231	0.501741
C	-3.230916	2.837825	-0.233192
C	-4.276905	3.924533	-0.540639
C	-4.743278	4.630015	0.735477
C	-3.560573	5.250107	1.478758
C	-2.501954	4.190096	1.781235
N	-2.788047	2.046659	-1.392353
C	-3.886517	1.327996	-2.018180
N	0.954087	1.538103	1.254910
C	2.208230	0.983921	0.981718
C	2.343409	-0.364957	1.347227
C	3.503317	-1.061140	1.059891
C	4.570170	-0.445065	0.411707
C	4.436661	0.895380	0.079687
C	3.285268	1.626296	0.363714
C	3.599725	-2.515721	1.417817
F	2.387519	-3.091600	1.512360
C	5.509797	1.555738	-0.736716
F	6.709106	0.985711	-0.550192
C	-2.041909	2.801226	-2.393290
F	4.290856	-3.202171	0.492927
F	4.217088	-2.712496	2.590632
F	5.233454	1.459623	-2.051495
F	5.631062	2.859118	-0.459038
H	-1.398047	1.589648	1.196172
H	0.327750	0.844239	1.664948
H	-2.911197	3.441727	2.474242
H	-1.624008	4.634128	2.262334
H	-3.115079	6.039581	0.858697
H	-3.893234	5.724287	2.407776
H	-5.487455	5.394545	0.489169
H	-5.240170	3.900492	1.389579
H	-3.842413	4.666227	-1.224518
H	-5.135844	3.478414	-1.052915
H	-1.562830	4.218216	-0.146781
H	-3.692311	2.111116	0.456009
H	-1.143147	3.244510	-1.953788
H	-1.721489	2.110305	-3.180418
H	-2.635850	3.597784	-2.871033
H	-4.460686	0.794962	-1.252896
H	-3.475860	0.601929	-2.731253
H	-4.577132	1.976035	-2.582663
H	1.502149	-0.872344	1.812330
H	5.467883	-0.998164	0.159638
H	3.214124	2.667478	0.082671
N	-3.301835	-1.361089	1.423080
O	-3.966602	-0.587911	0.746758
O	-3.755040	-2.047748	2.310557
C	-1.746142	-1.413798	1.160247
C	-1.457449	-0.855506	-0.173096
H	-2.054081	0.017135	-0.423197
O	-1.167394	-0.298217	1.638443
C	-0.160810	-0.965363	-0.860670
C	2.305983	-0.963581	-2.170745
C	0.608403	-2.137071	-0.913206
C	0.297477	0.189397	-1.508385
C	1.535088	0.197032	-2.143507

C	1.832294	-2.132738	-1.573763
H	0.254737	-3.050381	-0.447996
H	-0.313396	1.088301	-1.468854
H	1.903110	1.111676	-2.598099
H	2.434252	-3.035996	-1.593386
H	3.281205	-0.952732	-2.648407
C	-1.226956	-2.726516	1.696841
H	-1.655573	-3.591539	1.182825
H	-1.476226	-2.780854	2.757455
H	-0.141194	-2.730450	1.596956
N	-2.693211	-1.943007	-1.598647
H	-2.233292	-1.796907	-2.494671
H	-3.554558	-1.402052	-1.552364
C	-2.881503	-3.310457	-1.278824
C	-3.108734	-5.962746	-0.440146
C	-1.947645	-4.259351	-1.703238
C	-3.944246	-3.693907	-0.456634
C	-4.049635	-5.016591	-0.038776
C	-2.064795	-5.579528	-1.280174
H	-1.132848	-3.958384	-2.356378
H	-4.678812	-2.957235	-0.140827
H	-4.873488	-5.304840	0.605986
H	-1.335296	-6.311722	-1.611505
H	-3.193346	-6.992131	-0.108904

RS epoxide:Catalyst:Aniline, Transition State 2; Energy = -2737.297352; 6-31G(d) basis set.

N	3.580414	-0.131693	-0.665935
C	2.649258	0.750429	-0.254901
S	2.769660	1.598631	1.195723
C	4.867901	-0.352982	-0.011937
C	5.361177	-1.797735	-0.227830
C	6.718335	-1.969181	0.471980
C	7.753748	-0.946448	0.001586
C	7.242752	0.479786	0.204939
C	5.900149	0.671700	-0.498981
N	4.442273	-2.856393	0.193224
C	3.533908	-3.325913	-0.838276
N	1.594710	0.848604	-1.134233
C	0.452606	1.656441	-1.024262
C	0.512962	2.983181	-0.593170
C	-0.657571	3.727929	-0.501771
C	-1.889414	3.200157	-0.863119
C	-1.927736	1.895906	-1.343212
C	-0.777473	1.123442	-1.431668
C	-0.590030	5.104679	0.092713
F	-0.656324	5.053481	1.437657
C	-3.259572	1.313878	-1.719565
F	-3.141985	0.158536	-2.385124
C	3.753616	-2.596799	1.447125
F	0.552178	5.731195	-0.214880
F	-1.604372	5.878881	-0.315896
F	-4.002391	1.055128	-0.624531
F	-3.974908	2.156758	-2.476386
H	3.479963	-0.517059	-1.599811
H	1.464358	0.029039	-1.725216
H	6.030359	0.553206	-1.584438
H	5.501749	1.676485	-0.322978
H	7.116513	0.673382	1.278661
H	7.969480	1.209335	-0.166984
H	8.698771	-1.097279	0.533922
H	7.961239	-1.105974	-1.065733
H	6.575457	-1.866401	1.556666
H	7.061458	-2.992118	0.291943
H	4.699317	-0.194038	1.057373
H	5.530592	-1.937214	-1.307210
H	3.004512	-1.790543	1.381364
H	3.241199	-3.512196	1.761830
H	4.476049	-2.337368	2.227065
H	3.032064	-4.233261	-0.482005
H	4.103282	-3.592528	-1.734382
H	2.753201	-2.603228	-1.118312
H	1.462234	3.423803	-0.319180
H	-2.795427	3.791359	-0.784282
H	-0.840933	0.114670	-1.833749

N	0.208647	-2.051833	-0.926100
O	0.751998	-1.787261	0.133757
O	0.671474	-1.762638	-2.017110
C	-1.170497	-2.861030	-0.931357
C	-2.187953	-2.137487	-0.144232
H	-2.200752	-1.066227	-0.316020
O	-1.906403	-2.566219	-1.972760
C	-3.488144	-2.783566	0.181441
C	-5.970752	-3.911110	0.793715
C	-3.564291	-3.950946	0.948903
C	-4.664827	-2.181727	-0.269403
C	-5.900605	-2.745669	0.034537
C	-4.800111	-4.512956	1.251729
H	-2.656222	-4.417829	1.322531
H	-4.601922	-1.279116	-0.867153
H	-6.809447	-2.273015	-0.323613
H	-4.848763	-5.418371	1.848062
H	-6.934979	-4.348965	1.031445
C	-0.738783	-4.296077	-0.689764
H	-1.625940	-4.930552	-0.703893
H	-0.203308	-4.413939	0.256847
H	-0.087962	-4.597532	-1.515718
N	-1.585481	-1.754720	1.793415
H	-0.596467	-1.999357	1.809339
H	-2.114384	-2.360632	2.417244
C	-1.798365	-0.370244	2.063865
C	-2.254513	2.347955	2.447490
C	-0.729633	0.524577	2.008060
C	-3.096881	0.088105	2.291136
C	-3.317884	1.448697	2.484152
C	-0.962625	1.880299	2.213032
H	0.280896	0.172017	1.810737
H	-3.924264	-0.617240	2.309586
H	-4.328535	1.804533	2.658337
H	-0.123409	2.567952	2.175955
H	-2.427324	3.409736	2.591206

RS epoxide:Catalyst:Aniline, Transition State 3; Energy = -2737.289032; 6-31G(d) basis set.

N	-2.181827	1.280991	-0.865686
C	-1.051606	1.372583	-0.153950
S	-1.027118	1.289905	1.536087
C	-3.517812	0.990776	-0.328090
C	-4.164837	2.307669	0.165991
C	-4.674905	3.163569	-1.013902
C	-5.449937	2.397388	-2.095340
C	-4.668457	1.177083	-2.586179
C	-4.295236	0.252554	-1.423151
N	-5.104872	2.060366	1.267307
C	-6.475663	1.747647	0.899476
N	0.079523	1.453816	-0.935696
C	1.400263	1.747077	-0.539708
C	2.439822	1.158125	-1.259484
C	3.763137	1.418787	-0.911453
C	4.075096	2.264990	0.139737
C	3.026127	2.870421	0.830683
C	1.700103	2.631630	0.503607
C	4.842424	0.746922	-1.713021
F	4.650148	-0.581523	-1.770625
C	3.357518	3.854383	1.919215
F	4.402140	3.439457	2.650230
C	-5.093728	3.153025	2.227806
F	4.856116	1.187544	-2.979668
F	6.058629	0.957755	-1.198437
F	3.691612	5.050262	1.408759
F	2.328563	4.051313	2.750797
H	-2.100608	1.265473	-1.877261
H	-0.033018	1.219611	-1.920816
H	-3.699735	-0.601222	-1.768178
H	-5.207644	-0.159111	-0.979768
H	-5.252218	0.618157	-3.324269
H	-3.763925	1.512250	-3.116322
H	-6.422602	2.067491	-1.716156
H	-5.657532	3.072821	-2.932668
H	-5.275683	3.994703	-0.624119

H	-3.796691	3.621169	-1.489490
H	-3.387090	0.351651	0.549805
H	-3.341526	2.858746	0.631631
H	-4.076206	3.313016	2.594855
H	-5.472138	4.104760	1.811084
H	-5.726802	2.889172	3.080580
H	-7.008187	2.593526	0.428319
H	-7.025753	1.474210	1.805415
H	-6.514793	0.894850	0.219631
H	2.214951	0.489927	-2.086870
H	5.105788	2.451175	0.419135
H	0.905968	3.117061	1.054541
N	-0.418461	-1.261090	-2.546719
O	-1.166059	-0.394106	-2.956674
O	0.801812	-1.175092	-2.590324
C	-1.065122	-2.554819	-1.814852
C	-1.180412	-2.154818	-0.391639
H	-1.555479	-1.142156	-0.282526
O	-2.367273	-2.552911	-1.855943
C	-1.487803	-3.077134	0.712711
C	-2.035641	-4.680977	2.935849
C	-2.229521	-2.571246	1.788210
C	-0.999173	-4.387076	0.775403
C	-1.283288	-5.186085	1.878283
C	-2.502972	-3.367967	2.893677
H	-2.583184	-1.543577	1.754921
H	-0.369662	-4.777375	-0.015475
H	-0.899192	-6.200239	1.917485
H	-3.081155	-2.965526	3.718966
H	-2.250478	-5.306445	3.796688
C	-0.287101	-3.736568	-2.366888
H	0.749539	-3.750778	-2.025283
H	-0.306916	-3.694594	-3.459308
H	-0.801002	-4.647108	-2.058912
N	0.685123	-1.467648	0.362363
H	0.377492	-0.872386	1.136348
H	1.041814	-0.871322	-0.382430
C	1.633694	-2.451220	0.735864
C	3.429723	-4.473537	1.413013
C	1.554742	-3.060596	1.989880
C	2.609126	-2.852828	-0.180944
C	3.503224	-3.861436	0.162917
C	2.455156	-4.067492	2.322334
H	0.783217	-2.751270	2.691156
H	2.667265	-2.362507	-1.149372
H	4.265082	-4.163368	-0.548858
H	2.390597	-4.537554	3.298645
H	4.130637	-5.258131	1.678219

RS epoxide:Catalyst:Aniline, Transition State 4; Energy = -2737.292484; 6-31G(d) basis set.

N	2.783129	-0.945886	0.195691
C	2.589544	0.371261	-0.015879
S	3.601144	1.584155	0.562422
C	4.032870	-1.630067	0.520960
C	5.198339	-1.253108	-0.415268
C	6.365557	-2.217551	-0.139359
C	6.810322	-2.122602	1.323586
C	5.647064	-2.419652	2.273465
C	4.452913	-1.503579	1.990428
N	4.756014	-1.148012	-1.801917
C	4.358950	-2.401150	-2.416015
N	1.445541	0.592871	-0.748412
C	0.531326	1.650424	-0.735547
C	-0.779786	1.321111	-1.120253
C	-1.780945	2.274361	-1.072314
C	-1.519714	3.580936	-0.665199
C	-0.213964	3.903266	-0.328963
C	0.817941	2.967330	-0.367569
C	-3.194718	1.887927	-1.392559
F	-3.945734	1.805741	-0.274494
C	0.099355	5.281652	0.179619
F	1.317252	5.691476	-0.193178
C	5.696097	-0.423583	-2.636125
F	-3.792209	2.784259	-2.187067

F	-3.270993	0.690057	-1.991695
F	-0.787090	6.190078	-0.251109
F	0.071293	5.319345	1.526190
H	2.033629	-1.564674	-0.101926
H	1.073927	-0.241513	-1.195917
H	4.713456	-0.461393	2.199956
H	3.601393	-1.764145	2.629643
H	5.339283	-3.467394	2.147036
H	5.965552	-2.306739	3.315028
H	7.641164	-2.810570	1.513474
H	7.184282	-1.108646	1.518836
H	6.057051	-3.249549	-0.358973
H	7.203012	-1.984853	-0.807235
H	3.797227	-2.689617	0.352096
H	5.525254	-0.246329	-0.131059
H	5.927640	0.538868	-2.170193
H	6.642781	-0.964894	-2.814046
H	5.236581	-0.228972	-3.610371
H	5.192903	-3.110569	-2.560300
H	3.925114	-2.191611	-3.398622
H	3.587344	-2.895423	-1.816498
H	-1.009398	0.314182	-1.462007
H	-2.309435	4.323380	-0.627586
H	1.827571	3.252380	-0.106557
N	-0.327377	-2.509591	-0.901068
O	0.306278	-2.831188	0.098339
O	0.136708	-1.842833	-1.803515
C	-1.867607	-2.980563	-1.035742
C	-2.673013	-2.097017	-0.167355
H	-2.428205	-1.045155	-0.272496
O	-2.474389	-2.416422	-2.040291
C	-4.084940	-2.432014	0.150977
C	-6.753848	-2.978927	0.764380
C	-5.085594	-1.517769	-0.187516
C	-4.428287	-3.616650	0.812359
C	-5.758032	-3.888759	1.115869
C	-6.415759	-1.794053	0.115171
H	-4.815552	-0.600415	-0.699778
H	-3.654125	-4.322543	1.102554
H	-6.016488	-4.809371	1.628990
H	-7.187973	-1.082119	-0.157430
H	-7.791298	-3.192419	1.001083
C	-1.811267	-4.492875	-0.937467
H	-1.349031	-4.838918	-0.010341
H	-1.239351	-4.869403	-1.790163
H	-2.829869	-4.874615	-1.017672
N	-1.926976	-2.023929	1.752645
H	-2.685712	-2.320999	2.363913
H	-1.159215	-2.692993	1.799891
C	-1.493748	-0.690023	2.027760
C	-0.697234	1.944207	2.444623
C	-0.137400	-0.390505	2.155936
C	-2.451776	0.324034	2.081825
C	-2.047799	1.639140	2.291080
C	0.253597	0.927347	2.376537
H	0.607028	-1.180133	2.089961
H	-3.503868	0.080583	1.951412
H	-2.793416	2.427520	2.319153
H	1.310755	1.160747	2.470987
H	-0.382786	2.973309	2.585063

RS epoxide:Catalyst:Aniline, Transition State 5; Energy = -2737.294231; 6-31G(d) basis set.

N	1.224740	2.325963	0.774017
C	0.041378	2.351624	0.129456
S	-0.262487	3.094786	-1.344502
C	2.462574	3.035985	0.443335
C	3.006925	2.739831	-0.967103
C	4.370164	3.433541	-1.126632
C	4.239049	4.945854	-0.932653
C	3.672161	5.258520	0.452235
C	2.333790	4.550124	0.668673
N	3.002727	1.299042	-1.288430
C	2.890893	1.098699	-2.731771
N	-0.932271	1.657741	0.821620

C	-2.171752	1.204023	0.330606
C	-2.283334	0.615620	-0.934364
C	-3.494441	0.070731	-1.328254
C	-4.610952	0.097428	-0.493671
C	-4.485218	0.680237	0.757953
C	-3.276602	1.233216	1.176455
C	-3.621675	-0.604552	-2.664805
F	-4.070084	-1.865333	-2.524059
C	-5.646153	0.675015	1.712197
F	-6.815313	0.534978	1.073927
C	4.156514	0.578221	-0.762536
F	-4.502977	0.026721	-3.454628
F	-2.458407	-0.663147	-3.320297
F	-5.553535	-0.332859	2.593651
F	-5.703203	1.809398	2.424623
H	1.232573	1.852890	1.673789
H	-0.790140	1.517662	1.820662
H	1.583787	4.940795	-0.028462
H	1.961370	4.725247	1.683483
H	4.388291	4.927446	1.217207
H	3.544722	6.337820	0.583070
H	5.213265	5.427679	-1.065037
H	3.570614	5.354850	-1.701610
H	5.082358	3.041611	-0.387313
H	4.781988	3.209348	-2.117646
H	3.188556	2.648758	1.171612
H	2.315391	3.202965	-1.673787
H	4.262787	0.768013	0.311340
H	4.004894	-0.498136	-0.899551
H	5.102903	0.850032	-1.255803
H	2.846720	0.028561	-2.951796
H	3.744262	1.519073	-3.288630
H	1.967246	1.561809	-3.087999
H	-1.423214	0.564875	-1.590768
H	-5.553856	-0.332415	-0.814472
H	-3.194235	1.683583	2.160897
N	0.162605	-0.523451	2.838958
O	0.630196	0.565510	3.147397
O	-1.001954	-0.676882	2.517399
C	1.195420	-1.776956	2.754133
C	2.125329	-1.430012	1.645313
H	2.514808	-0.423407	1.741430
O	2.199810	-1.658622	3.571909
C	3.014614	-2.463475	1.074672
C	4.767514	-4.374629	0.030174
C	4.398885	-2.255303	1.115093
C	2.517787	-3.645980	0.514235
C	3.393423	-4.592876	-0.010500
C	5.271369	-3.205042	0.598938
H	4.785519	-1.351872	1.578158
H	1.448072	-3.821208	0.466611
H	2.996716	-5.500983	-0.452690
H	6.342414	-3.036960	0.644788
H	5.447414	-5.116563	-0.376757
C	0.339698	-3.026160	2.797057
H	-0.356545	-3.097777	1.959723
H	-0.223417	-3.033907	3.733694
H	1.016626	-3.881446	2.794856
N	1.056412	-0.758384	-0.039726
H	1.677566	-0.071025	-0.508051
H	0.304056	-0.221245	0.396177
C	0.508875	-1.732358	-0.916739
C	-0.542005	-3.729586	-2.558465
C	-0.774561	-2.232624	-0.676630
C	1.272663	-2.247914	-1.964376
C	0.742770	-3.240347	-2.783227
C	-1.296765	-3.224212	-1.500885
H	-1.358708	-1.832388	0.149938
H	2.287063	-1.889855	-2.116630
H	1.341024	-3.633873	-3.598886
H	-2.301948	-3.591354	-1.321881
H	-0.953414	-4.499246	-3.202773

RS epoxide:Catalyst:Aniline, Transition State 6; Energy = -2737.281663; 6-31G(d) basis set.

N	-1.916829	2.111843	-1.247337
C	-0.793763	2.419276	-0.568601
S	-0.768193	3.067145	0.977384
C	-3.301597	2.452591	-0.927643
C	-3.885726	1.689609	0.275916
C	-5.328958	2.213859	0.551874
C	-5.935226	2.994082	-0.618516
C	-5.076649	4.222601	-0.970994
C	-3.574724	3.950557	-0.745461
N	-3.759135	0.227909	0.122770
C	-4.462630	-0.316496	-1.032962
N	0.336695	2.116823	-1.307250
C	1.631092	1.793821	-0.865585
C	2.260016	2.367096	0.243205
C	3.522441	1.912870	0.615713
C	4.191699	0.925324	-0.094785
C	3.576660	0.402550	-1.228871
C	2.317257	0.830219	-1.620809
C	4.163408	2.473176	1.856155
F	5.498462	2.518658	1.739635
C	4.282916	-0.678834	-1.998953
F	3.629390	-1.011310	-3.117926
C	-4.174297	-0.471758	1.335519
F	3.734465	3.709998	2.128026
F	3.893345	1.713494	2.930663
F	5.523547	-0.307218	-2.341620
F	4.402534	-1.793482	-1.257359
H	-1.802522	1.551469	-2.084501
H	0.139360	1.717957	-2.221173
H	-3.275940	4.249397	0.262450
H	-2.960044	4.526179	-1.443877
H	-5.256556	4.504547	-2.014033
H	-5.381106	5.076648	-0.357817
H	-6.022829	2.334493	-1.490943
H	-6.955173	3.304318	-0.371098
H	-5.984752	1.378615	0.818833
H	-5.300343	2.867509	1.431281
H	-3.841940	2.147640	-1.830306
H	-3.255991	1.938871	1.134773
H	-3.705177	-0.000508	2.204598
H	-5.264680	-0.473973	1.489990
H	-3.846341	-1.516769	1.281020
H	-4.369875	-1.406886	-1.023298
H	-4.018030	0.041471	-1.965778
H	-5.538842	-0.075189	-1.034698
H	1.769586	3.145266	0.809625
H	5.176671	0.587402	0.210769
H	1.868305	0.415018	-2.519600
N	-0.024777	-1.214608	-2.819728
O	0.715448	-1.225502	-3.774961
O	-0.749945	-0.256943	-2.542667
C	-0.102398	-2.566697	-1.924376
C	-1.173931	-2.424668	-0.923441
H	-2.045386	-1.913963	-1.313800
O	-0.876019	-3.450006	-2.511161
C	-1.392172	-3.418229	0.147883
C	-1.940470	-5.243384	2.197193
C	-0.370219	-3.857290	0.996295
C	-2.691966	-3.898348	0.345109
C	-2.967173	-4.805343	1.362444
C	-0.645186	-4.768173	2.011767
H	0.633734	-3.459164	0.895318
H	-3.485154	-3.573903	-0.323981
H	-3.978202	-5.176073	1.498004
H	0.155224	-5.092720	2.668895
H	-2.151085	-5.951737	2.992452
C	1.339366	-2.902520	-1.613800
H	1.805813	-2.156634	-0.959801
H	1.900972	-2.965019	-2.547487
H	1.359524	-3.878478	-1.127376
N	-0.826276	-0.718861	0.297840
H	-0.304536	-0.135125	-0.353194
H	-1.786547	-0.336676	0.343494
C	-0.169250	-0.853398	1.544151
C	1.166899	-1.274292	3.966201

C	-0.877163	-1.265935	2.674880
C	1.214034	-0.670193	1.628669
C	1.875204	-0.875459	2.834494
C	-0.209576	-1.469054	3.877776
H	-1.943825	-1.454046	2.601433
H	1.772786	-0.362939	0.748543
H	2.946352	-0.709458	2.886457
H	-0.771741	-1.789188	4.749694
H	1.682568	-1.431422	4.907784

RS epoxide:Catalyst:Aniline, Transition State 7; Energy = -2737.307817; 6-31G(d) basis set.

N	2.530712	-0.856034	-0.574256
C	1.419840	-1.604501	-0.490349
S	1.420822	-3.217402	-0.000327
C	3.890859	-1.306366	-0.330954
C	4.841913	-0.572975	-1.298698
C	6.289803	-0.992066	-1.009518
C	6.678507	-0.744731	0.449509
C	5.730496	-1.481053	1.396760
C	4.281651	-1.074887	1.132079
N	4.536495	-0.724510	-2.721831
C	3.535398	0.181572	-3.260924
N	0.304097	-0.900237	-0.881049
C	-1.059149	-1.197510	-0.787928
C	-1.621021	-2.106910	0.119613
C	-2.999588	-2.274676	0.147132
C	-3.850495	-1.560363	-0.690313
C	-3.283867	-0.634623	-1.554390
C	-1.908954	-0.449736	-1.611430
C	-3.613348	-3.184423	1.173006
F	-2.738659	-4.069310	1.661981
C	-4.146983	0.201185	-2.455544
F	-5.435086	0.179807	-2.074090
C	4.266679	-2.088745	-3.142565
F	-4.091000	-2.483847	2.221693
F	-4.651152	-3.868427	0.669954
F	-3.752308	1.484437	-2.453519
F	-4.103547	-0.217237	-3.727725
H	2.411150	0.143848	-0.741825
H	0.499754	0.011795	-1.299974
H	4.141657	-0.008344	1.365613
H	3.588715	-1.636269	1.767393
H	5.835780	-2.563964	1.245561
H	5.991795	-1.279162	2.441262
H	7.714097	-1.057668	0.620088
H	6.633020	0.333213	0.659272
H	6.411370	-2.060465	-1.233883
H	6.945375	-0.445577	-1.694001
H	3.919018	-2.381292	-0.538547
H	4.765196	0.504232	-1.079504
H	5.046629	-2.765246	-2.782603
H	3.289547	-2.467038	-2.791673
H	4.268627	-2.129552	-4.236699
H	2.496192	-0.130346	-3.061529
H	3.658296	0.242030	-4.348566
H	3.670889	1.184376	-2.845273
H	-0.986889	-2.681269	0.780549
H	-4.924635	-1.702836	-0.648454
H	-1.487492	0.283904	-2.293163
N	-0.368648	3.351986	-1.313754
O	-0.803447	4.451397	-0.997743
O	-0.913040	2.583952	-2.071637
C	0.945641	2.872790	-0.595868
C	0.489354	2.035709	0.527380
H	-0.376185	1.431484	0.267143
O	1.404883	1.728696	-1.102358
C	1.299956	1.549310	1.655071
C	2.645424	0.560769	3.895630
C	2.296727	2.316583	2.273643
C	0.973549	0.292444	2.182180
C	1.646285	-0.200904	3.295555
C	2.966638	1.819564	3.385639
H	2.531453	3.309913	1.907612
H	0.186684	-0.295651	1.715953

H	1.393505	-1.181875	3.684430
H	3.736416	2.418701	3.861002
H	3.173692	0.177362	4.762832
C	1.881570	4.059048	-0.517271
H	1.500173	4.845552	0.135305
H	2.016332	4.468607	-1.521738
H	2.850128	3.705681	-0.162900
N	-0.900069	3.211728	1.680080
H	-0.478300	3.399292	2.586651
H	-1.041320	4.081524	1.166654
C	-2.068516	2.409406	1.757169
C	-4.237662	0.664062	1.779987
C	-2.999374	2.447927	0.715493
C	-2.207288	1.486857	2.796078
C	-3.290570	0.612844	2.799152
C	-4.089209	1.584240	0.744222
H	-2.867162	3.145949	-0.108967
H	-1.465758	1.453133	3.590417
H	-3.392121	-0.113054	3.599349
H	-4.818057	1.621246	-0.058961
H	-5.075847	-0.024538	1.784047

RS epoxide:Catalyst:Aniline, Transition State 8; Energy = -2737.294943; 6-31G(d) basis set.

N	-0.046491	1.853713	0.395866
C	-1.352257	1.709289	0.094572
S	-2.277119	2.857315	-0.721004
C	0.826749	3.012220	0.212485
C	1.254000	3.291121	-1.250219
C	2.298545	4.417552	-1.219359
C	1.769201	5.675221	-0.527968
C	1.361836	5.371687	0.911701
C	0.309361	4.265609	0.931359
N	1.757180	2.042266	-1.880525
C	0.700601	1.365137	-2.636753
N	-1.809617	0.470593	0.476226
C	-3.087838	-0.083147	0.355585
C	-4.269880	0.652439	0.492827
C	-5.494521	-0.000988	0.411252
C	-5.584018	-1.374980	0.220683
C	-4.401651	-2.098038	0.113860
C	-3.165757	-1.469030	0.175098
C	-6.754645	0.814220	0.491703
F	-6.610084	1.879282	1.292510
C	-4.457245	-3.593215	-0.012888
F	-3.408463	-4.077775	-0.693724
C	2.907962	2.195386	-2.764702
F	-7.122474	1.277643	-0.712574
F	-7.784033	0.092404	0.961986
F	-4.447670	-4.191772	1.190487
F	-5.570636	-3.999205	-0.639339
H	0.386595	1.053789	0.852580
H	-1.071745	-0.216632	0.650199
H	-0.603247	4.616469	0.443263
H	0.044917	3.988689	1.957596
H	2.248064	5.055963	1.480765
H	0.970904	6.269787	1.400601
H	2.534421	6.457958	-0.559627
H	0.899126	6.053904	-1.080117
H	3.191277	4.070056	-0.677008
H	2.614933	4.662842	-2.237263
H	1.750087	2.707549	0.724638
H	0.379061	3.656120	-1.810544
H	2.705425	2.830535	-3.643260
H	3.772130	2.604155	-2.235463
H	3.180719	1.204061	-3.143724
H	1.052466	0.374935	-2.950772
H	0.419799	1.932835	-3.539807
H	-0.193346	1.234134	-2.029934
H	-4.230963	1.718871	0.666230
H	-6.547055	-1.869120	0.163656
H	-2.252049	-2.045054	0.067376
N	0.844128	-1.714180	-1.181501
O	1.524772	-2.111984	-2.117437
O	-0.315104	-1.381430	-1.266320

C	1.542678	-1.591441	0.228894
C	2.408171	-0.402353	0.168830
H	2.059220	0.381161	-0.511502
O	0.806621	-0.860054	1.064851
C	3.300380	0.055571	1.254637
C	5.115824	1.012136	3.154823
C	4.039392	1.221724	1.011840
C	3.444525	-0.599647	2.480273
C	4.354568	-0.124116	3.419786
C	4.946673	1.696309	1.951236
H	3.891409	1.753718	0.072980
H	2.816063	-1.449350	2.717719
H	4.461642	-0.640349	4.368135
H	5.514385	2.598914	1.749255
H	5.824075	1.376231	3.892065
C	1.956721	-2.996684	0.626159
H	2.217462	-3.597266	-0.245425
H	1.110492	-3.448877	1.150968
H	2.823840	-2.974349	1.287573
N	3.967928	-0.845122	-1.245127
H	3.450238	-1.047941	-2.098641
H	4.492328	0.021235	-1.349611
C	4.785074	-1.940510	-0.846801
C	6.273358	-4.126777	0.043654
C	5.734114	-1.771926	0.165350
C	4.587130	-3.199642	-1.417809
C	5.330147	-4.286700	-0.969005
C	6.473985	-2.866416	0.602419
H	5.890488	-0.791211	0.606829
H	3.845493	-3.321357	-2.202372
H	5.171203	-5.262056	-1.417869
H	7.210905	-2.729408	1.387515
H	6.852091	-4.976367	0.390486

RS epoxide:Catalyst:Aniline, Transition State 9; Energy = -2737.278040; 6-31G(d) basis set.

N	3.759651	-1.701254	-0.608302
C	2.541235	-2.259344	-0.749311
S	2.311020	-3.618296	-1.711629
C	4.066162	-0.370215	-0.078078
C	5.599235	-0.241242	0.080521
C	6.255513	-0.286695	-1.310794
C	5.731495	0.836224	-2.208205
C	4.209129	0.746588	-2.348031
C	3.520361	0.747218	-0.980323
N	5.919015	1.015187	0.766568
C	7.358813	1.211881	0.892008
N	1.546585	-1.648081	-0.029449
C	0.181411	-1.984033	-0.022587
C	-0.478051	-2.057001	1.206792
C	-1.845856	-2.304747	1.245369
C	-2.579668	-2.474404	0.073848
C	-1.910530	-2.386531	-1.142949
C	-0.540474	-2.151951	-1.206059
C	-2.560402	-2.384493	2.567067
F	-3.279058	-1.267594	2.810734
C	-2.690677	-2.393753	-2.428371
F	-3.878130	-2.991098	-2.293047
C	5.282757	1.118504	2.073304
F	-3.424802	-3.403887	2.591418
F	-1.714539	-2.532585	3.591313
F	-2.922303	-1.129294	-2.833500
F	-2.026165	-3.003616	-3.413427
H	4.476444	-2.185623	-1.132671
H	1.825532	-1.031610	0.727833
H	2.437377	0.626419	-1.101708
H	3.695971	1.706332	-0.478347
H	3.829322	1.580082	-2.946361
H	3.945023	-0.175192	-2.884382
H	6.000651	1.804359	-1.770167
H	6.204826	0.777134	-3.193409
H	7.343295	-0.251364	-1.216561
H	6.049117	-1.254584	-1.784756
H	3.619607	-0.309637	0.921861
H	5.950168	-1.105080	0.681488

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H          4.211358        1.317856        1.974795
H          5.420699        0.212847        2.692784
H          5.708352        1.967552        2.611458
H          7.868554        0.351713        1.362462
H          7.542637        2.096546        1.505064
H          7.812539        1.394034       -0.083982
H          0.079513       -1.925530        2.129188
H         -3.647154       -2.665546        0.106525
H         -0.037244       -2.082553       -2.163670
N         -1.157470        3.881791       -1.360386
O         -1.841325        4.859307       -1.576231
O         -0.652369        3.195616       -2.240600
C         -0.826747        3.504196        0.161193
C         -0.394576        2.089368        0.185007
H          0.305498        1.879504       -0.612472
O          0.406212        3.847502        0.477438
C         -0.139894        1.411392        1.487754
C          0.454899        0.133761        3.908723
C          1.183070        1.091046        1.816151
C         -1.158787        1.094825        2.387792
C         -0.861237        0.459878        3.593454
C          1.481103        0.454588        3.017979
H          1.974501        1.400157        1.136819
H         -2.187495        1.350817        2.150646
H         -1.662869        0.213248        4.281291
H          2.513065        0.225663        3.272171
H          0.683031       -0.360850        4.847433
C         -1.967195        4.030522        1.004957
H         -2.942586        3.654384        0.681962
H         -1.964665        5.119995        0.943014
H         -1.777560        3.739986        2.040218
N         -1.754237        0.869949       -0.661523
H         -1.373034        0.791157       -1.605109
H         -1.635954       -0.024578       -0.185878
C         -3.132322        1.258735       -0.704996
C         -5.776714        2.138761       -0.697153
C         -4.007952        0.821888        0.289165
C         -3.583051        2.109736       -1.715507
C         -4.903041        2.547846       -1.702410
C         -5.326472        1.267665        0.291383
H         -3.664090        0.129186        1.050913
H         -2.907305        2.427347       -2.504000
H         -5.246543        3.214351       -2.486577
H         -6.002303        0.925402        1.068494
H         -6.803806        2.487632       -0.691101

RS epoxide:Catalyst:Aniline, Transition State 10; Energy = -2737.303660; 6-31G(d)
basis set.
N         -2.854704       -0.107671       -1.098003
C         -1.943794       -1.085351       -1.223952
S         -2.324038       -2.695223       -1.555033
C         -4.285866       -0.248436       -1.328702
C         -5.009367       -0.722399       -0.042525
C         -4.915853        0.390130        1.010278
C         -5.510620        1.713670        0.522441
C         -4.805616        2.179099       -0.753843
C         -4.854835        1.084885       -1.824721
N         -6.396802       -1.085631       -0.374098
C         -7.244534       -1.226065        0.801986
N         -0.664027       -0.602945       -1.115430
C          0.540027       -1.298892       -0.986353
C          1.678614       -0.711971       -1.550871
C          2.927082       -1.297289       -1.379445
C          3.070672       -2.485700       -0.672915
C          1.933254       -3.059226       -0.117375
C          0.675602       -2.482370       -0.255155
C          4.151771       -0.612778       -1.912221
F          4.763309        0.119285       -0.952424
C          2.047500       -4.316116        0.698482
F          3.324925       -4.605107        0.997808
C         -6.440280       -2.340899       -1.118649
F          5.061237       -1.483569       -2.361811
F          3.866208        0.239535       -2.906739
F          1.386849       -4.201104        1.864015
F          1.536281       -5.378121        0.065887
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H	-2.501245	0.808642	-0.824379
H	-0.590844	0.414852	-1.055486
H	-4.316380	1.394650	-2.726941
H	-5.898862	0.904858	-2.100927
H	-5.268203	3.093622	-1.140413
H	-3.760372	2.441263	-0.525044
H	-6.579730	1.585264	0.310243
H	-5.425671	2.475043	1.306439
H	-5.374982	0.071178	1.950174
H	-3.851501	0.530536	1.232753
H	-4.390044	-1.000895	-2.111686
H	-4.467111	-1.607197	0.340134
H	-6.052197	-3.188047	-0.525221
H	-7.475502	-2.558353	-1.397108
H	-5.852587	-2.282405	-2.035686
H	-8.227757	-1.583763	0.483677
H	-7.388229	-0.266692	1.303351
H	-6.840812	-1.948623	1.535314
H	1.571907	0.194637	-2.139835
H	4.045279	-2.942311	-0.542669
H	-0.192917	-2.931109	0.211824
N	-1.234860	1.758898	1.800256
O	-1.229706	2.184917	2.946661
O	-1.484038	0.616838	1.486509
C	-0.782853	2.744455	0.655093
C	0.640912	2.426651	0.423770
H	0.833062	1.357545	0.472517
O	-0.993190	2.245236	-0.560673
C	1.613700	3.222409	-0.334040
C	3.627417	4.580738	-1.717616
C	2.741509	2.539312	-0.808514
C	1.514747	4.604214	-0.542057
C	2.515692	5.273198	-1.236398
C	3.744519	3.210684	-1.497250
H	2.835652	1.476325	-0.613557
H	0.666963	5.161732	-0.164782
H	2.429213	6.342024	-1.401669
H	4.604262	2.658465	-1.861294
H	4.402072	5.112534	-2.260774
C	-1.360697	4.104249	0.998980
H	-0.834640	4.582628	1.826831
H	-2.411385	3.987292	1.277944
H	-1.317129	4.728303	0.107008
N	1.644936	2.458913	2.349791
H	2.348247	3.193696	2.326019
H	0.928235	2.676211	3.042056
C	2.193122	1.156535	2.501661
C	3.167326	-1.456020	2.548847
C	1.378454	0.117414	2.961418
C	3.490614	0.888728	2.059720
C	3.972051	-0.417220	2.087862
C	1.871246	-1.183047	2.981946
H	0.365394	0.327145	3.295958
H	4.115863	1.698140	1.690790
H	4.978400	-0.619520	1.735358
H	1.232899	-1.989476	3.327127
H	3.540564	-2.475339	2.554991

RS epoxide:Catalyst:Aniline, Transition State 11; Energy = -2737.290818; 6-31G(d) basis set.

N	3.228968	0.748559	0.298647
C	2.448465	1.833086	0.384162
S	2.889821	3.374441	-0.123764
C	4.575665	0.709218	-0.273247
C	5.316621	-0.460765	0.418801
C	4.852215	-1.831650	-0.129288
C	4.732841	-1.916785	-1.657647
C	3.887598	-0.767668	-2.212005
C	4.467900	0.586998	-1.800661
N	6.768280	-0.235850	0.481592
C	7.540952	-0.621377	-0.688113
N	1.254549	1.541642	1.020204
C	0.000872	2.120560	0.864672
C	-0.987713	1.735523	1.784149
C	-2.303857	2.147797	1.615104

C	-2.674270	2.972893	0.560217
C	-1.680580	3.370735	-0.329479
C	-0.359154	2.962630	-0.197325
C	-3.353352	1.621265	2.548033
F	-2.884679	1.415948	3.781403
C	-2.073091	4.156207	-1.549799
F	-2.400849	3.327556	-2.561759
C	7.350450	-0.852541	1.663407
F	-4.414315	2.424794	2.630551
F	-3.819596	0.417170	2.113881
F	-3.142797	4.930157	-1.323182
F	-1.084633	4.938356	-1.990416
H	2.757776	-0.148710	0.434407
H	1.231378	0.630458	1.478606
H	3.840752	1.409359	-2.160118
H	5.456834	0.727954	-2.250663
H	3.828552	-0.831979	-3.303730
H	2.861457	-0.858348	-1.831170
H	5.722283	-1.898470	-2.127302
H	4.280083	-2.878921	-1.924026
H	5.517888	-2.615789	0.253325
H	3.858006	-2.045773	0.289489
H	5.074026	1.641541	0.001585
H	4.995089	-0.408865	1.465437
H	8.406063	-0.572023	1.731215
H	6.844332	-0.491782	2.562888
H	7.298399	-1.957049	1.652419
H	7.573508	-1.714021	-0.849722
H	8.571024	-0.276195	-0.553820
H	7.148958	-0.150741	-1.590447
H	-0.715013	1.102837	2.626090
H	-3.699982	3.300749	0.437361
H	0.384487	3.273356	-0.919590
N	0.450329	-2.022668	2.311097
O	0.849111	-0.960854	2.754465
O	-0.033264	-2.911398	2.988016
C	0.497579	-2.214207	0.728001
C	-0.648475	-1.422255	0.227472
H	-0.768788	-0.495651	0.776706
O	1.283197	-1.320390	0.158010
C	-1.198052	-1.422499	-1.123615
C	-2.472672	-1.297959	-3.602363
C	-1.733586	-0.213248	-1.587595
C	-1.321105	-2.576307	-1.909458
C	-1.959060	-2.510454	-3.141391
C	-2.357620	-0.146193	-2.827042
H	-1.654774	0.678219	-0.969368
H	-0.952524	-3.529070	-1.547945
H	-2.065392	-3.409211	-3.739778
H	-2.752707	0.800630	-3.178952
H	-2.968458	-1.253830	-4.567083
C	0.736928	-3.686433	0.468355
H	-0.111767	-4.308167	0.758641
H	1.618035	-4.010401	1.028563
H	0.945923	-3.806040	-0.595062
N	-2.416816	-2.207443	1.289015
H	-2.042509	-2.846850	1.989812
H	-2.791413	-1.380766	1.752268
C	-3.357295	-2.812180	0.421188
C	-5.038344	-3.950666	-1.490447
C	-4.255852	-2.008440	-0.283966
C	-3.310302	-4.186419	0.181291
C	-4.153216	-4.750256	-0.771702
C	-5.088905	-2.580287	-1.237632
H	-4.284322	-0.940098	-0.088625
H	-2.616740	-4.809695	0.740736
H	-4.115312	-5.820065	-0.951252
H	-5.779249	-1.949433	-1.788643
H	-5.690243	-4.392526	-2.236615

RS epoxide:Catalyst:Aniline, Transition State 12; Energy = -2737.287443; 6-31G(d) basis set.

N	0.664522	-2.154954	-0.422618
C	1.902119	-1.875814	0.018795
S	2.730047	-2.827217	1.135409

C	-0.219382	-3.224132	0.023481
C	-1.544765	-2.617887	0.547072
C	-2.613930	-3.702854	0.730044
C	-2.843300	-4.517152	-0.540626
C	-1.538968	-5.195909	-0.953402
C	-0.460715	-4.142727	-1.187392
N	-1.483110	-1.776013	1.758245
C	-0.518122	-0.676094	1.750090
N	2.370257	-0.696873	-0.506090
C	3.608374	-0.067467	-0.312250
C	4.816073	-0.765470	-0.214935
C	6.002149	-0.055507	-0.075468
C	6.026749	1.335381	-0.052925
C	4.822136	2.015564	-0.175785
C	3.619864	1.329445	-0.300717
C	7.289446	-0.815627	0.084938
F	7.545427	-1.086069	1.373710
C	4.795665	3.516835	-0.116453
F	4.492128	3.955831	1.115423
C	-1.351522	-2.506368	3.017835
F	7.260666	-1.987762	-0.563481
F	8.336316	-0.119149	-0.382988
F	5.980915	4.049602	-0.442840
F	3.876407	4.027743	-0.947546
H	0.247172	-1.532054	-1.113953
H	1.661586	-0.103412	-0.934048
H	-0.767209	-3.508272	-2.032292
H	0.496627	-4.597440	-1.462194
H	-1.221769	-5.886545	-0.160742
H	-1.676358	-5.792249	-1.861072
H	-3.631491	-5.256684	-0.366710
H	-3.191123	-3.862019	-1.351596
H	-2.301747	-4.399639	1.517580
H	-3.540114	-3.221933	1.068795
H	0.296883	-3.769228	0.818883
H	-1.892558	-1.952810	-0.256289
H	-0.428887	-3.106774	3.061812
H	-1.313885	-1.778595	3.832919
H	-2.211181	-3.154218	3.191580
H	0.509233	-0.994805	1.977608
H	-0.820211	0.048916	2.516434
H	-0.514391	-0.171551	0.781960
H	4.825518	-1.846236	-0.257237
H	6.962740	1.873965	0.039160
H	2.686149	1.878264	-0.394278
N	-1.193089	0.662678	-1.527295
O	-1.482086	-0.461271	-1.914177
O	-0.072939	0.978151	-1.169657
C	-2.352665	1.830948	-1.447993
C	-2.788149	1.878853	-0.016346
H	-1.935511	1.834411	0.653207
O	-1.815027	2.994583	-1.283434
C	-3.907667	2.760892	0.391800
C	-5.984063	4.404462	1.286953
C	-3.712792	3.621389	1.477774
C	-5.158900	2.719581	-0.233730
C	-6.189434	3.542042	0.212762
C	-4.743472	4.442331	1.921190
H	-2.739218	3.658274	1.958879
H	-5.339532	2.029682	-1.051081
H	-7.156650	3.502370	-0.277851
H	-4.577074	5.114247	2.756890
H	-6.789777	5.045339	1.630727
C	-3.243448	1.571851	-2.647353
H	-3.955632	2.395407	-2.709708
H	-3.772735	0.619759	-2.592311
H	-2.625498	1.593323	-3.549099
N	-3.558824	0.179051	0.876862
H	-3.799770	0.613393	1.768994
H	-2.848661	-0.545562	1.103716
C	-4.728831	-0.400585	0.296688
C	-7.010737	-1.485116	-0.889761
C	-5.987888	-0.151583	0.845230
C	-4.611868	-1.184744	-0.853265
C	-5.752030	-1.729568	-1.436291

C	-7.123775	-0.691867	0.249342
H	-6.074878	0.467740	1.734355
H	-3.632952	-1.344064	-1.296846
H	-5.653275	-2.342147	-2.327080
H	-8.099020	-0.493642	0.682315
H	-7.897067	-1.909063	-1.349866

RS epoxide:Catalyst:Aniline, Transition State 13; Energy = -2737.300772; 6-31G(d) basis set.

N	-3.214312	-0.189443	-0.457565
C	-3.970827	-1.287856	-0.533252
S	-5.657849	-1.300154	-0.603969
C	-3.706625	1.162284	-0.270207
C	-2.769992	1.932394	0.675689
C	-3.350559	3.339366	0.904385
C	-3.507817	4.086549	-0.423808
C	-4.395197	3.309146	-1.396454
C	-3.858680	1.893476	-1.608085
N	-2.453331	1.154317	1.881217
C	-3.613946	0.651532	2.606151
N	-3.271856	-2.468480	-0.557536
C	-1.940292	-2.630409	-0.110030
C	-1.028478	-3.347977	-0.879062
C	0.284921	-3.493356	-0.441009
C	0.709558	-2.921272	0.749721
C	-0.214280	-2.206235	1.510799
C	-1.533010	-2.065973	1.103242
C	1.232469	-4.275922	-1.308971
F	2.463795	-4.333932	-0.799049
C	0.236177	-1.496902	2.752013
F	-0.741643	-1.366025	3.654372
C	-1.580560	1.880062	2.791447
F	0.797323	-5.545312	-1.445213
F	1.305201	-3.767285	-2.541871
F	1.269086	-2.110620	3.343053
F	0.663199	-0.236201	2.473224
H	-2.205811	-0.280958	-0.585134
H	-3.819609	-3.290724	-0.774791
H	-2.877912	1.930331	-2.104185
H	-4.527560	1.306722	-2.245840
H	-5.413360	3.248427	-0.989332
H	-4.467579	3.832640	-2.355350
H	-3.916186	5.086745	-0.245400
H	-2.512725	4.225071	-0.871413
H	-4.327067	3.258434	1.401578
H	-2.695382	3.909453	1.570896
H	-4.699622	1.080887	0.185033
H	-1.807488	2.063244	0.149746
H	-2.093198	2.689487	3.337389
H	-1.166422	1.184453	3.525846
H	-0.750733	2.328813	2.233381
H	-4.264896	1.450203	3.000980
H	-3.255958	0.062521	3.457155
H	-4.217310	-0.006723	1.973866
H	-1.337465	-3.762492	-1.834018
H	1.743528	-3.020578	1.060398
H	-2.233321	-1.487915	1.697148
N	0.416604	-0.458729	-1.662130
O	-0.304501	0.008604	-0.774085
O	-0.010572	-1.066253	-2.610656
C	2.032324	-0.336197	-1.533318
C	2.375779	0.038116	-0.141241
H	1.790993	-0.521617	0.573631
O	2.566502	-1.509039	-1.297182
C	3.745626	0.404996	0.276645
C	6.279254	1.100723	1.229793
C	4.233884	-0.150945	1.464833
C	4.528466	1.334365	-0.417592
C	5.791258	1.675257	0.058204
C	5.496588	0.189262	1.936329
H	3.615845	-0.856074	2.015410
H	4.145967	1.812516	-1.312491
H	6.392865	2.395747	-0.486584
H	5.869516	-0.256306	2.852773
H	7.265942	1.367222	1.595182

C	2.449624	0.411581	-2.782817
H	2.073207	-0.143302	-3.644917
H	3.539093	0.411564	-2.827721
H	2.070242	1.437851	-2.806883
N	1.427011	1.727145	0.563781
H	0.486502	1.333508	0.573439
H	1.784635	1.812468	1.513636
C	1.531068	2.929749	-0.179988
C	1.805014	5.239546	-1.720996
C	2.538771	3.849880	0.116011
C	0.661442	3.162171	-1.249948
C	0.801202	4.317486	-2.012541
C	2.670518	5.000127	-0.656075
H	3.214404	3.660466	0.945895
H	-0.114452	2.436061	-1.479577
H	0.119511	4.495295	-2.838395
H	3.453053	5.713761	-0.418880
H	1.909388	6.139313	-2.317813

RS epoxide:Catalyst:Aniline, Transition State 14; Energy = -2737.288704; 6-31G(d) basis set.

N	2.532397	-0.605202	-1.338834
C	1.533145	-1.358576	-0.849008
S	1.789101	-2.824941	-0.057770
C	3.959295	-0.951852	-1.353772
C	4.581930	-0.832954	0.084404
C	5.449073	-2.024187	0.528684
C	6.095485	-2.815538	-0.607892
C	4.998800	-3.359722	-1.516562
C	4.253957	-2.218081	-2.210033
N	5.308388	0.434183	0.265747
C	4.468386	1.595792	0.039676
N	0.300316	-0.795074	-1.075541
C	-0.995054	-1.239828	-0.783253
C	-2.017739	-0.696899	-1.570532
C	-3.341836	-1.047890	-1.345517
C	-3.687960	-1.942787	-0.343892
C	-2.669168	-2.448941	0.456560
C	-1.335794	-2.109649	0.262621
C	-4.392531	-0.433267	-2.224905
F	-4.201535	0.889200	-2.359726
C	-3.048778	-3.321655	1.619131
F	-3.512190	-2.587864	2.650952
C	6.546401	0.536454	-0.483385
F	-4.383291	-0.953650	-3.459792
F	-5.628044	-0.609462	-1.728217
F	-4.028202	-4.177955	1.293425
F	-2.017702	-4.036451	2.081062
H	2.293729	0.334275	-1.649485
H	0.322476	0.090012	-1.586268
H	3.312128	-2.585224	-2.626837
H	4.865967	-1.889734	-3.059415
H	5.417078	-4.022862	-2.281956
H	4.300200	-3.949594	-0.914843
H	6.782573	-2.187909	-1.192438
H	6.690794	-3.634314	-0.189159
H	6.194320	-1.650001	1.239298
H	4.802565	-2.717648	1.078356
H	4.385023	-0.118540	-1.919407
H	3.732642	-0.772115	0.773130
H	7.243238	-0.249922	-0.183887
H	6.410550	0.478799	-1.581214
H	7.014502	1.500989	-0.262982
H	4.245665	1.793718	-1.027102
H	4.963100	2.487842	0.440391
H	3.515797	1.461204	0.556462
H	-1.770973	0.001653	-2.365060
H	-4.722498	-2.218382	-0.172117
H	-0.568298	-2.523865	0.900680
N	-0.925467	3.200229	-1.807190
O	-1.548485	4.226425	-1.568478
O	-1.318304	2.299815	-2.511927
C	0.447629	3.011219	-1.067720
C	0.143141	2.263337	0.164615
H	-0.614362	1.496647	0.020971

O	1.069114	1.891480	-1.427451
C	1.085210	2.062617	1.282351
C	2.861667	1.562081	3.376881
C	1.804871	3.115742	1.860833
C	1.229245	0.767199	1.790147
C	2.124857	0.516143	2.826433
C	2.688867	2.863251	2.903626
H	1.667993	4.132433	1.504054
H	0.650695	-0.046335	1.360734
H	2.246810	-0.497554	3.194462
H	3.248691	3.681416	3.344830
H	3.564769	1.366973	4.179953
C	1.204382	4.317205	-1.150473
H	0.675040	5.134604	-0.658977
H	1.351117	4.569836	-2.204056
H	2.184423	4.169243	-0.694641
N	-1.338036	3.345847	1.237723
H	-1.640985	4.103159	0.625386
H	-0.908187	3.722072	2.079854
C	-2.365551	2.402924	1.508920
C	-4.262336	0.414015	1.940947
C	-3.393710	2.216122	0.582850
C	-2.262449	1.578011	2.630641
C	-3.212355	0.583354	2.840081
C	-4.348427	1.231316	0.816150
H	-3.440961	2.836317	-0.310026
H	-1.439947	1.715560	3.328189
H	-3.128230	-0.065361	3.705742
H	-5.154810	1.092474	0.103193
H	-4.997270	-0.366547	2.107031

RS epoxide:Catalyst:Aniline, Transition State 15; Energy = -2737.295660; 6-31G(d) basis set.

N	2.504061	-1.801745	-0.714932
C	1.420543	-1.967805	0.064937
S	1.435061	-1.806838	1.747082
C	3.922181	-1.943536	-0.346987
C	4.484618	-0.830840	0.560080
C	5.982389	-1.095959	0.801939
C	6.222991	-2.470771	1.425391
C	5.680012	-3.562674	0.504966
C	4.192731	-3.341842	0.229898
N	4.176547	0.503427	0.034078
C	4.227625	1.515803	1.076882
N	0.290607	-2.265266	-0.664489
C	-1.078941	-2.120023	-0.372191
C	-1.641066	-2.140274	0.907282
C	-3.005069	-1.898039	1.056427
C	-3.843592	-1.694457	-0.029072
C	-3.280287	-1.727544	-1.300811
C	-1.919486	-1.923409	-1.478399
C	-3.575105	-1.897100	2.448992
F	-2.731361	-1.337662	3.327591
C	-4.136703	-1.435609	-2.500079
F	-3.691673	-2.066722	-3.594933
C	5.031734	0.921992	-1.074364
F	-4.732339	-1.225350	2.512448
F	-3.817414	-3.144364	2.882288
F	-5.408698	-1.801324	-2.303603
F	-4.148819	-0.120632	-2.790433
H	2.336876	-1.636243	-1.703180
H	0.458778	-2.327291	-1.663482
H	3.630038	-3.453395	1.163266
H	3.811180	-4.090595	-0.472936
H	6.237536	-3.545513	-0.441827
H	5.829276	-4.554312	0.944526
H	7.291921	-2.620736	1.610510
H	5.716369	-2.529000	2.398124
H	6.525008	-1.043289	-0.151770
H	6.389913	-0.304792	1.441756
H	4.441509	-1.874141	-1.311250
H	3.967606	-0.912102	1.521246
H	6.057133	1.161883	-0.745485
H	5.087131	0.137804	-1.833631
H	4.582592	1.801630	-1.538991

H	3.904614	2.471126	0.648932
H	5.237818	1.660680	1.499419
H	3.550461	1.238968	1.893419
H	-1.020854	-2.308969	1.775760
H	-4.901152	-1.501882	0.108576
H	-1.500196	-1.903547	-2.481233
N	1.677941	0.714241	-2.439120
O	2.785307	0.438573	-2.821779
O	0.742498	-0.095023	-2.441950
C	1.381993	2.223291	-1.929179
C	1.194476	2.182841	-0.461227
H	1.918937	1.522684	0.009906
O	2.474671	2.893469	-1.682359
C	0.647698	3.307818	0.325620
C	-0.428866	5.304227	1.968453
C	1.200126	3.569901	1.583258
C	-0.471133	4.041222	-0.087909
C	-1.001716	5.034585	0.727662
C	0.671428	4.566283	2.397296
H	2.051469	2.988322	1.921788
H	-0.957564	3.813982	-1.029066
H	-1.873726	5.589586	0.397104
H	1.117059	4.762444	3.367251
H	-0.846015	6.079397	2.603537
C	0.403290	2.750564	-2.964555
H	-0.546772	2.211805	-2.959021
H	0.865699	2.656585	-3.951494
H	0.240302	3.810691	-2.771444
N	-0.303730	0.800139	0.069653
H	0.155425	0.262777	0.810104
H	-0.274022	0.264139	-0.797089
C	-1.618118	1.181433	0.421311
C	-4.215529	1.933223	1.103288
C	-1.964077	1.351553	1.763556
C	-2.565855	1.404744	-0.578648
C	-3.861476	1.776926	-0.235003
C	-3.262076	1.719576	2.098307
H	-1.221666	1.168733	2.536152
H	-2.297007	1.244636	-1.620045
H	-4.598242	1.924242	-1.018454
H	-3.532591	1.826986	3.144036
H	-5.229305	2.212280	1.371096

RS epoxide:Catalyst:Aniline, Transition State 16; Energy = -2737.294221; 6-31G(d) basis set.

N	-1.420075	2.272100	-0.841439
C	-0.241350	2.425377	-0.209033
S	0.004247	3.252293	1.230581
C	-2.719134	2.861564	-0.511782
C	-3.211845	2.553049	0.915562
C	-4.639330	3.103026	1.072809
C	-4.670877	4.614264	0.831124
C	-4.153159	4.942977	-0.569627
C	-2.750159	4.373005	-0.782772
N	-3.048023	1.131456	1.278103
C	-4.124375	0.276236	0.791621
N	0.788157	1.796767	-0.885705
C	2.030330	1.388017	-0.366063
C	2.148854	0.871468	0.927938
C	3.362914	0.350535	1.348690
C	4.475963	0.334110	0.512410
C	4.344784	0.850161	-0.770007
C	3.135481	1.375242	-1.215581
C	3.484155	-0.234947	2.728167
F	4.158380	-1.397614	2.700095
C	5.508152	0.779676	-1.718861
F	6.679442	0.842798	-1.070961
C	-2.897748	0.986465	2.724241
F	4.155811	0.578477	3.556792
F	2.290251	-0.474332	3.282155
F	5.506852	-0.368767	-2.413823
F	5.481751	1.777554	-2.612858
H	-1.393858	1.762007	-1.720248
H	0.657806	1.614838	-1.879430
H	-2.038059	4.860708	-0.107414

H	-2.408551	4.555043	-1.807108
H	-4.837597	4.515568	-1.315573
H	-4.141925	6.025335	-0.732729
H	-5.689382	4.994288	0.961476
H	-4.042439	5.115262	1.579123
H	-5.313843	2.614949	0.355670
H	-5.014753	2.868248	2.075746
H	-3.411131	2.379777	-1.216547
H	-2.566190	3.108991	1.598331
H	-2.023926	1.554305	3.053842
H	-3.783702	1.329996	3.283154
H	-2.739004	-0.066844	2.972561
H	-5.087895	0.459005	1.292971
H	-3.855971	-0.773242	0.955793
H	-4.265888	0.423302	-0.284914
H	1.289408	0.843900	1.586230
H	5.419757	-0.080265	0.850526
H	3.047960	1.764817	-2.224793
N	-0.171634	-0.513684	-2.872699
O	1.010831	-0.547890	-2.579881
O	-0.749651	0.518904	-3.184382
C	-1.076335	-1.858747	-2.733430
C	-1.981912	-1.588216	-1.582547
H	-2.473464	-0.626480	-1.671582
O	-2.123917	-1.844343	-3.503010
C	-2.737262	-2.697598	-0.962461
C	-4.240911	-4.762542	0.173566
C	-4.136409	-2.639229	-0.960040
C	-2.098756	-3.808789	-0.399573
C	-2.850738	-4.832145	0.171413
C	-4.885101	-3.665793	-0.398577
H	-4.632213	-1.792225	-1.425540
H	-1.015487	-3.869595	-0.388307
H	-2.345142	-5.683750	0.614928
H	-5.968910	-3.614096	-0.411601
H	-4.824062	-5.564150	0.615931
C	-0.110878	-3.023347	-2.811100
H	0.635842	-3.016873	-2.015728
H	0.394808	-2.993900	-3.779618
H	-0.703255	-3.937886	-2.759771
N	-0.914245	-0.788339	0.043869
H	-1.582261	-0.161874	0.529969
H	-0.243002	-0.183782	-0.433482
C	-0.228151	-1.689661	0.902156
C	1.096837	-3.552608	2.501966
C	-0.865822	-2.226934	2.019845
C	1.068177	-2.098294	0.573343
C	1.726009	-3.024399	1.375413
C	-0.199028	-3.152100	2.817902
H	-1.887943	-1.936828	2.246722
H	1.557277	-1.675109	-0.302057
H	2.739292	-3.321889	1.125199
H	-0.699199	-3.562040	3.689528
H	1.614923	-4.269653	3.129860

RS epoxide:Catalyst:Aniline, Transition State 17; Energy = -2737.295767; 6-31G(d) basis set.

N	3.072894	-0.381394	-0.110872
C	2.521133	0.643718	-0.787251
S	3.304273	2.071803	-1.231870
C	4.439829	-0.504150	0.409309
C	5.516038	-0.571587	-0.699541
C	6.887293	-0.801628	-0.048193
C	7.207904	0.261591	1.003568
C	6.135071	0.287060	2.092591
C	4.756672	0.544340	1.482555
N	5.272874	-1.565289	-1.744640
C	4.425067	-1.143539	-2.846464
N	1.225109	0.463592	-1.181904
C	0.292070	-0.504560	-0.765259
C	0.206043	-0.952085	0.552662
C	-0.813370	-1.832572	0.921030
C	-1.750006	-2.273832	0.001237
C	-1.663153	-1.808138	-1.313302
C	-0.658303	-0.939714	-1.703409

C	-0.872290	-2.276982	2.354815
F	-1.883474	-3.119652	2.587557
C	-2.687833	-2.289982	-2.303624
F	-2.734208	-3.633468	-2.322351
C	4.912512	-2.889610	-1.287331
F	0.262754	-2.893569	2.720629
F	-1.019406	-1.231250	3.191398
F	-3.925141	-1.875082	-1.980346
F	-2.432986	-1.875918	-3.545325
H	2.532982	-1.238952	-0.090646
H	0.821683	1.230575	-1.720248
H	4.729283	1.540806	1.032106
H	3.972290	0.510312	2.248149
H	6.133115	-0.677459	2.620489
H	6.359158	1.056706	2.838789
H	8.193916	0.071978	1.441339
H	7.255583	1.247346	0.521209
H	6.910054	-1.790463	0.432192
H	7.641073	-0.815998	-0.841371
H	4.437882	-1.481451	0.911847
H	5.539414	0.404572	-1.195792
H	5.580052	-3.223141	-0.488073
H	3.869982	-2.964265	-0.918988
H	5.008551	-3.596269	-2.118493
H	3.343963	-1.198334	-2.625602
H	4.617156	-1.788668	-3.712078
H	4.659060	-0.112792	-3.122552
H	0.896827	-0.576761	1.302174
H	-2.536147	-2.959556	0.297157
H	-0.623661	-0.554755	-2.716101
N	-3.338876	1.815971	-2.120005
O	-4.450542	2.263748	-1.854298
O	-3.143673	0.783034	-2.715607
C	-2.063829	2.578468	-1.528279
C	-1.790373	1.905826	-0.240364
H	-1.996699	0.837582	-0.269762
O	-0.944769	2.048199	-1.971493
C	-0.743553	2.350718	0.715437
C	1.239854	3.005009	2.579232
C	0.250810	3.277287	0.389480
C	-0.708925	1.727434	1.969584
C	0.268321	2.057556	2.899682
C	1.232955	3.601479	1.321738
H	0.307726	3.680643	-0.614917
H	-1.429471	0.949017	2.200073
H	0.282086	1.556368	3.863040
H	2.016375	4.298078	1.042873
H	2.015030	3.256049	3.296690
C	-2.327804	4.062559	-1.676372
H	-2.248564	4.321187	-2.735747
H	-1.569933	4.620432	-1.125558
H	-3.316881	4.342221	-1.312478
N	-3.524517	2.097517	0.914804
H	-4.163148	2.513456	0.234027
H	-3.346092	2.755800	1.670979
C	-3.989334	0.830386	1.377965
C	-4.713225	-1.726813	2.223932
C	-4.500585	-0.086861	0.456932
C	-3.844366	0.470866	2.719553
C	-4.198250	-0.808106	3.135732
C	-4.870551	-1.357162	0.890673
H	-4.614117	0.186565	-0.589266
H	-3.449091	1.189937	3.433034
H	-4.068258	-1.084816	4.177122
H	-5.266178	-2.064294	0.168762
H	-4.986668	-2.724548	2.551082

RS epoxide:Catalyst:Aniline, Transition State 18; Energy = -2737.298417; 6-31G(d) basis set.

N	2.972860	-0.300392	-0.161505
C	2.055490	0.662301	-0.358167
S	2.336375	2.310092	-0.156217
C	4.407700	-0.168773	0.116128
C	5.197051	0.524158	-1.020518
C	6.692526	0.506347	-0.670562

C	6.974181	1.133410	0.695544
C	6.198960	0.405211	1.793693
C	4.699066	0.433020	1.497091
N	4.984456	-0.031272	-2.356650
C	3.850835	0.491920	-3.098337
N	0.842784	0.154412	-0.782827
C	-0.359518	0.868458	-0.932587
C	-0.788735	1.791092	0.027044
C	-2.010185	2.430947	-0.138253
C	-2.831314	2.163808	-1.230338
C	-2.412335	1.210784	-2.150135
C	-1.189076	0.562412	-2.013206
C	-2.543298	3.300881	0.961326
F	-1.580428	3.775590	1.759367
C	-3.341209	0.814708	-3.262090
F	-2.682066	0.322653	-4.318284
C	5.045314	-1.475319	-2.456769
F	-3.235105	4.345169	0.485946
F	-3.393360	2.602225	1.745317
F	-4.206011	-0.129618	-2.859042
F	-4.073754	1.855505	-3.687466
H	2.664511	-1.256532	-0.310160
H	0.815740	-0.789330	-1.176188
H	4.334281	1.464345	1.526243
H	4.143380	-0.138955	2.250841
H	6.545417	-0.636417	1.850838
H	6.392213	0.859033	2.771303
H	8.048975	1.110631	0.904980
H	6.672510	2.189414	0.681033
H	7.059226	-0.530000	-0.666434
H	7.230177	1.030192	-1.466367
H	4.754357	-1.210656	0.147890
H	4.876858	1.570499	-1.060031
H	5.922202	-1.865707	-1.932755
H	4.146942	-1.983691	-2.057625
H	5.135084	-1.757439	-3.511165
H	2.886600	0.028085	-2.824824
H	4.008664	0.309740	-4.167965
H	3.765544	1.569544	-2.939744
H	-0.177812	1.990506	0.897848
H	-3.783636	2.670283	-1.348582
H	-0.883413	-0.189979	-2.731771
N	0.910722	-3.201167	0.094462
O	1.223726	-3.603929	1.201750
O	1.709889	-2.847049	-0.754350
C	-0.631369	-3.160197	-0.318783
C	-1.323041	-2.139096	0.500329
H	-0.767153	-1.210386	0.561881
O	-0.837905	-2.368144	-1.344642
C	-2.793216	-2.029103	0.591727
C	-5.550939	-1.658013	0.860220
C	-3.634333	-3.128832	0.807314
C	-3.344623	-0.745879	0.551603
C	-4.717211	-0.558632	0.677857
C	-5.005785	-2.940663	0.933879
H	-3.222106	-4.128085	0.899348
H	-2.686847	0.107067	0.434085
H	-5.124414	0.447110	0.642439
H	-5.652169	-3.796978	1.096840
H	-6.622960	-1.519229	0.957814
C	-1.014002	-4.625167	-0.425095
H	-0.931502	-5.145880	0.532010
H	-0.349600	-5.097591	-1.154150
H	-2.032223	-4.686832	-0.809164
N	-0.952537	-2.290893	2.557632
H	-0.202152	-2.976009	2.634282
H	-1.794535	-2.618763	3.025185
C	-0.567699	-0.977132	2.934403
C	0.156647	1.665899	3.446870
C	0.753379	-0.565425	2.732643
C	-1.532863	-0.061258	3.358527
C	-1.163909	1.256330	3.617347
C	1.111247	0.752735	2.999688
H	1.493351	-1.277295	2.372060
H	-2.564578	-0.380876	3.480900

H	-1.918123	1.968167	3.935948
H	2.135563	1.072073	2.835160
H	0.436058	2.697322	3.634706

RS epoxide:Catalyst:Aniline, Transition State 19; Energy = -2737.303776; 6-31G(d) basis set.

N	2.829679	-0.881705	0.150322
C	2.050988	-1.628991	0.934145
S	2.328074	-1.935795	2.559399
C	4.103110	-0.278867	0.517950
C	4.959053	-0.148301	-0.759342
C	6.294588	0.520989	-0.411680
C	6.089709	1.884585	0.251746
C	5.225515	1.755666	1.506880
C	3.889737	1.088267	1.179720
N	5.176574	-1.386345	-1.507221
C	4.117509	-1.779543	-2.421776
N	0.987906	-2.175359	0.209452
C	-0.362517	-2.231738	0.545999
C	-0.886657	-1.838506	1.783628
C	-2.267410	-1.813333	1.965856
C	-3.157310	-2.173117	0.962691
C	-2.621621	-2.562861	-0.262710
C	-1.253258	-2.599425	-0.478712
C	-2.792776	-1.201751	3.233708
F	-2.789841	0.145730	3.121469
C	-3.549386	-2.770372	-1.426510
F	-4.705225	-3.329117	-1.051249
C	5.608218	-2.517501	-0.707427
F	-4.050476	-1.570357	3.493635
F	-2.042805	-1.503697	4.296223
F	-3.855148	-1.580044	-1.986714
F	-3.010844	-3.530005	-2.382127
H	2.426590	-0.524650	-0.724176
H	1.154486	-2.217149	-0.793340
H	3.309794	1.716014	0.487984
H	3.287678	0.951559	2.084592
H	5.757826	1.151431	2.254272
H	5.050632	2.737964	1.958270
H	7.058674	2.332294	0.497024
H	5.595252	2.561572	-0.458137
H	6.863901	-0.125491	0.270161
H	6.879846	0.611059	-1.331684
H	4.590403	-0.953739	1.232020
H	4.417354	0.529682	-1.436146
H	6.443070	-2.237803	-0.059320
H	4.801578	-2.934555	-0.076435
H	5.954928	-3.314438	-1.373542
H	3.317067	-2.368624	-1.940311
H	4.539478	-2.399627	-3.221575
H	3.656335	-0.896116	-2.873390
H	-0.225248	-1.550037	2.591205
H	-4.229313	-2.129887	1.117915
H	-0.869741	-2.869914	-1.458857
N	-0.105375	-0.446945	-2.606777
O	-1.278313	-0.550430	-2.921370
O	0.692488	-1.366540	-2.622184
C	0.411334	0.966625	-2.101270
C	0.066971	1.043692	-0.664576
H	0.214197	0.097134	-0.158761
O	1.668307	0.913812	-1.696191
C	0.168096	2.233833	0.188047
C	0.310892	4.382315	1.964545
C	-0.140737	3.526999	-0.247959
C	0.520888	2.023771	1.528236
C	0.595220	3.092568	2.412786
C	-0.059101	4.596004	0.638661
H	-0.477958	3.699452	-1.263791
H	0.753209	1.015845	1.870418
H	0.877719	2.920113	3.446059
H	-0.301733	5.596114	0.294847
H	0.370020	5.219983	2.652282
C	0.029911	1.958843	-3.180849
H	-1.050350	2.090094	-3.260092
H	0.426145	1.603248	-4.136166

H	0.511859	2.909236	-2.952098
N	-2.046723	0.722170	-0.372647
H	-2.084838	0.433819	0.605294
H	-2.276950	-0.071766	-0.969927
C	-2.880725	1.837892	-0.635213
C	-4.396478	4.106099	-1.203072
C	-3.109944	2.787944	0.361455
C	-3.412393	2.015942	-1.915040
C	-4.167714	3.150730	-2.192307
C	-3.869004	3.917433	0.072481
H	-2.686622	2.641366	1.352706
H	-3.238786	1.257757	-2.674783
H	-4.585073	3.283936	-3.185361
H	-4.045784	4.653266	0.850568
H	-4.988302	4.988200	-1.423746

RS epoxide:Catalyst:Aniline, Transition State 20; Energy = -2737.294211; 6-31G(d) basis set.

N	-1.197829	2.336847	-0.755260
C	-0.013582	2.340271	-0.111623
S	0.301707	3.064843	1.369178
C	-2.425420	3.061191	-0.417323
C	-2.972628	2.761570	0.991276
C	-4.326364	3.472205	1.157016
C	-4.174775	4.984126	0.975147
C	-3.604103	5.300304	-0.407394
C	-2.275818	4.575177	-0.630573
N	-2.987388	1.318519	1.301943
C	-4.150951	0.617030	0.771377
N	0.949618	1.639198	-0.811045
C	2.186153	1.169511	-0.327117
C	2.295218	0.568958	0.932557
C	3.499948	0.002758	1.315638
C	4.613212	0.021017	0.476287
C	4.489884	0.615976	-0.769707
C	3.286598	1.187652	-1.178642
C	3.620783	-0.696190	2.640591
F	2.461549	-0.737691	3.304350
C	5.674784	0.694497	-1.690754
F	6.603951	-0.221620	-1.387729
C	-2.877939	1.106280	2.743794
F	4.038209	-1.964836	2.476702
F	4.522957	-0.098549	3.433093
F	5.317126	0.505174	-2.969075
F	6.268089	1.896248	-1.627627
H	-1.212582	1.872982	-1.659752
H	0.804966	1.511242	-1.811362
H	-1.519939	4.949679	0.069082
H	-1.901716	4.753352	-1.644240
H	-4.325108	4.985610	-1.174694
H	-3.461724	6.378776	-0.529352
H	-5.142314	5.478072	1.111756
H	-3.500653	5.377763	1.747156
H	-5.044119	3.095905	0.414966
H	-4.740816	3.245734	2.146417
H	-3.157541	2.690077	-1.147909
H	-2.274696	3.210270	1.700952
H	-3.724932	1.534994	3.303985
H	-2.849384	0.034075	2.956150
H	-1.947544	1.553322	3.102944
H	-4.013833	-0.462201	0.900766
H	-4.254909	0.815690	-0.301113
H	-5.093474	0.898098	1.266848
H	1.436293	0.521312	1.590753
H	5.547961	-0.435124	0.784307
H	3.201775	1.631931	-2.165689
N	-0.176379	-0.510092	-2.844023
O	0.986144	-0.683361	-2.525272
O	-0.627959	0.587872	-3.144223
C	-1.227587	-1.748267	-2.766542
C	-2.150586	-1.395889	-1.653759
H	-2.524636	-0.382715	-1.741302
O	-2.231547	-1.608621	-3.581600
C	-3.055136	-2.420309	-1.090711
C	-4.836529	-4.313387	-0.061760

C	-4.436208	-2.191858	-1.130964
C	-2.576007	-3.613962	-0.538681
C	-3.465799	-4.551837	-0.021533
C	-5.322856	-3.132563	-0.622516
H	-4.809147	-1.279581	-1.587895
H	-1.509032	-3.805307	-0.491986
H	-3.082756	-5.468882	0.414209
H	-6.391313	-2.948717	-0.668198
H	-5.527505	-5.048341	0.339139
C	-0.391142	-3.010066	-2.820148
H	0.304778	-3.098829	-1.984168
H	0.170715	-3.019279	-3.757540
H	-1.081128	-3.854856	-2.823661
N	-1.070145	-0.753633	0.034822
H	-0.311363	-0.223348	-0.398352
H	-1.680948	-0.061635	0.509981
C	-0.534212	-1.742137	0.902669
C	0.491584	-3.768460	2.524501
C	0.741163	-2.259023	0.654816
C	-1.302458	-2.254956	1.948389
C	-0.785049	-3.261989	2.757341
C	1.250803	-3.265343	1.469059
H	1.328785	-1.860645	-0.170217
H	-2.310900	-1.883095	2.106774
H	-1.386716	-3.653380	3.571517
H	2.249796	-3.645959	1.283953
H	0.893271	-4.549721	3.160942

RS epoxide:Catalyst:Aniline, Transition State 21; Energy = -2737.302745; 6-31G(d) basis set.

N	2.978743	-0.999754	-1.089234
C	2.022718	-1.723187	-0.480030
S	2.271591	-2.915143	0.688391
C	4.427936	-1.033567	-0.879040
C	4.858784	-0.568455	0.533134
C	6.392575	-0.523184	0.595816
C	7.023886	-1.863685	0.214914
C	6.586311	-2.290512	-1.186685
C	5.061693	-2.374373	-1.269381
N	4.294135	0.706215	0.978974
C	2.969794	0.638929	1.574157
N	0.767809	-1.410088	-0.938589
C	-0.444259	-1.633559	-0.256898
C	-1.554887	-2.055640	-0.983728
C	-2.788593	-2.189799	-0.350130
C	-2.941119	-1.890374	0.995659
C	-1.827369	-1.449833	1.708210
C	-0.584101	-1.330013	1.102149
C	-3.940713	-2.739000	-1.141831
F	-3.992485	-2.206295	-2.373631
C	-1.992864	-1.005898	3.133051
F	-2.987289	-1.654179	3.750922
C	4.368390	1.799064	0.027597
F	-3.840609	-4.066372	-1.300824
F	-5.122847	-2.502673	-0.550415
F	-0.877364	-1.176141	3.849611
F	-2.294476	0.312786	3.203720
H	2.638641	-0.199765	-1.618670
H	0.705212	-0.721972	-1.690785
H	4.697761	-3.155539	-0.595750
H	4.735176	-2.636730	-2.281891
H	6.957848	-1.559889	-1.919538
H	7.026803	-3.257666	-1.450838
H	8.115664	-1.795048	0.272879
H	6.712046	-2.630086	0.937191
H	6.768655	0.251081	-0.088393
H	6.681775	-0.221242	1.607202
H	4.806997	-0.284665	-1.588411
H	4.517293	-1.326047	1.246874
H	5.363466	1.852646	-0.423621
H	3.613473	1.734155	-0.777515
H	4.191331	2.742337	0.558465
H	2.156309	0.568770	0.831043
H	2.794877	1.549772	2.160719
H	2.906972	-0.224725	2.242285

H	-1.447509	-2.281500	-2.039908
H	-3.905448	-1.988634	1.480511
H	0.280722	-0.995308	1.666343
N	-0.682595	1.409458	-3.135973
O	-0.728820	0.197728	-3.118908
O	-1.456879	2.126971	-3.750294
C	0.395622	2.115425	-2.202624
C	-0.182083	1.996011	-0.849898
H	-0.732915	1.067507	-0.714888
O	1.313326	1.259683	-1.782797
C	0.306227	2.622099	0.387456
C	1.027555	3.730749	2.849745
C	1.227333	3.673028	0.439425
C	-0.239156	2.127941	1.579464
C	0.113669	2.679461	2.805264
C	1.585048	4.219449	1.667948
H	1.679059	4.056874	-0.466934
H	-0.952398	1.310505	1.538583
H	-0.319014	2.277825	3.715938
H	2.306607	5.029348	1.702924
H	1.314859	4.162910	3.802923
C	0.803351	3.399318	-2.900911
H	0.981954	3.200264	-3.959915
H	1.737378	3.747759	-2.461451
H	0.041606	4.176978	-2.820857
N	-2.067305	3.003543	-0.965314
H	-1.962220	3.837000	-0.390322
H	-2.157251	3.271420	-1.945932
C	-3.143583	2.174651	-0.539016
C	-5.206490	0.499575	0.297789
C	-3.752277	1.312480	-1.455152
C	-3.541823	2.176370	0.798932
C	-4.569581	1.333365	1.212695
C	-4.792943	0.492733	-1.033379
H	-3.421173	1.299365	-2.491300
H	-3.054701	2.840405	1.508475
H	-4.871111	1.335864	2.255271
H	-5.276486	-0.162285	-1.749386
H	-6.012927	-0.151639	0.618704

RS epoxide:Catalyst:Aniline, Transition State 22; Energy = -2737.296605; 6-31G(d) basis set.

N	-2.579617	-1.288592	-0.098761
C	-1.442984	-1.522051	-0.774188
S	-1.259840	-1.113257	-2.400449
C	-3.872614	-0.930817	-0.687420
C	-4.992309	-1.509133	0.203046
C	-6.358083	-1.139374	-0.390833
C	-6.512686	0.371064	-0.574792
C	-5.397619	0.923976	-1.461627
C	-4.025524	0.582980	-0.878686
N	-4.916551	-2.949457	0.453142
C	-4.103569	-3.377352	1.575183
N	-0.470529	-2.115906	0.003388
C	0.932618	-2.082970	-0.128675
C	1.666616	-2.056124	1.063623
C	3.050058	-1.946712	1.032354
C	3.737590	-1.851892	-0.170939
C	3.000736	-1.910343	-1.346437
C	1.615690	-2.049069	-1.348509
C	3.798699	-1.911050	2.335397
F	3.157293	-1.163907	3.251529
C	3.698759	-1.753895	-2.669805
F	4.997338	-2.072696	-2.589596
C	-4.663255	-3.770110	-0.715919
F	3.930944	-3.136162	2.863819
F	5.028228	-1.402652	2.192479
F	3.146272	-2.525730	-3.614811
F	3.630490	-0.487225	-3.111673
H	-2.574393	-1.392060	0.912724
H	-0.759188	-2.279365	0.963725
H	-3.894514	1.091201	0.086555
H	-3.232304	0.923980	-1.553631
H	-5.483764	0.490787	-2.467729
H	-5.491951	2.008961	-1.571127

H	-7.494194	0.597006	-1.004574
H	-6.470769	0.863594	0.405844
H	-6.478139	-1.633457	-1.364769
H	-7.131765	-1.541663	0.269600
H	-3.909110	-1.410562	-1.673153
H	-4.918032	-1.015217	1.182912
H	-5.325718	-3.486047	-1.537685
H	-3.618616	-3.706634	-1.073424
H	-4.867602	-4.816918	-0.468804
H	-3.029860	-3.488099	1.331707
H	-4.449086	-4.357281	1.923919
H	-4.202531	-2.668853	2.403324
H	1.149552	-2.069940	2.020541
H	4.813634	-1.727828	-0.190354
H	1.075258	-2.113669	-2.281892
N	-1.820584	0.643551	2.145180
O	-0.908854	-0.188406	2.177218
O	-2.980434	0.356884	2.320830
C	-1.458165	2.194758	1.830128
C	-1.058959	2.292558	0.406853
H	-1.693936	1.697803	-0.240920
O	-2.516706	2.873840	1.489654
C	-0.471853	3.519086	-0.173497
C	0.605837	5.792794	-1.385472
C	0.657180	4.139438	0.372062
C	-1.044329	4.036738	-1.339215
C	-0.511772	5.171938	-1.940064
C	1.190645	5.272882	-0.233067
H	1.141041	3.720531	1.248370
H	-1.919662	3.551252	-1.762543
H	-0.968384	5.571053	-2.839967
H	2.070577	5.744194	0.192593
H	1.024389	6.677393	-1.855132
C	-0.632002	2.636215	3.021488
H	0.282582	2.052057	3.139673
H	-1.248008	2.538677	3.919975
H	-0.388649	3.691320	2.890609
N	0.490333	0.969280	-0.065232
H	0.212451	0.249201	0.600241
H	0.239553	0.664516	-1.009292
C	1.869815	1.269114	0.057237
C	4.581282	1.855363	0.329335
C	2.607827	1.669775	-1.055731
C	2.482584	1.175774	1.309804
C	3.835336	1.467329	1.441936
C	3.963117	1.953189	-0.915577
H	2.125591	1.733565	-2.027570
H	1.905277	0.826978	2.162450
H	4.309948	1.368538	2.413204
H	4.538100	2.243657	-1.789091
H	5.639165	2.073654	0.431556

RS epoxide:Catalyst:Aniline, Transition State 23; Energy = -2737.290114; 6-31G(d) basis set.

N	3.027341	0.329082	-0.458995
C	2.337128	1.484986	-0.474816
S	2.938230	2.923588	0.159737
C	4.419061	0.170925	-0.035728
C	4.579584	-1.286481	0.484503
C	4.774975	-2.298553	-0.665135
C	5.670442	-1.861447	-1.831794
C	5.278452	-0.472275	-2.333070
C	5.358609	0.541229	-1.193369
N	5.541555	-1.458789	1.574787
C	5.093865	-0.848193	2.815203
N	1.110157	1.331716	-1.076602
C	-0.093012	2.025336	-0.913977
C	-0.216029	3.357522	-0.513044
C	-1.488372	3.897663	-0.333873
C	-2.643364	3.164138	-0.557917
C	-2.503044	1.849452	-0.997296
C	-1.255064	1.283598	-1.184698
C	-1.594558	5.295542	0.206640
F	-1.493224	5.304149	1.549955
C	-3.736844	1.020534	-1.202103

F	-3.468288	-0.144158	-1.812877
C	6.917667	-1.082835	1.300388
F	-0.624752	6.090534	-0.259662
F	-2.770079	5.863352	-0.096459
F	-4.322520	0.712848	-0.027223
F	-4.657335	1.662886	-1.930808
H	2.536881	-0.520034	-0.732237
H	0.978184	0.423384	-1.515132
H	5.093842	1.547519	-1.535288
H	6.388328	0.590595	-0.820775
H	5.928536	-0.163459	-3.157926
H	4.254184	-0.498004	-2.730614
H	6.726880	-1.849956	-1.540902
H	5.582523	-2.598478	-2.637658
H	5.128362	-3.236337	-0.223488
H	3.779117	-2.508231	-1.081404
H	4.574992	0.868577	0.792676
H	3.617357	-1.542867	0.947745
H	7.066635	0.007351	1.205668
H	7.546943	-1.428726	2.127032
H	7.272049	-1.564991	0.388025
H	5.747664	-1.175120	3.630073
H	4.074208	-1.174290	3.043309
H	5.106884	0.255927	2.801451
H	0.665264	3.956997	-0.331786
H	-3.624338	3.602283	-0.409028
H	-1.173948	0.261759	-1.549332
N	0.509951	-2.202414	-1.145179
O	1.296256	-2.295974	-0.209814
O	0.653529	-1.420751	-2.064628
C	-0.794841	-3.158480	-1.169991
C	-1.768888	-2.598731	-0.210801
H	-1.898823	-1.525128	-0.298816
O	-1.640003	-2.824315	-2.102307
C	-2.952767	-3.389215	0.214129
C	-5.217478	-4.803785	1.032296
C	-2.818396	-4.619060	0.868389
C	-4.228281	-2.866660	-0.013467
C	-5.355894	-3.575252	0.391143
C	-3.946834	-5.323596	1.273932
H	-1.829461	-5.020774	1.074255
H	-4.329242	-1.912612	-0.519715
H	-6.343359	-3.165977	0.204344
H	-3.834140	-6.276392	1.780931
H	-6.097630	-5.354425	1.348498
C	-0.230188	-4.565333	-1.126693
H	0.401905	-4.740055	-0.253175
H	0.355673	-4.726528	-2.035937
H	-1.067061	-5.264892	-1.134231
N	-0.919537	-2.286558	1.644163
H	-1.475961	-2.825731	2.305336
H	0.030083	-2.655176	1.604873
C	-0.941694	-0.886329	1.926757
C	-1.055117	1.858510	2.374642
C	0.237268	-0.140578	1.947526
C	-2.178268	-0.261724	2.099654
C	-2.229052	1.110581	2.324771
C	0.174396	1.229823	2.185188
H	1.196229	-0.629089	1.789290
H	-3.091580	-0.850453	2.049994
H	-3.192716	1.595267	2.446018
H	1.091767	1.811619	2.198598
H	-1.097428	2.931724	2.529629

RS epoxide:Catalyst:Aniline, Transition State 24; Energy = -2737.289051; 6-31G(d) basis set.

N	2.726062	-1.260208	-0.341349
C	2.103850	-1.798690	-1.407525
S	2.461016	-3.300040	-2.067065
C	3.933645	-1.778578	0.293348
C	5.012045	-0.668804	0.319736
C	4.531517	0.468888	1.235904
C	4.274734	-0.032691	2.659607
C	3.255543	-1.177756	2.665663
C	3.653424	-2.302714	1.705064

N	6.287186	-1.224134	0.786076
C	7.312239	-0.196233	0.916360
N	1.090582	-1.047736	-1.960387
C	0.740745	0.280261	-1.699873
C	1.699562	1.256734	-1.405702
C	1.300363	2.551702	-1.090787
C	-0.033622	2.926595	-1.121786
C	-0.972521	1.968320	-1.497750
C	-0.609501	0.661271	-1.783955
C	2.335178	3.519615	-0.593247
F	3.536445	3.302381	-1.141419
C	-2.422345	2.364322	-1.504851
F	-3.194324	1.466713	-2.124570
C	6.768291	-2.285708	-0.091879
F	1.994699	4.790572	-0.826290
F	2.492446	3.394008	0.742742
F	-2.888689	2.475394	-0.244314
F	-2.609627	3.553041	-2.091039
H	2.299965	-0.443507	0.079085
H	0.425182	-1.607073	-2.489533
H	2.871824	-3.068095	1.650260
H	4.570243	-2.781066	2.066922
H	3.140679	-1.577935	3.678309
H	2.268151	-0.784109	2.385628
H	5.220098	-0.388033	3.086440
H	3.919282	0.791163	3.288145
H	5.239346	1.301941	1.228128
H	3.607262	0.895094	0.819729
H	4.247181	-2.599369	-0.349568
H	5.122372	-0.280577	-0.714404
H	6.815051	-1.971923	-1.150298
H	7.772241	-2.579376	0.223426
H	6.135779	-3.173249	-0.023579
H	7.443970	0.394579	-0.008663
H	8.265416	-0.674652	1.153402
H	7.078050	0.487941	1.734796
H	2.756328	1.013334	-1.434097
H	-0.337645	3.937398	-0.872141
H	-1.369882	-0.055813	-2.086177
N	-1.734775	-2.472950	-1.269534
O	-1.414876	-2.411616	-2.439691
O	-0.955638	-2.704905	-0.354722
C	-3.287400	-2.247159	-0.947115
C	-3.441545	-1.127169	0.007900
H	-2.827378	-0.265687	-0.233101
O	-3.861242	-1.475574	-1.832703
C	-4.765894	-0.846013	0.627167
C	-7.226665	-0.227794	1.799659
C	-5.368617	0.390876	0.388715
C	-5.402937	-1.769721	1.463179
C	-6.628188	-1.462256	2.045475
C	-6.595319	0.696556	0.971195
H	-4.876829	1.101287	-0.266147
H	-4.937867	-2.730984	1.668262
H	-7.114120	-2.185775	2.692060
H	-7.058250	1.658368	0.775437
H	-8.182360	0.012169	2.254655
C	-3.817338	-3.650191	-0.713220
H	-3.307014	-4.156646	0.111058
H	-3.675777	-4.223277	-1.633743
H	-4.887634	-3.584337	-0.512527
N	-2.370556	-1.377017	1.719463
H	-3.012651	-1.622010	2.470236
H	-1.754768	-2.158414	1.494150
C	-1.656843	-0.172360	1.973856
C	-0.320214	2.247349	2.319896
C	-0.320241	-0.058925	1.587059
C	-2.331296	0.922131	2.516774
C	-1.658144	2.128063	2.687985
C	0.343350	1.148973	1.777974
H	0.185188	-0.917757	1.146939
H	-3.377950	0.826281	2.794355
H	-2.186225	2.978053	3.107901
H	1.389762	1.244737	1.500919
H	0.207587	3.186684	2.448859

RS epoxide:Catalyst:Aniline, Transition State 25; Energy = -2737.307607; 6-31G(d) basis set.

N	2.500847	-0.604828	-0.438869
C	1.464049	-1.450847	-0.316289
S	1.616328	-3.010151	0.308233
C	3.869088	-0.889598	-0.026405
C	4.659454	-1.515510	-1.201340
C	4.788212	-0.461246	-2.310517
C	5.506586	0.800670	-1.824149
C	4.744654	1.423462	-0.651094
C	4.535208	0.398109	0.467992
N	5.964734	-1.993462	-0.723077
C	6.849558	-2.373099	-1.816728
N	0.289019	-0.881459	-0.750625
C	-1.043522	-1.297647	-0.661395
C	-1.526766	-2.292360	0.196182
C	-2.887666	-2.586673	0.199020
C	-3.791072	-1.921263	-0.616893
C	-3.303429	-0.907566	-1.435480
C	-1.955262	-0.589781	-1.461508
C	-3.404156	-3.593306	1.187379
F	-4.518459	-4.196412	0.750634
C	-4.247960	-0.176188	-2.346500
F	-4.395829	-0.810997	-3.519625
C	5.808767	-3.137469	0.170074
F	-2.504826	-4.544544	1.461064
F	-3.717979	-3.006580	2.360748
F	-5.476570	-0.074797	-1.807059
F	-3.823462	1.063349	-2.619562
H	2.290115	0.356226	-0.707376
H	0.400971	0.029141	-1.201894
H	3.936208	0.822585	1.281596
H	5.509340	0.115529	0.881685
H	5.284455	2.291757	-0.256059
H	3.774641	1.798972	-1.009697
H	6.522871	0.544326	-1.499075
H	5.597292	1.520832	-2.644463
H	5.276750	-0.883973	-3.192609
H	3.772132	-0.196186	-2.629254
H	3.792807	-1.598670	0.798856
H	4.064669	-2.365127	-1.589921
H	5.273233	-3.974674	-0.312257
H	6.797637	-3.489127	0.476824
H	5.261479	-2.865364	1.074122
H	7.758153	-2.814253	-1.398271
H	7.146203	-1.500484	-2.402538
H	6.391864	-3.114064	-2.497984
H	-0.849563	-2.839311	0.836693
H	-4.846774	-2.168372	-0.602089
H	-1.598766	0.211183	-2.103550
N	-0.682916	3.389973	-1.332312
O	-1.109143	4.508579	-1.079495
O	-1.251944	2.567420	-2.010979
C	0.660619	2.972368	-0.638993
C	0.280740	2.159388	0.530248
H	-0.528647	1.467634	0.315302
O	1.153233	1.829617	-1.121236
C	1.168967	1.817878	1.654637
C	2.754561	1.070936	3.830943
C	2.024327	2.750973	2.256977
C	1.090879	0.520782	2.177843
C	1.891650	0.143536	3.251125
C	2.810697	2.376199	3.340497
H	2.057033	3.774557	1.899902
H	0.403710	-0.195826	1.735283
H	1.837381	-0.871859	3.629450
H	3.468568	3.103836	3.804227
H	3.378450	0.781223	4.670404
C	1.569493	4.181635	-0.626979
H	1.163564	5.005122	-0.038328
H	1.709056	4.518750	-1.657500
H	2.539591	3.873996	-0.235024
N	-1.225253	3.246693	1.620866
H	-1.310236	4.177491	1.213809

H	-0.903211	3.313262	2.583977
C	-2.408433	2.469306	1.474889
C	-4.607720	0.812641	1.060129
C	-3.340741	2.789631	0.487353
C	-2.556238	1.304884	2.234228
C	-3.656435	0.479956	2.022827
C	-4.442577	1.962644	0.292725
H	-3.195573	3.671849	-0.130765
H	-1.809982	1.050610	2.983505
H	-3.760414	-0.434334	2.598180
H	-5.165248	2.211307	-0.477233
H	-5.462249	0.165687	0.891532

RS epoxide:Catalyst:Aniline, Transition State 26; Energy = -2737.319148; 6-31G(d) basis set.

N	1.835903	2.107442	-0.529233
C	0.587439	2.502594	-0.209393
S	0.264478	3.620844	1.014725
C	3.053848	2.764313	-0.083528
C	4.194988	1.746598	0.049217
C	5.449570	2.478032	0.561624
C	5.847702	3.623472	-0.374316
C	4.700171	4.617737	-0.548375
C	3.440650	3.902916	-1.035966
N	3.783818	0.570963	0.837137
C	4.838912	-0.430553	0.904821
N	-0.362832	1.878461	-0.975940
C	-1.733110	1.679289	-0.773923
C	-2.579257	2.486502	-0.012520
C	-3.914022	2.111560	0.143116
C	-4.441114	0.978084	-0.454527
C	-3.591363	0.203385	-1.243334
C	-2.262344	0.542071	-1.407870
C	-4.764201	2.926918	1.074762
F	-4.509161	2.613758	2.357984
C	-4.137249	-1.031727	-1.898821
F	-4.910939	-1.730889	-1.049940
C	3.282539	0.888547	2.168310
F	-4.535301	4.239979	0.943758
F	-6.073884	2.720736	0.875012
F	-4.901620	-0.739998	-2.961927
F	-3.166442	-1.854716	-2.324256
H	1.941932	1.338016	-1.194816
H	0.026484	1.178832	-1.605732
H	3.607957	3.485489	-2.038315
H	2.595652	4.596294	-1.104281
H	4.488876	5.102676	0.414173
H	4.979600	5.410449	-1.249892
H	6.739672	4.127349	0.012337
H	6.116957	3.207151	-1.354662
H	5.256730	2.880264	1.565667
H	6.281972	1.772998	0.650875
H	2.844556	3.205008	0.895719
H	4.419672	1.358726	-0.955801
H	2.413944	1.551609	2.105864
H	2.958592	-0.040144	2.653169
H	4.035594	1.353279	2.825693
H	4.441038	-1.346767	1.355142
H	5.700672	-0.122432	1.518042
H	5.187037	-0.667789	-0.105129
H	-2.201780	3.377552	0.468713
H	-5.478106	0.697509	-0.307381
H	-1.601781	-0.097742	-1.986598
N	3.084850	-1.573684	-1.661074
O	3.666072	-2.578655	-1.268115
O	3.630409	-0.597598	-2.118548
C	1.513610	-1.562856	-1.561534
C	1.164306	-1.219363	-0.166459
H	1.860359	-0.492057	0.255411
O	1.024015	-0.368791	-1.871407
C	-0.178936	-1.292630	0.419654
C	-2.708068	-1.289618	1.606746
C	-1.102981	-2.301054	0.113928
C	-0.521821	-0.309892	1.358820
C	-1.785214	-0.298549	1.940019

C	-2.360326	-2.296057	0.707151
H	-0.836802	-3.105633	-0.562505
H	0.194456	0.473314	1.602850
H	-2.056223	0.495539	2.628981
H	-3.074005	-3.073614	0.455754
H	-3.700790	-1.275882	2.046604
C	1.028339	-2.756392	-2.359968
H	-0.053736	-2.674673	-2.469884
H	1.289133	-3.706011	-1.890714
H	1.472109	-2.708304	-3.358523
N	2.082586	-2.705812	1.157296
H	2.166763	-2.203207	2.038036
H	2.993550	-2.812168	0.714350
C	1.394583	-3.935117	1.289499
C	-0.067829	-6.307004	1.432598
C	0.358305	-4.061009	2.216998
C	1.701334	-4.996805	0.433823
C	0.967447	-6.176246	0.508404
C	-0.364935	-5.247115	2.286531
H	0.110560	-3.223492	2.864746
H	2.517082	-4.890590	-0.277082
H	1.212311	-6.999046	-0.155815
H	-1.169816	-5.337730	3.009102
H	-0.635838	-7.229541	1.488971

RS epoxide:Catalyst:Aniline, Transition State 27; Energy = -2737.294186; 6-31G(d) basis set.

N	-1.403254	2.286891	-0.826633
C	-0.221357	2.426857	-0.197239
S	0.035856	3.244876	1.245572
C	-2.696927	2.882740	-0.487403
C	-3.185178	2.568125	0.940238
C	-4.608315	3.126329	1.107475
C	-4.631195	4.639237	0.875467
C	-4.117894	4.973471	-0.525619
C	-2.719519	4.396015	-0.748764
N	-3.029047	1.143099	1.292662
C	-4.113533	0.298408	0.805932
N	0.801152	1.793399	-0.879950
C	2.038090	1.366286	-0.362075
C	2.147366	0.837237	0.928184
C	3.350637	0.289395	1.344197
C	4.463676	0.258338	0.507508
C	4.342611	0.788854	-0.769480
C	3.142398	1.339020	-1.211300
C	3.456299	-0.318149	2.715517
F	4.128224	0.477048	3.561547
C	5.532680	0.813254	-1.687156
F	6.175259	1.989641	-1.629013
C	-2.872605	0.987253	2.736972
F	2.255977	-0.554987	3.257003
F	4.120569	-1.486053	2.675395
F	6.422832	-0.137680	-1.372257
F	5.174486	0.628374	-2.965734
H	-1.383923	1.782380	-1.708823
H	0.667676	1.617774	-1.874457
H	-2.001295	4.875057	-0.073703
H	-2.381451	4.582279	-1.773513
H	-4.808449	4.555052	-1.271037
H	-4.100578	6.056736	-0.682008
H	-5.646600	5.024977	1.013046
H	-3.996012	5.131428	1.623613
H	-5.289241	2.647187	0.390367
H	-4.980700	2.887572	2.110612
H	-3.395226	2.409870	-1.191979
H	-2.532833	3.115362	1.623679
H	-3.753343	1.332977	3.302756
H	-2.720025	-0.068872	2.977302
H	-1.993259	1.546802	3.066082
H	-3.851287	-0.753945	0.961364
H	-4.259680	0.454049	-0.268768
H	-5.073229	0.484003	1.313567
H	1.285968	0.815915	1.584228
H	5.394876	-0.189414	0.836944
H	3.058225	1.723703	-2.222891

N	-0.187709	-0.494261	-2.882720
O	0.995087	-0.542805	-2.592923
O	-0.755835	0.546547	-3.184652
C	-1.105717	-1.830736	-2.750892
C	-2.000412	-1.562236	-1.590823
H	-2.483356	-0.595136	-1.667529
O	-2.158208	-1.797746	-3.513030
C	-2.762186	-2.670485	-0.976437
C	-4.277620	-4.732929	0.148405
C	-4.160784	-2.600561	-0.966884
C	-2.130314	-3.791992	-0.426680
C	-2.888109	-4.814071	0.138910
C	-4.915332	-3.625853	-0.410969
H	-4.651725	-1.745451	-1.422611
H	-1.047563	-3.862206	-0.421663
H	-2.387535	-5.673812	0.572314
H	-5.998720	-3.565053	-0.418408
H	-4.865329	-5.533580	0.586451
C	-0.153569	-3.004928	-2.846846
H	0.598880	-3.014321	-2.056959
H	0.345153	-2.971553	-3.818857
H	-0.755515	-3.913431	-2.799901
N	-0.914604	-0.787061	0.035548
H	-0.242427	-0.182734	-0.440767
H	-1.574563	-0.160609	0.532252
C	-0.229372	-1.703214	0.878766
C	1.090580	-3.598277	2.444652
C	1.057935	-2.124568	0.530897
C	-0.860114	-2.242332	1.999369
C	-0.195713	-3.183615	2.780505
C	1.712946	-3.067277	1.315604
H	1.542232	-1.698713	-0.345909
H	-1.875332	-1.940854	2.241862
H	-0.690414	-3.594997	3.654569
H	2.719155	-3.375461	1.050238
H	1.606803	-4.328108	3.059214

RS epoxide:Catalyst:Aniline, Transition State 28; Energy = -2737.300922; 6-31G(d) basis set.

N	-2.023568	-1.631484	0.279449
C	-1.676777	-2.910751	0.079248
S	-2.712765	-4.107256	-0.484344
C	-3.393533	-1.123211	0.298666
C	-3.370260	0.240252	1.012239
C	-4.817666	0.687270	1.255193
C	-5.528291	0.846511	-0.095391
C	-5.463359	-0.441430	-0.921613
C	-4.021491	-0.934148	-1.087568
N	-2.452067	0.239928	2.164048
C	-2.253762	1.585786	2.695867
N	-0.363357	-3.239594	0.332633
C	0.671498	-2.410629	0.792214
C	0.524674	-1.603220	1.925151
C	1.586645	-0.803076	2.341499
C	2.813194	-0.826631	1.687776
C	2.956827	-1.661417	0.579705
C	1.900288	-2.436108	0.122490
C	1.373438	0.175050	3.463596
F	0.404437	-0.221746	4.299185
C	4.272948	-1.682018	-0.152385
F	4.366275	-2.719421	-0.988368
C	-2.850629	-0.672243	3.232137
F	2.484442	0.366538	4.178207
F	1.003523	1.374344	2.975269
F	4.445366	-0.565456	-0.887570
F	5.300308	-1.740392	0.701458
H	-1.385675	-1.020577	0.782594
H	-0.097293	-4.133460	-0.062130
H	-3.439331	-0.197473	-1.660432
H	-3.998604	-1.880488	-1.633482
H	-6.051534	-1.224825	-0.424297
H	-5.914221	-0.282431	-1.905887
H	-6.569544	1.146838	0.060377
H	-5.039028	1.656319	-0.652657
H	-5.345474	-0.052182	1.872437

H	-4.833022	1.638723	1.797347
H	-4.008816	-1.841117	0.860275
H	-2.932761	0.958888	0.308567
H	-2.937558	-1.694316	2.848393
H	-2.082145	-0.661046	4.010797
H	-3.808756	-0.391910	3.696684
H	-2.034300	2.274857	1.872673
H	-1.411312	1.580756	3.391697
H	-3.137284	1.968165	3.230066
H	-0.402204	-1.605775	2.490736
H	3.638215	-0.212593	2.034983
H	2.015523	-3.053081	-0.762448
N	-1.441909	3.099929	-1.651754
O	-2.104869	2.696827	-0.700888
O	-1.349544	4.269257	-1.951917
C	-0.733826	1.997761	-2.588362
C	-0.523567	0.771976	-1.779598
H	-1.413916	0.495194	-1.231998
O	-1.622334	1.345854	-3.305308
C	0.285979	-0.352493	-2.324854
C	1.723477	-2.515190	-3.365305
C	1.654528	-0.229383	-2.590936
C	-0.352496	-1.571471	-2.574943
C	0.361833	-2.647339	-3.094956
C	2.369682	-1.306637	-3.107915
H	2.160422	0.712848	-2.400665
H	-1.418642	-1.663788	-2.386359
H	-0.151875	-3.583078	-3.293888
H	3.431171	-1.201674	-3.306882
H	2.281911	-3.351741	-3.774546
C	0.396008	2.710240	-3.301085
H	1.111106	3.165009	-2.608014
H	-0.031733	3.488496	-3.934800
H	0.900404	1.980911	-3.936955
N	0.437015	1.135164	-0.037615
H	0.965155	0.275714	0.114633
H	-0.329693	1.170500	0.640529
C	1.284440	2.284532	0.068917
C	2.923746	4.539246	0.120161
C	2.648952	2.160291	-0.194027
C	0.741099	3.530429	0.384360
C	1.564640	4.651356	0.404572
C	3.462790	3.288993	-0.171686
H	3.072859	1.185227	-0.411408
H	-0.318262	3.625791	0.602767
H	1.134743	5.618667	0.642730
H	4.522681	3.184544	-0.380358
H	3.558854	5.418522	0.133370

RS epoxide:Catalyst:Aniline, Transition State 29; Energy = -2737.300922; 6-31G(d) basis set.

N	2.023605	1.631438	0.279684
C	1.676838	2.910734	0.079630
S	2.712849	4.107292	-0.483808
C	3.393555	1.123133	0.298805
C	3.370255	-0.240442	1.012161
C	4.817655	-0.687495	1.255088
C	5.528315	-0.846526	-0.095503
C	5.463385	0.441534	-0.921543
C	4.021513	0.934258	-1.087455
N	2.452036	-0.240297	2.163948
C	2.253729	-1.586233	2.695567
N	0.363423	3.239573	0.333053
C	-0.671455	2.410566	0.792503
C	-0.524676	1.602994	1.925329
C	-1.586676	0.802816	2.341541
C	-2.813208	0.826484	1.687790
C	-2.956796	1.661431	0.579832
C	-1.900230	2.436163	0.122755
C	-1.373504	-0.175481	3.463499
F	-0.404560	0.221212	4.299202
C	-4.272896	1.682169	-0.152292
F	-4.366153	2.719666	-0.988166
C	2.850587	0.671703	3.232189
F	-2.484542	-0.367113	4.178017

F	-1.003527	-1.374692	2.975010
F	-4.445337	0.565697	-0.887606
F	-5.300279	1.740494	0.701526
H	1.385701	1.020474	0.782749
H	0.097381	4.133490	-0.061610
H	3.439365	0.197644	-1.660409
H	3.998622	1.880667	-1.633250
H	6.051539	1.224865	-0.424100
H	5.914271	0.282682	-1.905829
H	6.569569	-1.146862	0.060246
H	5.039076	-1.656258	-0.652900
H	5.345442	0.051865	1.872460
H	4.833000	-1.639031	1.797096
H	4.008858	1.840934	0.860526
H	2.932791	-0.958961	0.308345
H	2.937613	1.693821	2.848593
H	2.082051	0.660453	4.010799
H	3.808664	0.391239	3.696761
H	2.034238	-2.275191	1.872290
H	1.411295	-1.581294	3.391419
H	3.137261	-1.968694	3.229691
H	0.402187	1.605453	2.490940
H	-3.638250	0.212410	2.034886
H	-2.015425	3.053256	-0.762102
N	1.441764	-3.099827	-1.651965
O	2.104950	-2.696801	-0.701227
O	1.349031	-4.269165	-1.951985
C	0.733856	-1.997535	-2.588547
C	0.523599	-0.771816	-1.779665
H	1.413914	-0.495138	-1.231948
O	1.622487	-1.345610	-3.305333
C	-0.285890	0.352746	-2.324819
C	-1.723315	2.515615	-3.365011
C	-1.654443	0.229714	-2.590920
C	0.352629	1.571730	-2.574766
C	-0.361664	2.647682	-3.094657
C	-2.369563	1.307055	-3.107760
H	-2.160363	-0.712527	-2.400763
H	1.418779	1.663986	-2.386170
H	0.152077	3.583425	-3.293484
H	-3.431061	1.202154	-3.306718
H	-2.281721	3.352235	-3.774148
C	-0.395978	-2.709831	-3.301451
H	-1.111194	-3.164588	-2.608495
H	0.031735	-3.488085	-3.935188
H	-0.900227	-1.980390	-3.937308
N	-0.437084	-1.135104	-0.037740
H	0.329542	-1.170481	0.640488
H	-0.965229	-0.275657	0.114502
C	-1.284530	-2.284469	0.068681
C	-2.923865	-4.539162	0.119746
C	-2.649031	-2.160195	-0.194307
C	-0.741217	-3.530386	0.384082
C	-1.564771	-4.651305	0.404201
C	-3.462884	-3.288888	-0.172055
H	-3.072917	-1.185110	-0.411638
H	0.318137	-3.625774	0.602512
H	-1.134894	-5.618635	0.642321
H	-4.522766	-3.184417	-0.380759
H	-3.558985	-5.418432	0.132883

RS epoxide:Catalyst:Aniline, Transition State 30; Energy = -2737.292849; 6-31G(d) basis set.

N	1.369979	1.659588	-0.119120
C	0.074738	1.777441	-0.467320
S	-0.479964	2.707258	-1.747232
C	2.515727	2.265133	-0.794271
C	3.755015	1.883993	0.033333
C	5.002591	2.633800	-0.475553
C	4.951825	2.865069	-1.995593
C	4.187101	1.723326	-2.663778
C	2.708092	1.744729	-2.238210
N	3.506167	1.985447	1.478831
C	3.197291	3.330154	1.947338
N	-0.742011	1.009912	0.334627

C	-2.120074	0.777589	0.171413
C	-3.046757	1.815523	0.069622
C	-4.402050	1.512356	-0.017614
C	-4.859736	0.199214	0.019904
C	-3.924587	-0.824123	0.127260
C	-2.566081	-0.545213	0.186708
C	-5.392499	2.632465	-0.175997
F	-5.593394	2.935888	-1.466181
C	-4.384104	-2.253493	0.130763
F	-3.473584	-3.069615	0.688758
C	4.591193	1.399241	2.254935
F	-6.587789	2.310397	0.341308
F	-4.977060	3.752460	0.431383
F	-5.529270	-2.401608	0.811503
F	-4.610559	-2.712224	-1.110569
H	1.594026	1.334815	0.824483
H	-0.267962	0.292707	0.878081
H	2.319289	0.723999	-2.289817
H	2.121077	2.366140	-2.916823
H	4.252023	1.793243	-3.753736
H	4.635193	0.763372	-2.379075
H	4.444663	3.813179	-2.216085
H	5.966997	2.952503	-2.394495
H	5.107380	3.590894	0.048153
H	5.883580	2.032929	-0.223304
H	2.381359	3.356316	-0.809127
H	3.909253	0.812455	-0.158209
H	4.828866	0.400962	1.869300
H	5.512861	2.002942	2.228885
H	4.279908	1.305893	3.301783
H	4.033824	4.038344	1.840077
H	2.942553	3.282352	3.011017
H	2.331378	3.729100	1.410916
H	-2.709493	2.844434	0.070772
H	-5.921358	-0.019396	-0.019261
H	-1.845227	-1.354581	0.240383
N	4.406058	-1.860557	0.203840
O	4.354420	-2.252063	1.370809
O	5.266594	-1.128926	-0.220138
C	3.271615	-2.346131	-0.826782
C	1.958761	-1.849956	-0.358002
H	2.009903	-0.829387	0.015807
O	3.152051	-1.515709	-1.829265
C	0.690230	-2.219872	-1.057043
C	-1.715899	-2.772792	-2.380835
C	0.079917	-1.249840	-1.859218
C	0.090992	-3.478116	-0.940814
C	-1.111435	-3.748359	-1.590991
C	-1.111424	-1.525219	-2.521404
H	0.553419	-0.281044	-1.979803
H	0.562430	-4.263043	-0.354686
H	-1.573223	-4.724330	-1.481927
H	-1.569887	-0.754546	-3.132990
H	-2.655665	-2.983916	-2.879314
C	3.558743	-3.813023	-1.074581
H	3.606838	-4.385966	-0.144552
H	4.511703	-3.897423	-1.603683
H	2.770266	-4.209325	-1.718210
N	1.555764	-2.549697	1.513262
H	2.520554	-2.700726	1.819211
H	1.052523	-3.432825	1.481202
C	0.880470	-1.565684	2.280157
C	-0.426486	0.482671	3.650391
C	1.593799	-0.434881	2.689318
C	-0.485654	-1.671386	2.547452
C	-1.131535	-0.645841	3.236913
C	0.936909	0.584133	3.372610
H	2.655542	-0.360193	2.467268
H	-1.041651	-2.544836	2.214300
H	-2.195082	-0.729193	3.436828
H	1.497683	1.462323	3.677931
H	-0.937562	1.281323	4.176582

RS epoxide:Catalyst:Aniline, Transition State 31; Energy = -2737.302844; 6-31G(d) basis set.

C	-4.603843	-0.709909	0.128119
C	-4.359736	-3.228782	0.300871
C	-6.647542	-2.199450	0.358549
C	-5.777473	-3.352570	0.855455
C	-6.017746	-0.852421	0.720862
C	-3.736770	-1.868983	0.645247
H	-4.379605	-3.342030	-0.792553
H	-6.755576	-2.269066	-0.732602
H	-5.739763	-3.332937	1.952864
H	-5.965682	-0.768058	1.814588
H	-3.637036	-1.797492	1.731220
H	-4.679326	-0.817768	-0.964124
H	-3.710226	-4.016170	0.698401
H	-7.654655	-2.267205	0.782909
H	-6.208317	-4.317023	0.567668
H	-6.656162	-0.037087	0.366317
N	-3.965707	0.601302	0.347592
N	-2.392042	-1.791549	0.094727
H	-2.336477	-1.741780	-0.923211
C	-4.689418	1.656799	-0.352584
H	-5.696380	1.840545	0.054484
H	-4.774168	1.401007	-1.412263
H	-4.132451	2.593071	-0.262722
C	-3.789092	0.951729	1.756133
H	-3.167264	0.205983	2.261004
H	-4.741658	1.053934	2.300343
H	-3.267626	1.912744	1.813070
C	-1.254042	-1.938445	0.791283
S	-1.180439	-2.027109	2.471691
N	-0.143856	-1.986784	-0.026700
H	-0.335723	-2.137499	-1.014874
C	1.220671	-1.873788	0.279816
C	3.995990	-1.529747	0.606682
C	2.120816	-2.386048	-0.663316
C	1.720513	-1.181609	1.389409
C	3.093685	-1.015728	1.530948
C	3.487921	-2.217223	-0.490036
H	1.748613	-2.905216	-1.541819
H	1.047914	-0.772053	2.130801
H	5.064096	-1.379843	0.723289
C	4.442500	-2.821416	-1.484110
C	3.622439	-0.245045	2.709251
F	3.871433	-2.992472	-2.681597
F	4.037376	-1.052298	3.692591
F	4.673028	0.514887	2.357547
F	2.691830	0.570351	3.229236
F	5.526124	-2.051876	-1.649323
F	4.873268	-4.023992	-1.073623
N	-0.924696	1.175190	-0.036415
H	-0.553120	0.423588	0.545014
H	-1.922153	0.953092	-0.216960
C	-0.744174	2.426494	0.610536
C	-0.244484	4.933940	1.735098
C	0.265663	2.578307	1.562452
C	-1.498958	3.533857	0.218233
C	-1.253080	4.779818	0.786967
C	0.513147	3.828277	2.117563
H	0.871104	1.723195	1.851905
H	-2.261446	3.419091	-0.546416
H	-1.848808	5.633978	0.480286
H	1.304143	3.935541	2.853201
H	-0.051747	5.907433	2.173862
N	-1.674279	-0.169238	-2.681678
O	-2.818101	0.129930	-2.398257
O	-1.263050	-1.324317	-2.657386
C	-0.559784	1.014976	-3.007361
O	0.420718	0.566835	-3.719409
C	0.294520	0.984013	-1.791067
H	0.527826	-0.036713	-1.514610
C	-1.382564	2.196639	-3.478807
H	-0.690431	2.974673	-3.803085
H	-2.051141	2.581922	-2.706923
H	-1.979148	1.892886	-4.342656
C	1.326936	1.969396	-1.458447
C	3.271492	3.736303	-0.507032

C	2.483562	1.488453	-0.833795
C	1.156862	3.351648	-1.608315
C	2.128284	4.226908	-1.137129
C	3.452941	2.363040	-0.357959
H	2.621190	0.415547	-0.734649
H	0.253237	3.748064	-2.056200
H	1.983612	5.297016	-1.245572
H	4.336681	1.971413	0.135715
H	4.019290	4.426950	-0.129627

RS epoxide:Catalyst:Aniline, Transition State 32; Energy = -2737.318441; 6-31G(d) basis set.

C	4.397926	-1.258013	-0.085835
C	3.861041	-3.550945	0.831799
C	6.218525	-3.006037	0.152374
C	5.167435	-4.109695	0.268748
C	5.696834	-1.831765	-0.681254
C	3.353742	-2.380719	-0.020428
H	4.013172	-3.200210	1.861735
H	6.475823	-2.644379	1.157311
H	4.976682	-4.537115	-0.724877
H	5.511725	-2.170302	-1.710021
H	3.165112	-2.760197	-1.028864
H	4.613541	-0.938294	0.944576
H	3.082482	-4.320804	0.857348
H	7.140710	-3.397086	-0.289957
H	5.532652	-4.925187	0.901378
H	6.461163	-1.049851	-0.731437
N	3.870544	-0.059026	-0.760804
N	2.088848	-1.876756	0.490235
H	2.135187	-1.166449	1.224884
C	4.837327	1.030840	-0.750188
H	5.690434	0.867218	-1.427741
H	5.211543	1.177714	0.267142
H	4.350629	1.961504	-1.062009
C	3.371232	-0.301858	-2.108001
H	2.580416	-1.058666	-2.095617
H	4.152249	-0.617467	-2.819159
H	2.933431	0.625457	-2.499027
C	0.876573	-2.352137	0.139787
S	0.643800	-3.385095	-1.176966
N	-0.119376	-1.880611	0.955235
H	0.208279	-1.191695	1.631327
C	-1.504975	-1.802708	0.770754
C	-4.270612	-1.353740	0.501605
C	-2.275276	-2.645050	-0.032664
C	-2.137095	-0.763428	1.473814
C	-3.494364	-0.546454	1.331665
C	-3.641496	-2.395770	-0.161174
H	-1.817517	-3.467144	-0.563782
H	-1.537639	-0.099720	2.090801
H	-5.331669	-1.168724	0.375115
C	-4.423937	-3.234089	-1.131300
C	-4.155503	0.588995	2.057701
F	-4.292278	-2.769566	-2.386785
F	-3.268273	1.465783	2.552206
F	-4.980647	1.271255	1.243996
F	-4.901672	0.159070	3.086283
F	-4.011007	-4.507848	-1.143154
F	-5.735720	-3.234592	-0.852087
N	1.846503	3.061103	-0.843367
H	2.372499	2.590189	-1.574905
H	2.489915	3.507435	-0.190114
C	0.835098	3.904707	-1.352299
C	-1.344700	5.410412	-2.232339
C	0.427481	5.030140	-0.633144
C	0.159763	3.542362	-2.520616
C	-0.925810	4.293289	-2.953764
C	-0.659519	5.777638	-1.076634
H	0.962605	5.318128	0.268438
H	0.472513	2.656926	-3.068345
H	-1.451108	3.998640	-3.856795
H	-0.969727	6.652378	-0.513718
H	-2.194550	5.992998	-2.571789
N	3.010544	1.781637	1.854529

O	3.502551	2.853302	1.523539
O	3.639920	0.825793	2.242484
C	1.439130	1.649721	1.779751
O	1.054601	0.410503	2.051843
C	1.091394	1.357336	0.372930
H	1.843002	0.725038	-0.102505
C	0.887801	2.778831	2.628699
H	1.066037	3.757889	2.180133
H	1.363768	2.743794	3.612558
H	-0.181265	2.614689	2.766814
C	-0.254757	1.348211	-0.198311
C	-2.760923	1.243944	-1.428819
C	-0.504775	0.428349	-1.225131
C	-1.266084	2.243175	0.180560
C	-2.507842	2.193883	-0.438565
C	-1.758437	0.361218	-1.824915
H	0.279279	-0.263198	-1.529873
H	-1.080729	2.995956	0.937072
H	-3.285337	2.887842	-0.137301
H	-1.954082	-0.389227	-2.584565
H	-3.742860	1.191439	-1.889467

RS epoxide:Catalyst:Aniline, Transition State 33; Energy = -2737.299860; 6-31G(d) basis set.

N	1.019336	2.365454	-0.017607
C	-0.214821	2.189475	0.494553
S	-0.694652	2.764433	1.995412
C	2.056669	3.217178	0.542281
C	3.431641	2.544119	0.401483
C	4.505833	3.474532	0.994696
C	4.491197	4.850847	0.323793
C	3.117869	5.508443	0.447783
C	2.036516	4.596096	-0.128513
N	3.425690	1.169210	0.943686
C	2.949736	1.081440	2.326141
N	-1.023516	1.455568	-0.357936
C	-2.337644	1.002677	-0.132565
C	-3.223362	1.020906	-1.211980
C	-4.507298	0.510794	-1.065227
C	-4.933438	-0.024784	0.143999
C	-4.036094	-0.050829	1.205854
C	-2.746884	0.453931	1.085801
C	-5.437315	0.492711	-2.246145
F	-6.713402	0.653577	-1.868630
C	-4.435827	-0.724097	2.488496
F	-5.750924	-0.616641	2.718723
C	4.731821	0.530428	0.814735
F	-5.146639	1.461861	-3.124478
F	-5.369532	-0.672187	-2.907810
F	-4.156153	-2.041908	2.450035
F	-3.790530	-0.220521	3.545660
H	1.192490	2.027775	-0.963037
H	-0.772005	1.506449	-1.345948
H	2.192655	4.468419	-1.209134
H	1.039676	5.028055	0.009034
H	2.900287	5.703131	1.506294
H	3.104440	6.475947	-0.063781
H	5.265091	5.486233	0.766103
H	4.743382	4.736288	-0.739422
H	4.331227	3.595023	2.072116
H	5.494993	3.021297	0.877720
H	1.822091	3.347559	1.602055
H	3.644341	2.439640	-0.676112
H	5.481507	0.923270	1.518155
H	4.629680	-0.544143	1.002207
H	5.109990	0.667829	-0.204536
H	3.031523	0.042793	2.657905
H	1.895625	1.366696	2.389398
H	3.532682	1.703394	3.022880
H	-2.907967	1.433950	-2.165016
H	-5.940789	-0.409873	0.257325
H	-2.064065	0.414385	1.924911
N	0.488146	0.000623	-2.791715
O	0.710640	1.210992	-2.719812
O	-0.626076	-0.464396	-2.717383

C	1.747223	-1.043701	-2.896017
C	1.567114	-1.948686	-1.745414
H	0.539329	-2.271709	-1.631520
O	1.484298	-2.071977	-3.654223
C	2.614730	-2.868406	-1.264331
C	4.483374	-4.633039	-0.165189
C	3.931275	-2.451993	-1.037914
C	2.241660	-4.170154	-0.919474
C	3.173274	-5.051879	-0.379762
C	4.860645	-3.330351	-0.492220
H	4.224888	-1.432058	-1.260878
H	1.213886	-4.486510	-1.072719
H	2.872395	-6.061093	-0.118618
H	5.878895	-2.996812	-0.317224
H	5.210156	-5.316960	0.261708
C	2.968314	-0.188518	-3.161013
H	2.805502	0.411432	-4.058772
H	3.804775	-0.864246	-3.342718
H	3.200343	0.479645	-2.326387
N	1.318694	-0.823049	0.010096
H	2.136801	-0.228355	0.235912
H	0.536517	-0.201911	-0.207115
C	0.940624	-1.715836	1.047159
C	0.160719	-3.567873	2.984718
C	-0.407434	-2.047222	1.198757
C	1.903691	-2.341256	1.841644
C	1.508506	-3.260105	2.808461
C	-0.795675	-2.960972	2.173462
H	-1.148688	-1.581003	0.552743
H	2.957297	-2.122503	1.684681
H	2.262007	-3.740306	3.424893
H	-1.849483	-3.185915	2.300189
H	-0.141582	-4.279217	3.746004

RS epoxide:Catalyst:Aniline, Transition State 1; "TS-RS2"; Energy = -2738.179136; TZVP basis set.

N	-0.881663	2.523742	0.779377
C	0.448433	2.552595	0.614741
S	1.255893	3.807912	-0.178150
C	-1.811911	3.595345	0.471965
C	-3.064683	3.025735	-0.207228
C	-4.042636	4.174441	-0.499523
C	-4.410862	4.934215	0.774699
C	-3.163201	5.485560	1.457893
C	-2.173822	4.361472	1.747573
N	-2.716702	2.190983	-1.368404
C	-3.883496	1.548415	-1.952524
N	1.053450	1.446902	1.160064
C	2.281440	0.842148	0.890821
C	2.361800	-0.512400	1.244063
C	3.503268	-1.238268	0.982189
C	4.608274	-0.652949	0.374721
C	4.527184	0.689689	0.055828
C	3.391467	1.450747	0.308998
C	3.568823	-2.693910	1.348507
F	2.359919	-3.210550	1.611165
C	5.671916	1.354037	-0.659240
F	6.820207	0.681227	-0.513223
C	-1.944255	2.873991	-2.399283
F	4.102132	-3.428931	0.359546
F	4.327752	-2.907246	2.432915
F	5.438918	1.438039	-1.981606
F	5.883210	2.601734	-0.227171
H	-1.287120	1.679343	1.182720
H	0.392278	0.786141	1.565778
H	-2.608513	3.659817	2.467923
H	-1.251858	4.750383	2.184570
H	-2.688267	6.225054	0.804818
H	-3.426203	5.999759	2.383968
H	-5.107775	5.740542	0.538600
H	-4.928541	4.255720	1.461113
H	-3.584995	4.868762	-1.211801
H	-4.945555	3.778663	-0.967639
H	-1.306576	4.281614	-0.207365
H	-3.547603	2.344374	0.507479

H	-1.001022	3.245384	-1.996509
H	-1.708160	2.157053	-3.188355
H	-2.486177	3.710774	-2.862403
H	-4.472794	1.070970	-1.167275
H	-3.550624	0.787049	-2.663777
H	-4.534706	2.240033	-2.505336
H	1.501593	-0.990538	1.698532
H	5.498539	-1.228701	0.160545
H	3.362119	2.496325	0.047592
N	-3.403222	-1.154646	1.489675
O	-4.024723	-0.347258	0.824058
O	-3.875409	-1.791340	2.396429
C	-1.849253	-1.320251	1.184173
C	-1.559369	-0.797593	-0.162560
H	-2.105274	0.103726	-0.416830
O	-1.192746	-0.241408	1.635621
C	-0.292044	-1.006467	-0.871680
C	2.123336	-1.219531	-2.241090
C	0.376244	-2.233924	-0.928219
C	0.240746	0.098592	-1.541346
C	1.454971	-0.001342	-2.205097
C	1.573478	-2.337022	-1.619654
H	-0.040699	-3.108519	-0.449137
H	-0.294081	1.041488	-1.502440
H	1.879493	0.871978	-2.684044
H	2.090064	-3.287563	-1.658511
H	3.073194	-1.300053	-2.755019
C	-1.412389	-2.658532	1.718938
H	-1.898166	-3.490559	1.207489
H	-1.655588	-2.698629	2.778527
H	-0.332450	-2.728856	1.611893
N	-2.908946	-1.838629	-1.565748
H	-2.449017	-1.722749	-2.462273
H	-3.729079	-1.243691	-1.503717
C	-3.166068	-3.187352	-1.229309
C	-3.525744	-5.810920	-0.367748
C	-2.303277	-4.189988	-1.668361
C	-4.226977	-3.504301	-0.383425
C	-4.398695	-4.812207	0.046135
C	-2.485663	-5.495030	-1.234123
H	-1.493212	-3.943658	-2.344738
H	-4.913438	-2.729116	-0.061714
H	-5.220597	-5.048050	0.709550
H	-1.811102	-6.268883	-1.577521
H	-3.661227	-6.828809	-0.027530

RS epoxide:Catalyst:Aniline, Transition State 2; "TS-RS1"; Energy = -2738.183381; TZVP basis set.

N	1.767634	2.157495	-0.522091
C	0.510634	2.480904	-0.176676
S	0.157765	3.571628	1.066862
C	2.962549	2.847907	-0.065274
C	4.133676	1.867253	0.044824
C	5.367198	2.627483	0.556436
C	5.720449	3.798063	-0.361836
C	4.542600	4.756976	-0.507252
C	3.305631	4.012009	-0.998695
N	3.768464	0.672315	0.825717
C	4.859783	-0.289963	0.884755
N	-0.421984	1.812285	-0.925414
C	-1.787331	1.598623	-0.725416
C	-2.640706	2.407217	0.019884
C	-3.975084	2.038764	0.158195
C	-4.495723	0.905467	-0.436047
C	-3.637845	0.127692	-1.206829
C	-2.309969	0.461159	-1.358122
C	-4.847913	2.889613	1.039890
F	-4.602583	2.659035	2.341550
C	-4.191691	-1.099596	-1.873482
F	-4.907882	-1.846450	-1.016741
C	3.256701	0.956989	2.159965
F	-4.646545	4.196843	0.837847
F	-6.150943	2.652629	0.844928
F	-5.017109	-0.789699	-2.884946
F	-3.235049	-1.888457	-2.377732

H	1.900635	1.412508	-1.205818
H	-0.015196	1.113333	-1.543277
H	3.480137	3.617420	-2.005343
H	2.440320	4.676014	-1.048534
H	4.324119	5.215363	0.462903
H	4.789645	5.567890	-1.194669
H	6.596731	4.321644	0.024915
H	5.991794	3.408454	-1.348760
H	5.170775	3.005765	1.565226
H	6.217722	1.947741	0.624578
H	2.742787	3.262413	0.919125
H	4.358829	1.498306	-0.963734
H	2.366631	1.585936	2.107599
H	2.970437	0.015363	2.636468
H	3.992827	1.442920	2.815594
H	4.488876	-1.239591	1.276854
H	5.684008	0.027566	1.537873
H	5.252748	-0.465570	-0.117803
H	-2.267165	3.300257	0.494398
H	-5.535082	0.633084	-0.310950
H	-1.649101	-0.170162	-1.940869
N	3.181985	-1.522092	-1.751014
O	3.782501	-2.517068	-1.377876
O	3.701863	-0.540494	-2.208845
C	1.598451	-1.539311	-1.620187
C	1.272236	-1.230870	-0.212167
H	1.961947	-0.505040	0.217203
O	1.089666	-0.351391	-1.903207
C	-0.053292	-1.342459	0.393055
C	-2.549482	-1.417316	1.628376
C	-0.961081	-2.359354	0.083710
C	-0.396301	-0.388033	1.356155
C	-1.642282	-0.417336	1.963368
C	-2.203181	-2.390956	0.698441
H	-0.693518	-3.142102	-0.612371
H	0.306807	0.401755	1.602096
H	-1.907958	0.347007	2.682617
H	-2.902522	-3.178882	0.450767
H	-3.527765	-1.437428	2.092493
C	1.130509	-2.731534	-2.423736
H	0.050777	-2.665196	-2.534658
H	1.405740	-3.674250	-1.955863
H	1.575387	-2.675932	-3.418066
N	2.248485	-2.760172	1.089868
H	2.396812	-2.239902	1.947191
H	3.121865	-2.899351	0.590781
C	1.518834	-3.952515	1.280376
C	-0.030700	-6.250199	1.543845
C	0.537642	-4.022069	2.266268
C	1.725916	-5.034745	0.426582
C	0.949762	-6.176600	0.560728
C	-0.227415	-5.171575	2.397475
H	0.365736	-3.169742	2.914697
H	2.503036	-4.978289	-0.327557
H	1.118239	-7.015772	-0.102068
H	-0.988447	-5.218174	3.165901
H	-0.631647	-7.143874	1.647428

RS epoxide:Catalyst:Aniline, Transition State 3, "TS-RS"; Energy = -2738.183378; TZVP basis set.

C	4.324144	-1.469011	-0.049494
C	3.621676	-3.744472	0.788945
C	6.022211	-3.331863	0.202104
C	4.903907	-4.368633	0.247985
C	5.604338	-2.107261	-0.612438
C	3.214322	-2.523772	-0.040485
H	3.766316	-3.431401	1.828443
H	6.263192	-3.016587	1.222865
H	4.719462	-4.750985	-0.761424
H	5.436715	-2.405173	-1.652949
H	3.025106	-2.860190	-1.060354
H	4.520353	-1.179388	0.990553
H	2.797351	-4.460200	0.770057
H	6.931150	-3.765171	-0.219449
H	5.194741	-5.221380	0.863905

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H          6.412527       -1.374506       -0.611157
N          3.895220       -0.231078       -0.724181
N          1.975828       -1.953248        0.464885
H          2.057986       -1.271231        1.218705
C          4.933008        0.790725       -0.683902
H          5.763725        0.590815       -1.374264
H          5.327820        0.873689        0.329366
H          4.510545        1.760753       -0.954886
C          3.407649       -0.423312       -2.083324
H          2.553906       -1.103005       -2.096233
H          4.173000       -0.806715       -2.772560
H          3.070276        0.539247       -2.478580
C          0.744039       -2.343998        0.096791
S          0.467047       -3.347257       -1.236464
N         -0.231540       -1.814471        0.899137
H          0.122805       -1.129989        1.564486
C         -1.611705       -1.699685        0.716294
C         -4.370245       -1.218747        0.479589
C         -2.403170       -2.537485       -0.063488
C         -2.219163       -0.643381        1.410658
C         -3.571485       -0.413607        1.285505
C         -3.764792       -2.273577       -0.175262
H         -1.963066       -3.372780       -0.584127
H         -1.606304        0.008604        2.022210
H         -5.429787       -1.027475        0.375226
C         -4.572915       -3.154935       -1.088041
C         -4.218717        0.726491        2.019508
F         -4.320022       -2.886815       -2.380536
F         -3.326903        1.541279        2.596222
F         -4.969250        1.480654        1.199107
F         -5.038660        0.294171        2.989679
F         -4.299282       -4.452458       -0.905819
F         -5.890421       -2.997808       -0.910922
N          2.045257        3.068920       -0.821576
H          2.564516        2.575283       -1.537917
H          2.682933        3.491447       -0.152739
C          1.060526        3.930343       -1.341797
C         -1.058455        5.489939       -2.255832
C          0.660024        5.053967       -0.622574
C          0.405210        3.594807       -2.525164
C         -0.648044        4.373835       -2.976553
C         -0.395205        5.828984       -1.083079
H          1.177641        5.319658        0.292282
H          0.711010        2.712648       -3.076382
H         -1.156435        4.101589       -3.892710
H         -0.699063        6.702580       -0.520464
H         -1.883183        6.094263       -2.609567
N          3.107254        1.699577        1.924551
O          3.633994        2.748939        1.593306
O          3.696893        0.739348        2.341678
C          1.521711        1.612332        1.806709
O          1.100001        0.384653        2.056389
C          1.202514        1.349335        0.387842
H          1.942987        0.703676       -0.082018
C          0.991765        2.748554        2.653360
H          1.197724        3.719820        2.207029
H          1.460739        2.700532        3.636721
H         -0.078529        2.609254        2.784324
C         -0.124422        1.397485       -0.210833
C         -2.601862        1.396843       -1.485730
C         -0.387865        0.498708       -1.248175
C         -1.107340        2.322787        0.157894
C         -2.335421        2.322529       -0.481199
C         -1.626924        0.484801       -1.871505
H          0.373828       -0.215147       -1.545389
H         -0.910509        3.058207        0.923798
H         -3.089589        3.043074       -0.193119
H         -1.829360       -0.241418       -2.648462
H         -3.571549        1.388704       -1.967921

SR epoxide:Catalyst:Aniline, Transition State 1; Energy = -2737.307181; 6-31G(d) basis
set.
C         -4.106610        0.780976       -0.323422
C         -4.129036       -1.676745        0.227624
C         -6.145330       -0.630631       -0.849429
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C	-5.651670	-1.719983	0.104245
C	-5.642636	0.753155	-0.424467
C	-3.665828	-0.290775	0.684848
H	-3.672061	-1.886190	-0.748982
H	-5.777917	-0.847405	-1.861910
H	-6.098453	-1.567366	1.096026
H	-6.076234	1.015929	0.550345
H	-4.101645	-0.085147	1.667773
H	-3.696735	0.485328	-1.303048
H	-3.759189	-2.428101	0.934185
H	-7.239309	-0.631741	-0.901900
H	-5.972144	-2.708065	-0.241627
H	-5.983726	1.507004	-1.141561
N	-3.505441	2.086815	-0.027967
N	-2.223040	-0.245613	0.844180
H	-1.685894	-0.299579	-0.030687
C	-3.809755	3.075402	-1.051264
H	-4.864559	3.397388	-1.047863
H	-3.574696	2.664099	-2.037813
H	-3.187112	3.958428	-0.892989
C	-3.790373	2.611311	1.299985
H	-3.448055	1.915218	2.072247
H	-4.858698	2.828627	1.469654
H	-3.232542	3.544744	1.424642
C	-1.577300	-0.412534	1.993023
S	-2.262591	-0.853150	3.464496
N	-0.202011	-0.211677	1.916395
H	0.287140	-0.585754	2.721331
C	0.464870	0.837132	1.267259
C	1.976275	2.914454	0.103792
C	1.863271	0.857240	1.377482
C	-0.177279	1.860433	0.558251
C	0.592173	2.876679	-0.004087
C	2.597446	1.883853	0.804016
H	2.370791	0.063644	1.919073
H	-1.260258	1.883541	0.430672
H	2.551738	3.718204	-0.339053
C	4.096757	1.824661	0.874826
C	-0.141839	3.955394	-0.750332
F	4.525131	1.374629	2.063692
F	0.682652	4.906041	-1.209627
F	-0.808055	3.458909	-1.801934
F	-1.051074	4.560259	0.034666
F	4.599087	0.994699	-0.057537
F	4.655848	3.024526	0.670442
N	-1.414066	-3.254649	-0.549314
O	-2.294168	-4.016138	-0.891236
O	-1.079531	-3.066669	0.610965
C	-0.702796	-2.390743	-1.666328
C	0.568471	-1.847228	-1.156269
H	0.496257	-1.438315	-0.154966
C	1.584487	-1.282616	-2.082207
C	3.580414	-0.175655	-3.696894
C	2.247220	-2.072565	-3.029517
C	1.917099	0.067160	-1.968760
C	2.910657	0.619207	-2.771433
C	3.242013	-1.522283	-3.830129
H	1.990387	-3.123038	-3.141740
H	1.369249	0.685482	-1.267931
H	3.161911	1.670115	-2.666013
H	3.753548	-2.144166	-4.557585
H	4.361293	0.250995	-4.318253
O	-1.126266	-1.121051	-1.665726
C	-0.805810	-3.155367	-2.964762
H	-0.311934	-2.571180	-3.741964
H	-0.350082	-4.148098	-2.896453
H	-1.859702	-3.268875	-3.221413
H	1.040756	-4.043067	0.021223
N	1.715949	-3.356338	-0.310713
H	2.316140	-3.779732	-1.015078
C	2.464267	-2.806129	0.770768
C	3.915661	-1.714141	2.883046
C	3.687235	-2.180171	0.520913
C	1.938524	-2.842722	2.064132
C	2.673370	-2.303034	3.117643

C	4.413250	-1.647919	1.582443
H	4.069418	-2.121387	-0.495339
H	0.967634	-3.299227	2.240155
H	2.271333	-2.349546	4.125189
H	5.363564	-1.163140	1.387083
H	4.485734	-1.294586	3.705249

SR epoxide:Catalyst:Aniline, Transition State 2; Energy = -2737.282849; 6-31G(d) basis set.

C	-2.120550	-3.075387	-0.809212
C	-1.425080	-3.995140	1.475262
C	-3.191853	-5.169091	0.138335
C	-2.702191	-4.831241	1.545033
C	-3.410824	-3.899226	-0.687195
C	-1.651720	-2.738960	0.624679
H	-0.616856	-4.588863	1.039231
H	-2.448477	-5.802024	-0.363690
H	-3.484215	-4.271253	2.076537
H	-4.190055	-3.290481	-0.203486
H	-2.494373	-2.192865	1.072390
H	-1.360266	-3.713642	-1.283221
H	-1.101515	-3.686584	2.475282
H	-4.123498	-5.742503	0.181360
H	-2.518677	-5.744880	2.119092
H	-3.780336	-4.166109	-1.681267
N	-2.271192	-1.829770	-1.607355
N	-0.547187	-1.779239	0.715634
H	-0.792261	-0.896222	1.156000
C	-1.096934	-1.630611	-2.462690
H	-1.044560	-2.392395	-3.257901
H	-0.180088	-1.696584	-1.876954
H	-1.146571	-0.643058	-2.934546
C	-3.457934	-1.762689	-2.459934
H	-4.376756	-1.850008	-1.878316
H	-3.463276	-2.528350	-3.252039
H	-3.468356	-0.785166	-2.954261
C	0.776705	-1.990217	0.523012
S	1.411235	-3.311002	-0.295793
N	1.527266	-0.961422	1.041070
H	0.993492	-0.230027	1.503100
C	2.825121	-0.529156	0.719929
C	5.347355	0.562030	0.140435
C	3.897608	-1.372655	0.418943
C	3.029432	0.855568	0.766361
C	4.276835	1.386253	0.469413
C	5.137886	-0.811608	0.128163
H	3.766143	-2.445490	0.420352
H	2.199154	1.514011	1.017155
H	6.322093	0.979473	-0.084394
C	6.271502	-1.724253	-0.251931
C	4.432139	2.879616	0.415011
F	7.461949	-1.186328	0.051118
F	5.704007	3.257183	0.594125
F	4.045616	3.362436	-0.782277
F	3.685923	3.493627	1.339785
F	6.189605	-2.906985	0.371251
F	6.279426	-1.974463	-1.570233
N	-1.181568	2.014820	1.730124
O	-0.470647	1.005230	1.729064
O	-0.759538	3.130436	1.590927
C	-2.767969	1.809822	1.855966
C	-3.326854	2.074931	0.509431
H	-2.971627	3.014357	0.102147
C	-4.717706	1.631143	0.218893
C	-7.329616	0.817917	-0.339061
C	-5.734948	2.578473	0.090963
C	-5.015704	0.272932	0.064072
C	-6.317131	-0.131855	-0.214901
C	-7.037122	2.171349	-0.184391
H	-5.501049	3.628865	0.233844
H	-4.220918	-0.467601	0.148205
H	-6.540405	-1.188040	-0.333736
H	-7.824694	2.912257	-0.275786
H	-8.345359	0.502871	-0.555580
O	-3.399220	2.880977	2.259203

C	-2.998814	0.520337	2.618985
H	-4.077674	0.395293	2.722553
H	-2.579634	-0.362285	2.134521
H	-2.562056	0.618372	3.615993
H	-2.181675	0.123594	-0.886498
N	-2.382084	1.129182	-1.030016
H	-3.136984	1.176112	-1.714870
C	-1.249800	1.885696	-1.464686
C	0.926248	3.457534	-2.217060
C	-1.459143	3.143566	-2.034119
C	0.047853	1.410582	-1.274276
C	1.128855	2.196382	-1.662309
C	-0.371126	3.926667	-2.405199
H	-2.473558	3.503874	-2.190081
H	0.203468	0.429482	-0.832087
H	2.137806	1.820574	-1.533583
H	-0.541626	4.905160	-2.842179
H	1.778228	4.066560	-2.499799

SR epoxide:Catalyst:Aniline, Transition State 3; Energy = -2737.303089; 6-31G(d) basis set.

C	-3.640405	1.759588	0.901296
C	-3.680993	3.662389	-0.756819
C	-5.877804	2.826271	0.227060
C	-5.211468	3.829859	-0.734843
C	-4.934035	2.472793	1.379659
C	-3.315889	2.187672	-0.545296
H	-3.215101	4.262394	0.028925
H	-6.813776	3.238054	0.617351
H	-5.617764	3.694800	-1.743113
H	-5.450381	1.854911	2.122647
H	-3.938153	1.599964	-1.229718
H	-2.810842	2.112621	1.517662
H	-3.264727	4.005306	-1.708740
H	-6.149540	1.913626	-0.316246
H	-5.453400	4.853981	-0.432816
H	-4.652551	3.396013	1.899702
N	-3.640010	0.287931	1.060658
N	-1.955523	1.848476	-0.962252
H	-1.903657	1.136242	-1.691728
C	-3.479146	-0.048762	2.472466
H	-4.275670	0.364367	3.112658
H	-2.516782	0.325140	2.835729
H	-3.508686	-1.135883	2.613010
C	-4.824156	-0.374209	0.518442
H	-4.940139	-0.146604	-0.543889
H	-5.753520	-0.104764	1.046499
H	-4.702127	-1.460492	0.602905
C	-0.784273	2.335553	-0.506869
S	-0.627540	3.387171	0.803845
N	0.278216	1.855131	-1.239059
H	0.002281	1.165536	-1.935525
C	1.633322	1.723315	-0.905868
C	4.327566	1.159396	-0.313876
C	2.288326	0.630922	-1.501996
C	2.351376	2.558958	-0.050240
C	3.680767	2.250514	0.242145
C	3.609767	0.360025	-1.203376
H	1.728465	-0.031026	-2.157152
H	1.880609	3.421928	0.397935
H	5.357512	0.930596	-0.063301
C	4.298195	-0.820096	-1.825004
C	4.384036	3.089838	1.269858
F	4.990431	-1.519893	-0.908592
F	4.092437	4.390743	1.141013
F	4.021670	2.731567	2.514950
F	5.717064	2.963557	1.199380
F	3.437267	-1.666668	-2.408269
F	5.180833	-0.443870	-2.763407
N	-2.951574	-1.543147	-2.125678
O	-3.419340	-0.461592	-2.411005
O	-3.609957	-2.543346	-1.885393
C	-1.376596	-1.649058	-2.007638
C	-1.061308	-1.279789	-0.616262
H	-1.752223	-0.540867	-0.207529

C	0.233620	-1.382484	0.053138
C	2.640728	-1.451500	1.463935
C	0.494856	-0.441301	1.057943
C	1.176471	-2.384433	-0.213209
C	2.370727	-2.418331	0.494125
C	1.701302	-0.463636	1.750311
H	-0.241445	0.333031	1.271873
H	0.973987	-3.148549	-0.954311
H	3.101457	-3.190453	0.277858
H	1.914565	0.301273	2.490778
H	3.589182	-1.468099	1.992402
O	-0.800901	-0.499693	-2.339035
C	-0.966965	-2.914900	-2.730245
H	0.117809	-2.909106	-2.838034
H	-1.288163	-3.813583	-2.201264
H	-1.406457	-2.914810	-3.731206
H	-2.597297	-2.118625	1.244551
N	-2.114008	-2.773166	0.635423
H	-2.775648	-3.213702	-0.002274
C	-1.263047	-3.669788	1.314798
C	0.630059	-5.329599	2.523252
C	-0.638053	-3.272460	2.499717
C	-0.949544	-4.905508	0.744034
C	-0.007377	-5.729822	1.351230
C	0.306353	-4.100060	3.094896
H	-0.876939	-2.305437	2.934838
H	-1.445768	-5.218617	-0.171371
H	0.228353	-6.689900	0.902918
H	0.794629	-3.778357	4.009446
H	1.368642	-5.972232	2.990551

SR epoxide:Catalyst:Aniline, Transition State 4; Energy = -2737.300858; 6-31G(d) basis set.

C	-3.455488	-2.335314	0.742751
C	-2.372851	-4.493017	-0.003934
C	-4.782715	-4.494821	0.709461
C	-3.490087	-5.306939	0.647942
C	-4.552313	-3.165742	1.432657
C	-2.152426	-3.155400	0.715285
H	-2.627382	-4.287982	-1.053972
H	-5.136303	-4.294821	-0.310990
H	-3.186783	-5.585418	1.665932
H	-4.260157	-3.367801	2.471927
H	-1.820304	-3.355644	1.737224
H	-3.759597	-2.174016	-0.302205
H	-1.428736	-5.047884	0.002059
H	-5.570442	-5.063300	1.214230
H	-3.643820	-6.238841	0.094635
H	-5.485127	-2.593116	1.465794
N	-3.259180	-0.984956	1.304924
N	-1.073149	-2.427158	0.061735
H	-1.212834	-2.252122	-0.933211
C	-4.458442	-0.163741	1.165632
H	-5.243026	-0.417753	1.894611
H	-4.876931	-0.279091	0.160149
H	-4.196184	0.890692	1.316553
C	-2.809718	-0.968929	2.698169
H	-1.868986	-1.513520	2.804891
H	-3.556991	-1.387199	3.390239
H	-2.625993	0.068829	2.993693
C	0.154779	-2.209606	0.574296
S	0.606636	-2.563704	2.153681
N	1.016167	-1.652135	-0.347109
H	0.751966	-1.753651	-1.323002
C	2.328958	-1.190113	-0.129138
C	4.912061	-0.129978	0.121298
C	3.299371	-1.469671	-1.086288
C	2.648140	-0.372223	0.962951
C	3.928173	0.144740	1.071869
C	4.581255	-0.936236	-0.955138
H	3.061766	-2.109723	-1.931135
H	1.892931	-0.129063	1.698938
H	5.910972	0.280763	0.222246
C	5.588327	-1.213386	-2.035302
C	4.277689	1.071933	2.201900

F	5.377522	-0.436707	-3.110492
F	5.327364	0.620689	2.903119
F	4.625776	2.285908	1.733436
F	3.262543	1.249110	3.051738
F	6.841054	-0.986723	-1.622397
F	5.519702	-2.483989	-2.457732
N	-1.869649	-0.629905	-2.652672
O	-2.793921	-1.379020	-2.429648
O	-0.691253	-0.982013	-2.597656
C	-2.201686	0.953561	-2.883871
C	-2.671514	1.402460	-1.554231
H	-3.381298	0.705881	-1.127711
C	-2.793538	2.816310	-1.168766
C	-3.038880	5.435285	-0.226759
C	-3.966235	3.232449	-0.529161
C	-1.741536	3.726068	-1.328697
C	-1.864832	5.027937	-0.857549
C	-4.092311	4.537690	-0.065931
H	-4.786621	2.529141	-0.414481
H	-0.810038	3.406302	-1.782777
H	-1.037978	5.721247	-0.971724
H	-5.009692	4.852975	0.420531
H	-3.131186	6.451861	0.142527
O	-3.411449	1.158847	-3.315491
C	-1.017914	1.521607	-3.638352
H	-1.239856	2.568053	-3.851803
H	-0.080577	1.441602	-3.084787
H	-0.915618	0.991606	-4.588684
H	-0.597132	0.181815	-0.593230
N	-1.269550	0.751735	-0.078795
H	-1.886176	0.115800	0.466656
C	-0.607473	1.736791	0.688675
C	0.668240	3.779591	2.106938
C	0.700213	2.108402	0.365798
C	-1.283028	2.407825	1.710983
C	-0.644785	3.424070	2.412532
C	1.338516	3.116198	1.081621
H	1.218384	1.593401	-0.440850
H	-2.313147	2.144791	1.936380
H	-1.178035	3.940809	3.204292
H	2.366276	3.372195	0.843718
H	1.165640	4.565465	2.665336

SR epoxide:Catalyst:Aniline, Transition State 5; Energy = -2737.300260; 6-31G(d) basis set.

C	3.465875	2.465280	0.419427
C	2.302842	4.527856	-0.487893
C	4.733196	4.645543	0.130995
C	3.418917	5.420555	0.052804
C	4.570805	3.380343	0.977289
C	2.146795	3.254043	0.352264
H	2.524848	4.244922	-1.526739
H	5.050394	4.364708	-0.882631
H	3.144806	5.774889	1.055292
H	4.321630	3.665923	2.007943
H	1.840378	3.541537	1.361364
H	3.743668	2.199473	-0.614364
H	1.342830	5.054565	-0.491755
H	5.526601	5.273010	0.549370
H	3.528733	6.306729	-0.580074
H	5.519130	2.834819	1.014656
N	3.310517	1.179362	1.127897
N	1.078008	2.425944	-0.185547
H	1.246583	2.024257	-1.107002
C	2.814701	1.299433	2.499864
H	2.715716	0.294327	2.921764
H	1.824655	1.762436	2.512822
H	3.491957	1.870843	3.153080
C	4.541295	0.394334	1.101729
H	4.965358	0.407776	0.093163
H	4.319397	-0.647249	1.360377
H	5.304047	0.762336	1.804694
C	-0.164841	2.312653	0.324416
S	-0.650627	2.969292	1.791281
N	-0.994183	1.569711	-0.491289

H	-0.750853	1.529795	-1.480522
C	-2.290304	1.104229	-0.189779
C	-4.827379	0.006829	0.261846
C	-3.268444	1.170855	-1.177128
C	-2.575055	0.479098	1.029496
C	-3.833690	-0.061280	1.237877
C	-4.528209	0.622851	-0.943231
H	-3.048457	1.646554	-2.127805
H	-1.809885	0.397661	1.791147
H	-5.810110	-0.416807	0.440521
C	-5.550868	0.658799	-2.043777
C	-4.144614	-0.788607	2.515332
F	-6.798788	0.565733	-1.566073
F	-5.193729	-0.246632	3.149930
F	-4.469539	-2.072116	2.269043
F	-3.112241	-0.795660	3.364112
F	-5.469540	1.791917	-2.755644
F	-5.381624	-0.355487	-2.906028
N	0.318866	-0.303675	-2.711185
O	0.839043	0.805450	-2.767378
O	-0.877657	-0.462561	-2.562240
C	1.317276	-1.592606	-2.736797
C	2.297242	-1.339187	-1.658540
H	2.703955	-0.336407	-1.698152
C	3.164265	-2.416708	-1.139741
C	4.878842	-4.389261	-0.150568
C	4.551604	-2.237748	-1.183934
C	2.643084	-3.598616	-0.601127
C	3.499948	-4.577246	-0.105102
C	5.405863	-3.218760	-0.695396
H	4.953948	-1.333255	-1.631080
H	1.569446	-3.746376	-0.546121
H	3.085956	-5.485705	0.320225
H	6.480260	-3.073946	-0.743837
H	5.543956	-5.155709	0.234826
O	2.307672	-1.455251	-3.576020
C	0.427331	-2.812796	-2.820987
H	1.081114	-3.684507	-2.873942
H	-0.249656	-2.905306	-1.969160
H	-0.160155	-2.762044	-3.740640
H	1.999843	-0.112508	0.509328
N	1.282640	-0.732033	0.082836
H	0.549941	-0.122549	-0.284215
C	0.708871	-1.679360	0.965404
C	-0.439688	-3.595504	2.639623
C	-0.612639	-2.088160	0.761388
C	1.463065	-2.250759	1.991895
C	0.885304	-3.205384	2.823462
C	-1.186618	-3.033102	1.605410
H	-1.186662	-1.646992	-0.051751
H	2.500767	-1.956008	2.125583
H	1.475464	-3.642744	3.622583
H	-2.223889	-3.318079	1.460703
H	-0.888573	-4.330825	3.298785

SR epoxide:Catalyst:Aniline, Transition State 6; Energy = -2737.299270; 6-31G(d) basis set.

C	3.652424	2.221405	0.590462
C	2.517649	4.087594	-0.682075
C	4.883921	4.383371	0.115704
C	3.562801	5.088384	-0.190834
C	4.675429	3.242965	1.116101
C	2.321607	2.945775	0.324245
H	2.830984	3.656710	-1.644449
H	5.302660	3.975080	-0.814783
H	3.191723	5.577081	0.719729
H	4.319322	3.658819	2.067999
H	1.941515	3.374864	1.255843
H	4.023600	1.852014	-0.378483
H	1.549526	4.573885	-0.840738
H	5.618080	5.094005	0.508255
H	3.708741	5.875584	-0.937190
H	5.629048	2.744349	1.318689
N	3.478501	1.018379	1.423620
N	1.313084	2.009381	-0.148348

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H          1.634336        1.346939       -0.849738
C          4.702756        0.226067        1.503088
H          4.472696       -0.754381        1.935441
H          5.479325        0.687864        2.131503
H          5.120230        0.076851        0.501978
C          2.994112        1.299330        2.775300
H          2.082872        1.902354        2.742516
H          3.740479        1.821527        3.393248
H          2.750881        0.351354        3.267018
C         -0.013671        2.114077        0.070785
S         -0.692673        3.232588        1.127401
N         -0.729712        1.171084       -0.619248
H         -0.175060        0.445114       -1.064751
C         -2.085449        0.819618       -0.460044
C         -4.747740       -0.014907       -0.226155
C         -3.111971        1.762117       -0.475901
C         -2.390411       -0.538016       -0.337460
C         -3.712199       -0.943994       -0.225217
C         -4.430008        1.332174       -0.350562
H         -2.882601        2.815105       -0.579092
H         -1.590158       -1.272981       -0.289993
H         -5.779864       -0.334911       -0.130333
C         -5.533152        2.350540       -0.432228
C         -4.038893       -2.397441       -0.026433
F         -6.643981        1.930142        0.188552
F         -5.088300       -2.768091       -0.774633
F         -3.010546       -3.193727       -0.342966
F         -4.367084       -2.659719        1.250301
F         -5.173698        3.516843        0.117941
F         -5.868986        2.606433       -1.707182
N          2.427662       -4.515458        0.152230
O          2.948351       -4.248259        1.233837
O          1.652350       -5.423102       -0.026806
C          2.728266       -3.533815       -1.064261
C          1.750481       -2.428038       -0.933959
H          0.751805       -2.783642       -0.700534
C          1.850692       -1.240973       -1.824355
C          1.975821        0.949489       -3.567124
C          0.781392       -0.951799       -2.679293
C          2.985630       -0.423617       -1.851230
C          3.053759        0.655300       -2.731446
C          0.837971        0.145665       -3.537513
H         -0.086701       -1.606299       -2.683412
H          3.813792       -0.629678       -1.179299
H          3.946273        1.273820       -2.758554
H         -0.002431        0.364571       -4.187895
H          2.025855        1.799085       -4.240129
O          2.085238       -3.855657       -2.158232
C          4.234570       -3.351677       -1.096855
H          4.699499       -4.328263       -1.258107
H          4.480844       -2.716261       -1.948668
H          4.626726       -2.919618       -0.173411
H          2.303139       -0.621903        0.901431
N          1.881606       -1.566798        0.905951
H          2.533192       -2.236893        1.323028
C          0.619792       -1.582027        1.581781
C         -1.898183       -1.588489        2.789236
C          0.054746       -0.389093        2.033390
C         -0.072222       -2.787121        1.743995
C         -1.330351       -2.780055        2.342426
C         -1.198339       -0.393682        2.637305
H          0.600815        0.540625        1.915833
H          0.365603       -3.727267        1.417916
H         -1.871933       -3.714328        2.449813
H         -1.626730        0.547807        2.967963
H         -2.884841       -1.592050        3.239746

SR epoxide:Catalyst:Aniline, Transition State 7; Energy = -2737.286316; 6-31G(d) basis
set.
C         -0.816175        3.515918        1.105274
C         -1.543613        4.226016       -1.180504
C         -2.138612        5.695976        0.774079
C         -1.434661        5.641214       -0.581113
C         -1.434123        4.765376        1.778885
C         -1.688742        3.133310       -0.099683
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H	-0.654981	3.998113	-1.781713
H	-2.157851	6.717009	1.165815
H	-1.858351	6.374165	-1.273128
H	-2.148156	4.448854	2.547344
H	-2.734753	3.082600	0.225911
H	0.170858	3.792348	0.709138
H	-2.407933	4.154866	-1.849826
H	-3.183907	5.390461	0.647031
H	-0.380468	5.912374	-0.445643
H	-0.635497	5.312098	2.291217
N	-0.552644	2.396171	2.026164
N	-1.468707	1.799995	-0.716399
H	-2.158621	1.675479	-1.456437
C	0.470578	2.731347	3.014408
H	1.371712	3.088803	2.505273
H	0.725391	1.832200	3.583164
H	0.136036	3.502534	3.724206
C	-1.736215	1.843024	2.679186
H	-2.541718	1.706651	1.954095
H	-2.105579	2.482684	3.494272
H	-1.473560	0.869282	3.107214
C	-0.257293	1.272651	-1.130417
S	-0.136190	0.492259	-2.611567
N	0.703014	1.333259	-0.180421
H	0.325932	1.552375	0.772879
C	2.004174	0.807933	-0.235317
C	4.599276	-0.246018	-0.183078
C	2.476531	0.153197	0.905156
C	2.838559	0.956991	-1.343340
C	4.124600	0.427707	-1.302566
C	3.759461	-0.375499	0.918329
H	1.822692	0.024652	1.762976
H	2.488729	1.483908	-2.222306
H	5.603954	-0.654776	-0.165866
C	4.222357	-1.185424	2.095281
C	5.001358	0.549927	-2.518349
F	4.158736	-2.503161	1.831337
F	6.301632	0.544775	-2.190902
F	4.806873	-0.466881	-3.370180
F	4.756534	1.681115	-3.193319
F	5.497609	-0.918387	2.409706
F	3.477607	-0.966197	3.186247
N	-4.387284	0.669656	-0.507196
O	-4.299620	1.442183	-1.438092
O	-4.298870	1.005765	0.669531
C	-4.520130	-0.914388	-0.843200
C	-3.122456	-1.389120	-0.964742
H	-2.509765	-0.726617	-1.570480
C	-2.768143	-2.821856	-1.007755
C	-1.930746	-5.481802	-1.100213
C	-3.095358	-3.698781	0.031061
C	-2.003845	-3.282342	-2.082891
C	-1.594325	-4.610992	-2.133648
C	-2.677494	-5.023440	-0.015723
H	-3.645988	-3.335364	0.894294
H	-1.739703	-2.590940	-2.878511
H	-1.006484	-4.963037	-2.975106
H	-2.925674	-5.696688	0.798434
H	-1.603407	-6.516250	-1.133573
O	-4.664873	-1.152477	-2.112859
C	-5.534693	-1.460423	0.143106
H	-5.635577	-2.530936	-0.042291
H	-5.261808	-1.283163	1.185140
H	-6.500024	-0.987761	-0.057875
H	-1.796805	0.101168	0.446814
N	-2.103576	-0.826492	0.760528
H	-2.833466	-0.674169	1.456209
C	-1.035159	-1.627891	1.256163
C	1.054028	-3.223103	2.191552
C	0.040203	-1.927387	0.417559
C	-1.080454	-2.150822	2.549807
C	-0.034532	-2.943624	3.014489
C	1.081009	-2.719494	0.891904
H	0.058916	-1.535833	-0.598255
H	-1.929308	-1.928135	3.192535

H	-0.070211	-3.336959	4.025536
H	1.924654	-2.934445	0.243000
H	1.877923	-3.826001	2.558037

SR epoxide:Catalyst:Aniline, Transition State 8; Energy = -2737.282849; 6-31G(d) basis set.

C	-2.121400	3.076404	0.808560
C	-1.425092	3.996577	-1.475372
C	-3.192807	5.169983	-0.139210
C	-2.702317	4.832460	-1.545702
C	-3.411802	3.899994	0.686130
C	-1.652080	2.740176	-0.625218
H	-0.617251	4.590339	-1.038680
H	-2.449896	5.803112	0.363255
H	-3.483941	4.272413	-2.077732
H	-4.190735	3.291103	0.202130
H	-2.494616	2.194215	-1.073355
H	-1.361411	3.714827	1.282832
H	-1.100839	3.688347	-2.475269
H	-4.124613	5.743103	-0.182656
H	-2.518665	5.746238	-2.119497
H	-3.781711	4.166762	1.680085
N	-2.272061	1.830756	1.606620
N	-0.547604	1.780373	-0.716083
H	-0.792961	0.897360	-1.156274
C	-1.097881	1.631705	2.462087
H	-1.045806	2.393355	3.257451
H	-0.180970	1.698022	1.876494
H	-1.147339	0.644063	2.933775
C	-3.458869	1.763620	2.459086
H	-4.377642	1.850831	1.877377
H	-3.464356	2.529337	3.251142
H	-3.469265	0.786126	2.953479
C	0.776314	1.991369	-0.523633
S	1.410872	3.311611	0.296021
N	1.526981	0.963167	-1.042721
H	0.993356	0.232831	-1.506531
C	2.824388	0.529974	-0.720893
C	5.345862	-0.562526	-0.140794
C	3.897081	1.372875	-0.419078
C	3.027977	-0.854859	-0.767539
C	4.275069	-1.386173	-0.470402
C	5.137007	0.811185	-0.127979
H	3.766062	2.445776	-0.420215
H	2.197378	-1.512817	-1.018548
H	6.320340	-0.980495	0.084177
C	6.270786	1.723349	0.252773
C	4.429869	-2.879605	-0.416355
F	6.190741	2.905390	-0.371987
F	5.701464	-3.257569	-0.596679
F	4.044333	-3.362472	0.781222
F	3.682624	-3.493229	-1.340540
F	6.276844	1.975211	1.570763
F	7.461282	1.184159	-0.047805
N	-1.179970	-2.015133	-1.728978
O	-0.470262	-1.004710	-1.725776
O	-0.756760	-3.130452	-1.591059
C	-2.766381	-1.811466	-1.855321
C	-3.325292	-2.076122	-0.508732
H	-2.969597	-3.015107	-0.100841
C	-4.716389	-1.632878	-0.218549
C	-7.328830	-0.820771	0.338509
C	-5.733235	-2.580660	-0.090770
C	-5.015048	-0.274775	-0.064063
C	-6.316749	0.129445	0.214473
C	-7.035671	-2.174096	0.184146
H	-5.498803	-3.630963	-0.233427
H	-4.220593	0.466120	-0.148137
H	-6.540568	1.185541	0.333060
H	-7.822931	-2.915349	0.275435
H	-8.344779	-0.506154	0.554685
O	-3.396856	-2.883287	-2.257977
C	-2.998057	-0.522530	-2.619056
H	-2.561366	-0.620886	-3.616065
H	-4.076997	-0.398158	-2.722599

H	-2.579347	0.360598	-2.135077
H	-2.180731	-0.123518	0.885898
N	-2.380789	-1.129031	1.030164
H	-3.135682	-1.175711	1.715042
C	-1.248270	-1.884880	1.465420
C	0.928188	-3.455571	2.219001
C	0.049251	-1.409318	1.275194
C	-1.457271	-3.142574	2.035367
C	-0.369049	-3.925100	2.407066
C	1.130449	-2.194569	1.663769
H	0.204631	-0.428375	0.832572
H	-2.471586	-3.503190	2.191265
H	-0.539287	-4.903461	2.844444
H	2.139277	-1.818431	1.535037
H	1.780322	-4.064176	2.502181

SR epoxide:Catalyst:Aniline, Transition State 9; Energy = -2737.292137; 6-31G(d) basis set.

C	-2.802589	3.000267	-0.017650
C	-0.853651	4.540637	0.473932
C	-3.148318	5.510091	0.179743
C	-1.651703	5.749979	-0.009840
C	-3.594504	4.222536	-0.518514
C	-1.305588	3.258989	-0.236829
H	-0.987880	4.413596	1.557953
H	-3.369294	5.431837	1.253285
H	-1.439741	5.918349	-1.073955
H	-3.452064	4.328265	-1.602407
H	-1.114554	3.381269	-1.306533
H	-2.976226	2.919604	1.069412
H	0.216774	4.674477	0.286886
H	-3.727505	6.357148	-0.201445
H	-1.333070	6.650155	0.525127
H	-4.663798	4.066596	-0.348131
N	-3.227734	1.707276	-0.586554
N	-0.507395	2.119424	0.199560
H	-0.719026	1.771026	1.131649
C	-4.651951	1.453825	-0.382723
H	-5.298627	2.102752	-0.992108
H	-4.906296	1.601775	0.672664
H	-4.870760	0.415946	-0.647002
C	-2.873490	1.516634	-1.992802
H	-3.314197	2.273352	-2.659471
H	-3.250050	0.536807	-2.306495
H	-1.786374	1.519725	-2.120945
C	0.694392	1.790919	-0.331959
S	1.296080	2.472484	-1.746481
N	1.347537	0.813738	0.368058
H	0.841874	0.340442	1.112896
C	2.674512	0.365124	0.160988
C	5.297097	-0.575134	-0.092846
C	3.732430	1.270616	0.053180
C	2.926075	-1.003540	0.147393
C	4.236219	-1.460592	0.029487
C	5.027624	0.791540	-0.084483
H	3.539237	2.336103	0.077864
H	2.102693	-1.709298	0.176896
H	6.314237	-0.937971	-0.193224
C	6.163479	1.759992	-0.260775
C	4.497697	-2.939765	0.082725
F	5.880983	2.960866	0.262702
F	5.613412	-3.270947	-0.581705
F	4.657355	-3.361049	1.349357
F	3.484842	-3.642044	-0.437343
F	7.283632	1.314130	0.328281
F	6.454654	1.951373	-1.555264
N	-0.441044	-3.162799	-1.019013
O	-0.103751	-4.220620	-0.551779
O	0.287916	-2.168513	-1.071357
C	-1.993688	-2.995342	-1.489380
C	-2.681827	-2.548224	-0.257988
H	-2.277386	-3.018370	0.635348
C	-4.121969	-2.194090	-0.195627
C	-6.816994	-1.480102	0.067965
C	-4.984713	-2.280109	-1.293238

C	-4.633635	-1.785975	1.042273
C	-5.970463	-1.426366	1.173378
C	-6.322061	-1.917251	-1.159365
H	-4.626509	-2.695492	-2.226980
H	-3.979180	-1.761225	1.909804
H	-6.352420	-1.114804	2.140471
H	-6.984004	-1.995424	-2.015868
H	-7.862136	-1.204591	0.166822
O	-2.650011	-4.115324	-1.392100
C	-1.927793	-2.214117	-2.789222
H	-1.280217	-1.338799	-2.716826
H	-1.540486	-2.880073	-3.565229
H	-2.929249	-1.895810	-3.080398
H	-1.005982	-0.815880	-0.355007
N	-1.822387	-0.756154	0.261107
H	-2.392445	0.072663	-0.004460
C	-1.431045	-0.692458	1.620943
C	-0.683716	-0.585631	4.314098
C	-0.400610	-1.514384	2.096723
C	-2.100179	0.164275	2.503718
C	-1.723566	0.213938	3.843459
C	-0.029298	-1.449695	3.437948
H	0.098335	-2.203824	1.418530
H	-2.916598	0.777905	2.127295
H	-2.244956	0.883260	4.520343
H	0.773463	-2.085476	3.797125
H	-0.389859	-0.540972	5.357054

SR epoxide:Catalyst:Aniline, Transition State 10; Energy = -2737.290609; 6-31G(d) basis set.

C	-3.470796	2.469378	-0.432436
C	-2.369959	4.427418	0.725068
C	-4.284876	4.884029	-0.841122
C	-3.751009	5.091508	0.574484
C	-4.531535	3.388745	-1.096703
C	-2.161064	3.254037	-0.254899
H	-2.244110	4.053623	1.748312
H	-5.212559	5.442602	-0.997011
H	-3.684267	6.155126	0.819812
H	-4.551737	3.203077	-2.176074
H	-1.831604	3.637076	-1.223419
H	-3.823658	2.204337	0.576764
H	-1.565953	5.150152	0.551755
H	-3.558270	5.277081	-1.562714
H	-4.459475	4.649488	1.286066
H	-5.520234	3.112193	-0.714400
N	-3.282109	1.180129	-1.125050
N	-1.086302	2.403360	0.230906
H	-1.254140	1.954898	1.130936
C	-2.663454	1.293053	-2.446658
H	-3.272617	1.862091	-3.165699
H	-2.527798	0.285968	-2.854050
H	-1.677695	1.759158	-2.371303
C	-4.541887	0.446711	-1.213872
H	-5.021947	0.420320	-0.231113
H	-4.346531	-0.586020	-1.522575
H	-5.246643	0.890841	-1.934001
C	0.165205	2.335689	-0.266460
S	0.665948	3.069859	-1.690093
N	0.993452	1.565439	0.526531
H	0.755977	1.505121	1.516253
C	2.286023	1.105642	0.203285
C	4.811508	0.005788	-0.301276
C	2.552797	0.503718	-1.031618
C	3.276246	1.149305	1.179365
C	4.530485	0.600113	0.918824
C	3.805663	-0.038625	-1.266485
H	1.777130	0.440781	-1.784860
H	3.070046	1.607361	2.141707
H	5.789561	-0.419722	-0.499911
C	4.097198	-0.743138	-2.561165
C	5.566450	0.610975	2.007458
F	5.134828	-0.188162	-3.203320
F	6.807541	0.508237	1.514365
F	5.507117	1.736833	2.732785

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F          5.394379       -0.410771        2.860301
F          4.428134       -2.029868       -2.342184
F          3.051103       -0.737309       -3.393087
N         -0.294042       -0.342545        2.728759
O         -0.800458        0.771887        2.807885
O          0.898064       -0.512654        2.559568
C         -1.307897       -1.621009        2.748507
C         -2.286244       -1.341911        1.676178
H         -2.673489       -0.331796        1.724514
C         -3.176341       -2.390923        1.141559
C         -4.937053       -4.297752        0.106464
C         -2.685853       -3.593215        0.619171
C         -4.556119       -2.156835        1.142806
C         -5.433674       -3.105028        0.631186
C         -3.565697       -4.539718        0.101835
H         -1.617379       -3.780171        0.590302
H         -4.934800       -1.234445        1.574121
H         -6.502444       -2.917493        0.645867
H         -3.175588       -5.464709       -0.310230
H         -5.620047       -5.039001       -0.296523
O         -2.293586       -1.477937        3.591934
C         -0.430278       -2.850970        2.819715
H         -1.092588       -3.715933        2.876684
H          0.237231       -2.947031        1.960758
H          0.166915       -2.809984        3.733607
H         -0.530175       -0.133777        0.287489
N         -1.267226       -0.746280       -0.066257
H         -1.994498       -0.134528       -0.484267
C         -0.706109       -1.701763       -0.947830
C          0.421458       -3.626036       -2.627264
C          0.619242       -2.106777       -0.760906
C         -1.474735       -2.282334       -1.958642
C         -0.907337       -3.240896       -2.792885
C          1.182465       -3.055510       -1.607842
H          1.204370       -1.660117        0.041211
H         -2.515445       -1.991578       -2.077267
H         -1.508791       -3.685113       -3.579713
H          2.222447       -3.337132       -1.476933
H          0.862209       -4.364217       -3.288715

SR epoxide:Catalyst:Aniline, Transition State 11; Energy = -2737.283508; 6-31G(d)
basis set.
C         -2.454662        2.987116        0.325907
C         -0.878891        3.897053        2.066866
C         -2.543084        5.470320        1.041580
C         -2.023329        4.885210        2.352902
C         -3.164177        4.361372        0.174464
C         -0.984543        3.258212        0.665962
H         -0.875343        3.094188        2.813621
H         -3.285501        6.252290        1.226088
H         -1.681229        5.673743        3.029076
H         -3.135787        4.666579       -0.877898
H         -0.579033        3.948064       -0.078220
H         -2.907744        2.455955        1.179506
H          0.094682        4.394774        2.129201
H         -1.712382        5.948162        0.508499
H         -2.847548        4.370524        2.862288
H         -4.220069        4.239467        0.437932
N         -2.637295        2.088729       -0.833373
N         -0.145242        2.070796        0.600524
H         -0.488641        1.246162        1.086570
C         -4.054114        1.995205       -1.187266
H         -4.643060        1.753217       -0.295403
H         -4.190083        1.194566       -1.921771
H         -4.452526        2.923803       -1.622702
C         -1.857207        2.478306       -2.008424
H         -2.117754        3.480238       -2.384866
H         -2.058976        1.764688       -2.813801
H         -0.787214        2.453540       -1.788596
C          1.176626        2.099137        0.282896
S          1.887306        3.385910       -0.531466
N          1.823424        0.970085        0.699362
H          1.265564        0.360484        1.292636
C          3.081681        0.422506        0.415568
C          5.508805       -0.934049       -0.027508
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C	4.034688	0.957355	-0.454232
C	3.352806	-0.797096	1.058559
C	4.547797	-1.457711	0.833601
C	5.230187	0.269941	-0.656111
H	3.847663	1.888032	-0.970260
H	2.614628	-1.236392	1.726190
H	6.438921	-1.459768	-0.210736
C	6.260385	0.895329	-1.556579
C	4.837618	-2.740788	1.561802
F	6.978729	1.824025	-0.907028
F	5.499162	-3.606639	0.781183
F	5.606765	-2.525370	2.641457
F	3.719865	-3.341201	1.985490
F	7.125839	-0.012239	-2.029719
F	5.695510	1.504453	-2.608014
N	0.034377	-1.948319	0.971784
O	-0.182656	-0.899682	1.606009
O	0.753132	-2.821820	1.370647
C	-0.619385	-2.114328	-0.490445
C	-2.075199	-2.282770	-0.339807
H	-2.355661	-2.922078	0.491339
C	-2.983703	-2.268344	-1.510085
C	-4.809915	-2.238288	-3.625392
C	-2.987873	-1.209641	-2.423535
C	-3.909305	-3.302575	-1.656889
C	-4.816728	-3.289833	-2.712849
C	-3.893421	-1.196838	-3.478975
H	-2.303640	-0.376765	-2.287408
H	-3.912982	-4.119470	-0.941270
H	-5.531017	-4.099736	-2.818888
H	-3.888588	-0.370079	-4.183235
H	-5.518341	-2.226307	-4.447548
O	-0.606312	-3.356385	-0.888821
C	0.055342	-1.028709	-1.312784
H	-0.220897	-1.184387	-2.356427
H	-0.237790	-0.022196	-0.995552
H	1.141923	-1.138698	-1.232409
H	-2.222129	-0.513290	1.377792
N	-2.902637	-0.649253	0.631680
H	-2.848698	0.154374	-0.012379
C	-4.193680	-0.969556	1.125687
C	-6.692640	-1.770518	2.085924
C	-4.329507	-1.422199	2.440961
C	-5.309124	-0.941086	0.282619
C	-6.551528	-1.333487	0.770673
C	-5.575320	-1.817472	2.916532
H	-3.457002	-1.458229	3.089088
H	-5.198904	-0.627151	-0.751499
H	-7.413212	-1.304089	0.111240
H	-5.670462	-2.161106	3.941623
H	-7.664186	-2.076746	2.459058

SR epoxide:Catalyst:Aniline, Transition State 12; Energy = -2737.289748; 6-31G(d) basis set.

C	2.440618	3.692930	-0.037650
C	0.886480	4.935217	-1.592529
C	2.414326	6.279887	-0.121423
C	1.962275	6.035436	-1.558718
C	3.099245	5.021455	0.433090
C	0.971885	3.970894	-0.389024
H	0.979329	4.346122	-2.512290
H	3.101958	7.129044	-0.063319
H	1.578880	6.952539	-2.014996
H	3.095286	5.060864	1.528185
H	0.469176	4.415434	0.472859
H	2.937622	3.361268	-0.961771
H	-0.119197	5.369061	-1.594361
H	1.543331	6.540210	0.492333
H	2.831807	5.728448	-2.153215
H	4.150549	5.018482	0.124982
N	2.617199	2.578704	0.914732
N	0.247083	2.751551	-0.707664
H	0.718143	2.147248	-1.380479
C	1.867560	2.730917	2.159830
H	1.999181	1.821878	2.757668

H	0.799277	2.840580	1.952076
H	2.198912	3.584852	2.772046
C	4.035867	2.373949	1.190839
H	4.569841	2.198632	0.250175
H	4.160310	1.496220	1.834144
H	4.508542	3.221338	1.710367
C	-1.034984	2.486792	-0.382482
S	-1.869045	3.308496	0.827669
N	-1.552459	1.450918	-1.121758
H	-0.916599	1.069409	-1.820217
C	-2.591113	0.558216	-0.802318
C	-4.486701	-1.419159	-0.161467
C	-3.773469	0.910699	-0.145772
C	-2.398375	-0.771472	-1.191949
C	-3.330033	-1.742810	-0.861354
C	-4.693933	-0.085608	0.172305
H	-3.966496	1.940434	0.119972
H	-1.497713	-1.048350	-1.732374
H	-5.214238	-2.179507	0.097783
C	-5.923049	0.297316	0.949646
C	-3.005368	-3.170281	-1.196892
F	-6.358279	1.520776	0.622436
F	-2.117926	-3.684754	-0.327146
F	-4.089295	-3.955345	-1.166654
F	-2.453313	-3.279270	-2.414729
F	-6.930745	-0.562415	0.740583
F	-5.683748	0.306088	2.270524
N	1.517112	-0.237327	-1.974268
O	0.447227	-0.177592	-2.561147
O	2.182554	0.753004	-1.718772
C	2.111601	-1.734517	-1.617696
C	3.273942	-1.522026	-0.742528
H	3.842122	-0.638665	-1.003099
C	4.017675	-2.634841	-0.099148
C	5.438122	-4.643185	1.244479
C	5.043304	-2.309656	0.797726
C	3.755830	-3.983226	-0.361639
C	4.457663	-4.977184	0.313422
C	5.741674	-3.302897	1.474153
H	5.307163	-1.266078	0.957946
H	3.047338	-4.251265	-1.135249
H	4.244008	-6.019265	0.098756
H	6.528678	-3.030674	2.169873
H	5.980236	-5.422646	1.770061
O	2.960588	-2.119378	-2.538664
C	0.880955	-2.564866	-1.311498
H	1.178372	-3.491739	-0.821033
H	0.179444	-2.051885	-0.650150
H	0.388818	-2.804689	-2.257380
H	2.509186	0.481627	0.686658
N	2.596527	-0.511246	0.958047
H	3.357041	-0.622051	1.625028
C	1.371927	-1.021405	1.477811
C	-1.057954	-2.080618	2.329268
C	1.332149	-2.303597	2.030760
C	0.206567	-0.263478	1.363089
C	-1.005725	-0.793472	1.800188
C	0.113387	-2.828281	2.447607
H	2.246633	-2.885566	2.115254
H	0.266191	0.740097	0.946516
H	-1.907010	-0.190945	1.732703
H	0.079062	-3.828914	2.866851
H	-2.005965	-2.496460	2.654141

SR epoxide:Catalyst:Aniline, Transition State 13; Energy = -2737.302103; 6-31G(d) basis set.

C	4.201739	1.458860	-0.383997
C	3.567670	3.699636	0.618982
C	5.695288	3.487280	-0.699476
C	5.000721	4.205073	0.456186
C	5.650906	1.974420	-0.480802
C	3.514851	2.172806	0.793508
H	2.978546	3.969925	-0.265161
H	5.189363	3.736555	-1.641676
H	5.562108	4.022545	1.382934

H	6.190823	1.737752	0.446456
H	4.075040	1.923107	1.703430
H	3.671858	1.757765	-1.293529
H	3.087613	4.166346	1.486100
H	6.732862	3.824369	-0.793436
H	4.994507	5.288070	0.295969
H	6.173075	1.457389	-1.292973
N	4.080220	-0.006539	-0.309285
N	2.144533	1.737127	1.104590
H	2.009449	1.460645	2.073838
C	4.926254	-0.615931	0.712106
H	4.682350	-1.679020	0.787223
H	4.726687	-0.168061	1.688357
H	6.001493	-0.530745	0.488210
C	4.343423	-0.611184	-1.612619
H	3.630622	-0.219671	-2.345780
H	4.207789	-1.693877	-1.544992
H	5.365250	-0.423935	-1.979900
C	1.024458	2.004107	0.399596
S	0.986568	2.143319	-1.282877
N	-0.097250	2.103504	1.190170
H	0.051666	1.892907	2.173745
C	-1.449570	1.960316	0.797490
C	-4.095174	1.434375	0.053252
C	-2.243236	1.112696	1.574130
C	-1.996424	2.605718	-0.312799
C	-3.309960	2.318951	-0.676725
C	-3.548830	0.845681	1.187964
H	-1.813136	0.587324	2.422625
H	-1.402897	3.295814	-0.895775
H	-5.110676	1.209099	-0.254344
C	-4.328292	-0.205174	1.928225
C	-3.857875	2.896216	-1.949901
F	-3.977392	-0.275692	3.216158
F	-3.644844	2.063888	-2.986569
F	-5.181497	3.094430	-1.879380
F	-3.285745	4.064967	-2.262995
F	-5.649228	0.041160	1.878970
F	-4.137919	-1.416696	1.390180
N	1.208280	-0.968652	2.547608
O	0.887147	0.065060	3.116912
O	2.357542	-1.271603	2.290444
C	0.017278	-1.929876	2.030928
C	-0.334241	-1.356068	0.712074
H	-0.269974	-0.276342	0.723024
C	-1.299845	-1.914728	-0.248482
C	-3.121371	-2.817326	-2.167614
C	-1.896881	-1.016551	-1.142376
C	-1.604210	-3.275253	-0.343339
C	-2.516554	-3.719902	-1.294767
C	-2.805034	-1.461671	-2.095411
H	-1.640116	0.039905	-1.093024
H	-1.123432	-3.991669	0.312079
H	-2.750070	-4.777743	-1.358721
H	-3.266792	-0.745724	-2.768321
H	-3.834680	-3.171099	-2.905491
O	-1.155688	-1.504590	2.424833
C	0.456947	-3.340557	2.372932
H	-0.392541	-4.005551	2.219219
H	1.306906	-3.677026	1.780835
H	0.715999	-3.375751	3.434950
H	0.984382	-0.656058	-1.310789
N	1.331498	-1.306406	-0.603471
H	2.151792	-0.856050	-0.160655
C	1.620811	-2.585942	-1.133053
C	2.112998	-5.167895	-2.085787
C	0.963504	-3.048403	-2.275704
C	2.517796	-3.424001	-0.462718
C	2.763658	-4.706192	-0.942478
C	1.213257	-4.334264	-2.745779
H	0.251265	-2.403068	-2.784699
H	3.009815	-3.056071	0.434511
H	3.467070	-5.346421	-0.419072
H	0.697143	-4.684162	-3.634430
H	2.306004	-6.168554	-2.458067

SR epoxide:Catalyst:Aniline, Transition State 14; Energy = -2737.301884; 6-31G(d) basis set.

C	3.856792	1.686484	-0.645392
C	3.778357	3.577873	1.078972
C	5.371468	3.725852	-0.899593
C	4.193474	4.375850	-0.158818
C	5.296016	2.186036	-0.860407
C	3.437423	2.088327	0.780898
H	2.910799	4.049209	1.549475
H	5.377644	4.074390	-1.937672
H	4.452589	5.397665	0.137576
H	5.918162	1.807460	-0.038543
H	4.028213	1.468421	1.463886
H	3.190388	2.199840	-1.344479
H	4.591409	3.605624	1.814051
H	6.320871	4.047450	-0.457941
H	3.331117	4.449086	-0.825965
H	5.712080	1.761644	-1.780884
N	3.665717	0.242493	-0.888735
N	2.063384	1.722536	1.130189
H	1.983091	0.963216	1.808008
C	4.741031	-0.588164	-0.352407
H	4.932482	-0.343090	0.694348
H	5.682571	-0.492949	-0.916501
H	4.443947	-1.643086	-0.381104
C	3.499893	-0.008627	-2.314731
H	2.622169	0.527674	-2.687001
H	3.351188	-1.079496	-2.498049
H	4.376324	0.294000	-2.912774
C	0.912998	2.228460	0.647302
S	0.821271	3.316589	-0.638597
N	-0.180981	1.742186	1.324467
H	0.055788	1.015065	1.996831
C	-1.531748	1.679895	0.959273
C	-4.240095	1.269592	0.308151
C	-2.202123	2.593310	0.144655
C	-2.240795	0.585651	1.484729
C	-3.569031	0.390676	1.157786
C	-3.539696	2.361500	-0.177874
H	-1.689375	3.460277	-0.246125
H	-1.719215	-0.133738	2.110044
H	-5.276305	1.101805	0.036093
C	-4.196273	3.293464	-1.155616
C	-4.315179	-0.791200	1.704691
F	-3.841946	2.997678	-2.418882
F	-5.193403	-0.431218	2.653230
F	-5.023673	-1.408234	0.742327
F	-3.498606	-1.705901	2.248400
F	-5.534283	3.224263	-1.098792
F	-3.846922	4.569238	-0.944265
N	2.890299	-1.836956	2.170987
O	3.492205	-2.871480	1.924004
O	3.413909	-0.796071	2.504448
C	1.316923	-1.836911	1.991701
C	1.084907	-1.418803	0.595372
H	1.836577	-0.713098	0.231545
C	-0.190172	-1.406631	-0.115648
C	-2.547374	-1.250815	-1.601117
C	-0.350903	-0.411233	-1.088999
C	-1.210647	-2.347319	0.083211
C	-2.378779	-2.270842	-0.662868
C	-1.533163	-0.320696	-1.816921
H	0.445148	0.315659	-1.246574
H	-1.088688	-3.149652	0.801328
H	-3.168304	-2.997001	-0.501016
H	-1.667125	0.484488	-2.532690
H	-3.475578	-1.180713	-2.160345
O	0.808029	-0.665808	2.346396
C	0.799704	-3.094987	2.657819
H	1.196386	-3.150409	3.674951
H	-0.286264	-3.023511	2.722560
H	1.085763	-3.997851	2.115986
H	2.623468	-3.519193	0.028012
N	2.050053	-3.004914	-0.639973

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H          2.647660       -2.439739       -1.237118
C          1.136834       -3.801649       -1.365733
C         -0.863728       -5.236536       -2.683143
C          0.680121       -5.010654       -0.837158
C          0.600265       -3.318370       -2.562118
C         -0.396733       -4.034387       -3.212782
C         -0.316375       -5.722589       -1.498433
H          1.106854       -5.392915        0.086866
H          0.947586       -2.369189       -2.962285
H         -0.814961       -3.646155       -4.136097
H         -0.664184       -6.662939       -1.082457
H         -1.643922       -5.791983       -3.192699
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SR epoxide:Catalyst:Aniline, Transition State 15; Energy = -2737.287570; 6-31G(d) basis set.

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C          0.868511       -3.605135       -0.019579
C          2.352510       -3.781819       -2.111215
C         -0.136266       -4.011361       -2.316430
C          1.109065       -3.263566       -2.827333
C          0.056261       -4.564288       -0.893959
C          2.287814       -3.424626       -0.615459
H          3.275225       -3.367501       -2.526751
H         -1.004652       -3.344897       -2.309886
H          1.209889       -3.370254       -3.911751
H          0.565827       -5.535923       -0.906380
H          2.985017       -4.059566       -0.062395
H          0.347110       -2.630920       -0.061978
H          2.419122       -4.870945       -2.217876
H         -0.373609       -4.844983       -2.986519
H          1.010731       -2.187569       -2.628419
H         -0.931567       -4.719850       -0.458893
N          0.936078       -4.057185        1.376713
N          2.725559       -2.033603       -0.422741
H          2.002140       -1.316676       -0.486211
C          1.720891       -3.147276        2.203228
H          1.293841       -2.126098        2.216489
H          2.756155       -3.092428        1.857939
H          1.733866       -3.523450        3.230138
C         -0.400684       -4.161953        1.956591
H         -0.996410       -3.246199        1.787943
H         -0.306446       -4.328997        3.032981
H         -0.946451       -5.009116        1.538512
C          4.007997       -1.654211       -0.428963
S          5.322604       -2.706725       -0.532174
N          4.252626       -0.302080       -0.360735
H          5.222517       -0.059801       -0.518855
C          3.393592        0.725385        0.073465
C          1.830439        2.862741        0.993774
C          3.414825        1.949554       -0.591586
C          2.577026        0.564302        1.199592
C          1.807221        1.627853        1.641617
C          2.637501        3.006817       -0.124822
H          4.036340        2.071973       -1.473793
H          2.560825       -0.383100        1.728140
H          1.227601        3.690360        1.353336
C          2.677223        4.304171       -0.882177
C          0.966435        1.500929        2.880040
F          3.923861        4.783085       -0.977129
F          1.418254        2.299960        3.856577
F         -0.310192        1.892915        2.646558
F          0.924313        0.259311        3.360175
F          2.230340        4.141387       -2.141318
F          1.917734        5.246124       -0.311172
N         -0.604009       -0.444643       -0.179710
O          0.280643       -0.294210       -1.006185
O         -0.410029       -0.387311        1.023793
C         -2.065697       -0.925127       -0.693656
C         -3.026259       -0.687374        0.404879
H         -2.636694       -1.011607        1.359763
C         -4.488264       -0.787830        0.210888
C         -7.267206       -0.984900       -0.015361
C         -5.221803       -1.551210        1.125431
C         -5.162421       -0.111389       -0.813405
C         -6.545862       -0.210060       -0.921861
C         -6.603499       -1.656375        1.009206
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H	-4.697801	-2.078125	1.917906
H	-4.611111	0.507230	-1.513031
H	-7.061286	0.318160	-1.717536
H	-7.160854	-2.261568	1.716610
H	-8.345809	-1.063797	-0.107111
O	-2.215084	-2.215761	-0.478820
C	-2.212218	-0.414510	-2.109371
H	-2.191936	0.677421	-2.175063
H	-1.395399	-0.824558	-2.706844
H	-3.152869	-0.801724	-2.502619
H	-3.736304	1.420006	1.622417
N	-2.884345	1.271503	1.084363
H	-2.086789	1.190162	1.715560
C	-2.677637	2.274336	0.096776
C	-2.258008	4.100106	-1.969110
C	-3.766944	2.912341	-0.498753
C	-1.378596	2.561707	-0.328252
C	-1.173473	3.472419	-1.358748
C	-3.550826	3.820610	-1.531397
H	-4.774753	2.696573	-0.153851
H	-0.534152	2.077207	0.151436
H	-0.161104	3.688224	-1.685721
H	-4.400262	4.315354	-1.991409
H	-2.095892	4.808284	-2.774543

SR epoxide:Catalyst:Aniline, Transition State 16; Energy = -2737.282778; 6-31G(d) basis set.

C	-1.658251	3.327975	0.912649
C	-0.511576	4.676743	-0.910786
C	-2.637541	5.585696	0.167382
C	-1.568361	5.793130	-0.925321
C	-2.085625	4.756688	1.331481
C	-1.153769	3.331729	-0.546985
H	0.274206	4.900547	-0.186230
H	-2.996322	6.551807	0.535517
H	-2.052478	5.837066	-1.907136
H	-2.815407	4.704175	2.147193
H	-2.021527	3.202196	-1.207683
H	-0.807291	3.036956	1.533576
H	-0.027036	4.588895	-1.888157
H	-3.511139	5.082789	-0.261392
H	-1.065456	6.754563	-0.782167
H	-1.209261	5.268773	1.745364
N	-2.679373	2.276305	1.134973
N	-0.308660	2.176845	-0.864355
H	-0.646854	1.604039	-1.630670
C	-2.781548	1.959809	2.560019
H	-3.123765	2.813427	3.165786
H	-1.809743	1.630647	2.938494
H	-3.502530	1.147774	2.703283
C	-4.006569	2.609710	0.625257
H	-3.970614	2.834552	-0.444256
H	-4.467495	3.464441	1.145593
H	-4.666514	1.746854	0.767062
C	0.946404	1.912258	-0.436929
S	1.734266	2.758448	0.792832
N	1.499494	0.831930	-1.072059
H	0.890059	0.305073	-1.697194
C	2.699162	0.170756	-0.730937
C	5.022529	-1.240452	-0.060047
C	3.906945	0.848111	-0.586644
C	2.655206	-1.217157	-0.567855
C	3.810531	-1.905702	-0.229200
C	5.054643	0.134047	-0.247737
H	3.948398	1.920905	-0.728800
H	1.710376	-1.740264	-0.675835
H	5.920200	-1.784184	0.214288
C	6.351220	0.885307	-0.138114
C	3.763413	-3.382863	0.035167
F	7.303025	0.159182	0.464256
F	4.014593	-3.651546	1.330540
F	2.572543	-3.916440	-0.256337
F	4.691803	-4.042261	-0.674528
F	6.821797	1.230035	-1.347797
F	6.205638	2.021583	0.557111

N	-1.256188	-0.968004	-2.044229
O	-0.824821	-0.032209	-2.716387
O	-0.534959	-1.765178	-1.488931
C	-2.863810	-1.212897	-1.996399
C	-3.157226	-1.948030	-0.759549
H	-2.405211	-2.692628	-0.529959
C	-4.553912	-2.223262	-0.334971
C	-7.143491	-2.833319	0.523721
C	-5.475366	-1.201138	-0.085317
C	-4.937827	-3.552154	-0.136619
C	-6.228388	-3.856142	0.284746
C	-6.764471	-1.504987	0.340655
H	-5.180592	-0.163899	-0.216308
H	-4.223680	-4.345856	-0.335926
H	-6.519068	-4.891973	0.426301
H	-7.471682	-0.704289	0.531674
H	-8.149438	-3.069827	0.855306
O	-3.174301	-2.317281	-2.633948
C	-3.496876	0.104706	-2.376596
H	-3.185024	0.382279	-3.384351
H	-4.579369	-0.029872	-2.369432
H	-3.215949	0.903180	-1.679151
H	-2.551593	0.178425	0.715401
N	-2.565064	-0.838768	0.896916
H	-3.338744	-1.041284	1.529416
C	-1.313624	-1.265939	1.444406
C	1.158927	-2.127915	2.397208
C	-1.141286	-2.599323	1.817568
C	-0.258241	-0.362542	1.556858
C	0.973050	-0.793308	2.040847
C	0.097887	-3.025182	2.287494
H	-1.971175	-3.297536	1.736363
H	-0.410305	0.676482	1.277036
H	1.785401	-0.075941	2.122531
H	0.234657	-4.065382	2.565540
H	2.127355	-2.469992	2.747099

SR epoxide:Catalyst:Aniline, Transition State 17; Energy = -2737.281735; 6-31G(d) basis set.

C	-1.962076	3.960188	0.241245
C	-2.987494	2.041208	-1.087952
C	-3.969876	4.339709	-1.283949
C	-4.276722	2.842035	-1.275591
C	-3.257060	4.753740	0.004091
C	-2.293076	2.445874	0.220055
H	-2.316237	2.224613	-1.930904
H	-3.329646	4.569648	-2.145982
H	-4.977252	2.619408	-0.457328
H	-3.940452	4.601147	0.851141
H	-3.010951	2.262091	1.032625
H	-1.288190	4.158777	-0.600192
H	-3.211178	0.967355	-1.071730
H	-4.890571	4.919728	-1.405700
H	-4.768153	2.538661	-2.205817
H	-3.000886	5.817055	-0.009827
N	-1.286681	4.443471	1.441446
N	-1.149213	1.595353	0.589023
H	-1.180418	1.251211	1.545706
C	-1.857314	4.027448	2.705355
H	-1.449962	4.652691	3.506546
H	-1.633317	2.975874	2.969763
H	-2.943036	4.154476	2.704478
C	0.162082	4.346074	1.458030
H	0.561533	4.581445	0.467828
H	0.541994	3.352933	1.756523
H	0.562030	5.074875	2.172497
C	0.046925	1.476001	-0.033299
S	0.357104	2.020977	-1.598609
N	0.968859	0.809545	0.727503
H	0.608878	0.305354	1.540322
C	2.319649	0.541269	0.429860
C	5.017639	-0.073730	-0.006053
C	3.169939	1.495313	-0.132344
C	2.823202	-0.707627	0.799076
C	4.164109	-1.001919	0.578499

C	4.503880	1.171640	-0.352182
H	2.794706	2.479410	-0.383394
H	2.157963	-1.444563	1.243386
H	6.062993	-0.308082	-0.172175
C	5.396773	2.187579	-1.008822
C	4.672064	-2.378366	0.902753
F	5.074441	3.437187	-0.646854
F	4.037508	-2.910640	1.953226
F	4.493830	-3.222986	-0.131211
F	5.983959	-2.373137	1.174313
F	6.685083	1.992514	-0.693616
F	5.306628	2.131867	-2.345958
N	-0.880425	-1.755208	1.904322
O	-0.747189	-0.668591	2.459272
O	0.049771	-2.444875	1.546481
C	-2.419888	-2.233182	1.621959
C	-2.876467	-1.376634	0.481659
H	-2.574429	-0.348173	0.639108
C	-4.234998	-1.579010	-0.093322
C	-6.796947	-1.852605	-1.181393
C	-4.603341	-2.758633	-0.746652
C	-5.164871	-0.540623	0.012433
C	-6.439063	-0.675141	-0.527700
C	-5.878698	-2.894764	-1.287241
H	-3.892508	-3.575204	-0.834030
H	-4.887342	0.365256	0.544641
H	-7.152322	0.137561	-0.434681
H	-6.153825	-3.815146	-1.791895
H	-7.790004	-1.958990	-1.605891
O	-3.251157	-1.606293	2.394539
C	-2.389897	-3.745919	1.620025
H	-3.394161	-4.098796	1.377118
H	-1.659041	-4.157358	0.923930
H	-2.152597	-4.078349	2.634416
H	-1.501433	-0.467570	-1.384160
N	-1.804726	-1.437473	-1.248670
H	-2.539053	-1.624953	-1.932740
C	-0.691334	-2.330967	-1.419256
C	1.474403	-4.069243	-1.625676
C	0.603777	-1.821533	-1.461517
C	-0.910986	-3.703652	-1.520785
C	0.173852	-4.569203	-1.618420
C	1.682173	-2.694361	-1.564383
H	0.766400	-0.746492	-1.440108
H	-1.923652	-4.096051	-1.525997
H	-0.001375	-5.637941	-1.688706
H	2.689551	-2.293683	-1.598359
H	2.320979	-4.744656	-1.690498

SR epoxide:Catalyst:Aniline, Transition State 18; Energy = -2737.278907; 6-31G(d) basis set.

C	-5.649599	-0.476201	0.538827
C	-5.427165	0.086624	-1.916518
C	-7.375059	-1.375452	-1.154219
C	-6.700533	-0.667741	-2.346587
C	-7.145494	-0.604822	0.149950
C	-4.779402	-0.639778	-0.732723
H	-5.668381	1.108495	-1.614488
H	-8.448120	-1.486647	-1.339183
H	-6.458165	-1.406846	-3.118124
H	-7.677226	-1.069931	0.986044
H	-4.740659	-1.705269	-0.990599
H	-5.479666	0.541880	0.903825
H	-4.713776	0.160559	-2.743153
H	-6.976825	-2.392558	-1.058023
H	-7.397961	0.043099	-2.801480
H	-7.565855	0.400997	0.034060
N	-5.311054	-1.357353	1.657212
N	-3.374830	-0.304113	-0.489542
H	-2.737922	-1.097679	-0.487352
C	-5.404738	-2.777483	1.388904
H	-4.616000	-3.155380	0.710674
H	-6.378947	-3.023013	0.957582
H	-5.310626	-3.325126	2.332547
C	-4.081603	-1.039539	2.360243

H	-3.975312	0.046125	2.452934
H	-3.170685	-1.435940	1.874283
H	-4.122036	-1.470243	3.367717
C	-2.842568	0.869062	-0.107088
S	-3.599765	2.366957	-0.175358
N	-1.572609	0.688944	0.405217
H	-1.364360	-0.240721	0.767754
C	-0.544736	1.618875	0.576421
C	1.765221	3.208107	0.811094
C	-0.334689	2.692038	-0.299372
C	0.389637	1.371726	1.586251
C	1.539554	2.151761	1.680628
C	0.807064	3.468258	-0.165588
H	-1.038766	2.882310	-1.099880
H	0.221499	0.554748	2.284757
H	2.675782	3.792247	0.867651
C	1.034283	4.591354	-1.139906
C	2.543603	1.830625	2.750108
F	0.426574	5.720813	-0.753957
F	2.154457	2.266189	3.954867
F	2.722136	0.496235	2.867833
F	3.741771	2.367037	2.495896
F	2.339168	4.871556	-1.277009
F	0.560728	4.287854	-2.359366
N	-0.376671	-2.590823	0.230784
O	-1.214225	-2.537767	-0.639168
O	-0.393553	-1.880751	1.239113
C	0.886181	-3.605593	0.029806
C	1.929613	-2.799486	-0.635312
H	1.533366	-2.170664	-1.425209
C	3.329107	-3.253414	-0.796280
C	5.996755	-3.985582	-1.181294
C	3.923172	-3.119499	-2.053209
C	4.089436	-3.735498	0.275401
C	5.415912	-4.103212	0.080896
C	5.250316	-3.490572	-2.247023
H	3.336057	-2.732389	-2.880952
H	3.652675	-3.809653	1.267039
H	5.998850	-4.477577	0.916158
H	5.700497	-3.389454	-3.229029
H	7.032609	-4.273304	-1.330086
O	0.815667	-4.267608	-1.087265
C	1.010638	-4.333739	1.352261
H	0.083674	-4.883876	1.535732
H	1.819525	-5.059441	1.260082
H	1.198465	-3.657157	2.187884
H	2.997800	-1.333777	1.223165
N	2.348095	-1.097689	0.474998
H	1.452029	-0.858701	0.902545
C	2.848373	-0.046874	-0.345522
C	3.783901	2.008776	-1.975456
C	4.151283	0.423683	-0.188273
C	2.020925	0.487174	-1.335098
C	2.489354	1.519421	-2.140647
C	4.613571	1.451803	-1.004813
H	4.788683	0.002154	0.584692
H	1.001196	0.123254	-1.445303
H	1.830500	1.958589	-2.883401
H	5.623490	1.825735	-0.870700
H	4.139835	2.824112	-2.596126

SR epoxide:Catalyst:Aniline, Transition State 19; Energy = -2737.301937; 6-31G(d) basis set.

C	-4.767115	-1.161353	-0.167807
C	-4.649439	0.531730	1.671011
C	-6.614818	-1.062235	1.536888
C	-6.139872	0.330431	1.960413
C	-6.271992	-1.344962	0.070087
C	-4.369141	0.286457	0.184355
H	-4.049460	-0.176032	2.260507
H	-7.692947	-1.163585	1.699836
H	-6.712780	1.090668	1.412377
H	-6.833119	-0.657910	-0.577438
H	-4.965060	1.004476	-0.398580
H	-4.232374	-1.806288	0.547476

H	-4.332951	1.542015	1.939944
H	-6.125806	-1.816798	2.168304
H	-6.339227	0.493090	3.024576
H	-6.571781	-2.363395	-0.203067
N	-4.249382	-1.544287	-1.479652
N	-2.971247	0.436295	-0.184380
H	-2.592061	-0.413738	-0.607909
C	-4.212448	-2.980126	-1.686155
H	-5.211160	-3.436381	-1.799057
H	-3.703760	-3.456424	-0.842433
H	-3.641931	-3.194085	-2.596112
C	-4.872405	-0.859184	-2.600353
H	-4.829069	0.224031	-2.453727
H	-5.924647	-1.150105	-2.758175
H	-4.315882	-1.095414	-3.512098
C	-2.315494	1.591902	-0.383726
S	-2.918466	3.096849	0.066612
N	-1.115480	1.380316	-1.027729
H	-0.998042	0.423253	-1.350689
C	0.105610	2.050960	-0.930837
C	2.693761	3.130567	-0.674944
C	1.241145	1.266190	-1.193904
C	0.273350	3.394049	-0.587028
C	1.564008	3.903774	-0.454659
C	2.507579	1.803585	-1.057603
H	1.121431	0.231092	-1.506988
H	-0.588172	4.023872	-0.410606
H	3.689226	3.546744	-0.565490
C	3.711163	0.928996	-1.249269
C	1.718255	5.316236	0.033133
F	3.399849	-0.237014	-1.838030
F	0.772902	6.125169	-0.458965
F	1.622104	5.376567	1.375594
F	2.910186	5.834678	-0.293551
F	4.651420	1.524394	-1.992694
F	4.289967	0.622176	-0.070957
N	-0.703072	-2.274760	-0.864790
O	-0.830338	-1.461257	-1.759028
O	-1.462855	-2.362935	0.090537
C	0.568306	-3.267501	-0.939032
C	1.612832	-2.678847	-0.073484
H	1.756591	-1.615537	-0.235840
C	2.806530	-3.467610	0.324261
C	5.091346	-4.876370	1.095929
C	4.075729	-2.973717	0.012903
C	2.689482	-4.665497	1.038876
C	3.827776	-5.367018	1.421249
C	5.213195	-3.679621	0.394168
H	4.163867	-2.044289	-0.539633
H	1.706996	-5.043776	1.309369
H	3.728550	-6.294786	1.975347
H	6.195246	-3.292915	0.142205
H	5.979186	-5.424733	1.394178
O	1.357000	-3.006956	-1.942725
C	-0.019275	-4.657278	-0.783177
H	0.799061	-5.377232	-0.823422
H	-0.584560	-4.776955	0.143473
H	-0.679456	-4.845233	-1.634928
H	1.471060	-2.749382	2.456643
N	0.879066	-2.246173	1.798070
H	-0.070744	-2.615720	1.830227
C	0.912394	-0.832500	2.004475
C	1.036061	1.930603	2.317531
C	2.152909	-0.202669	2.119613
C	-0.265425	-0.084598	2.009932
C	-0.197179	1.295436	2.180215
C	2.208413	1.178931	2.277885
H	3.064640	-0.794482	2.079406
H	-1.227135	-0.575908	1.884944
H	-1.114974	1.877895	2.183687
H	3.174397	1.667780	2.356341
H	1.083381	3.009760	2.422402

SR epoxide:Catalyst:Aniline, Transition State 20; Energy = -2737.298633; 6-31G(d) basis set.

C	2.796259	-2.820616	-0.125960
C	1.315401	-4.035092	1.536993
C	3.586471	-4.953063	1.020430
C	2.152218	-5.305300	1.406767
C	3.623695	-4.114044	-0.259531
C	1.354800	-3.202329	0.248309
H	1.690627	-3.422881	2.369204
H	4.051505	-4.383237	1.836744
H	1.712597	-5.950206	0.634442
H	3.233476	-4.707973	-1.097507
H	0.928695	-3.806817	-0.556524
H	3.224329	-2.238911	0.708846
H	0.268316	-4.273714	1.751782
H	4.186146	-5.858814	0.884744
H	2.130412	-5.869066	2.344705
H	4.662418	-3.867266	-0.496777
N	2.857072	-1.929789	-1.307451
N	0.502360	-2.028053	0.384173
H	0.851415	-1.304549	1.009453
C	2.069098	-2.386907	-2.453436
H	2.162197	-1.643359	-3.251887
H	1.010890	-2.465532	-2.190752
H	2.410564	-3.355410	-2.850964
C	4.236378	-1.673099	-1.721262
H	4.834951	-1.369739	-0.855470
H	4.248155	-0.854566	-2.449634
H	4.716123	-2.540301	-2.197031
C	-0.832522	-2.027206	0.125104
S	-1.572103	-3.205539	-0.824205
N	-1.467158	-0.943726	0.659618
H	-0.858343	-0.257917	1.110258
C	-2.783748	-0.480956	0.502152
C	-5.336642	0.667120	0.258159
C	-3.900467	-1.296142	0.311707
C	-2.953792	0.906862	0.604390
C	-4.215561	1.464127	0.474326
C	-5.157472	-0.707325	0.187338
H	-3.794670	-2.371054	0.267733
H	-2.087405	1.543673	0.770136
H	-6.322927	1.107097	0.163430
C	-6.339324	-1.599493	-0.072596
C	-4.361270	2.958795	0.484168
F	-7.492306	-1.017044	0.287439
F	-3.380385	3.556138	1.170243
F	-4.328526	3.460247	-0.765044
F	-5.529402	3.340019	1.020244
F	-6.445695	-1.909225	-1.373944
F	-6.243710	-2.756966	0.596449
N	0.878420	1.810082	1.416781
O	0.665371	0.641179	1.730341
O	0.009208	2.591907	1.112247
C	2.430361	2.274964	1.474066
C	3.202509	1.279887	0.691197
H	2.885298	0.266826	0.904460
C	4.649224	1.505255	0.423265
C	7.380634	1.852801	-0.061878
C	5.097147	2.565022	-0.370900
C	5.582177	0.622682	0.973329
C	6.941520	0.795149	0.732064
C	6.456839	2.738965	-0.611447
H	4.378691	3.255945	-0.806238
H	5.234063	-0.184556	1.611759
H	7.658268	0.107303	1.168904
H	6.793667	3.565625	-1.228522
H	8.440808	1.987354	-0.250796
O	3.032044	1.783095	2.528964
C	2.444446	3.768111	1.246026
H	1.954819	4.062191	0.316915
H	1.932641	4.247482	2.084124
H	3.486575	4.091929	1.249517
H	2.583705	0.001344	-1.265451
N	2.587047	1.038354	-1.244299
H	3.348682	1.397534	-1.817375
C	1.318460	1.562378	-1.626448
C	-1.209404	2.584747	-2.203394

C	0.211218	0.714295	-1.636921
C	1.171342	2.913562	-1.941674
C	-0.094242	3.420762	-2.219256
C	-1.046852	1.226870	-1.934480
H	0.350865	-0.342631	-1.426110
H	2.042513	3.564013	-1.964854
H	-0.208202	4.475531	-2.448036
H	-1.901132	0.556968	-1.959523
H	-2.197438	2.985583	-2.402730

SR epoxide:Catalyst:Aniline, Transition State 21; Energy = -2737.300818; 6-31G(d) basis set.

C	-3.426332	-2.366845	0.756481
C	-2.313189	-4.511402	0.016821
C	-4.722495	-4.545150	0.731532
C	-3.418431	-5.338980	0.671953
C	-4.510475	-3.210627	1.450194
C	-2.111494	-3.168084	0.730928
H	-2.570992	-4.313906	-1.033867
H	-5.079487	-4.353584	-0.289354
H	-3.110725	-5.609771	1.690692
H	-4.214345	-3.405205	2.489770
H	-1.775569	-3.359617	1.753329
H	-3.733414	-2.213756	-0.288864
H	-1.361230	-5.052687	0.024407
H	-5.501750	-5.123103	1.238681
H	-3.559099	-6.274792	0.121776
H	-5.451315	-2.651240	1.482566
N	-3.249397	-1.011795	1.313607
N	-1.043318	-2.427084	0.073358
H	-1.185644	-2.260723	-0.922690
C	-2.800066	-0.983974	2.706707
H	-2.630832	0.057415	2.998050
H	-1.851818	-1.514944	2.815456
H	-3.541390	-1.409910	3.400480
C	-4.460061	-0.207994	1.171243
H	-4.877046	-0.333148	0.166312
H	-4.212504	0.850599	1.317897
H	-5.240970	-0.470091	1.901313
C	0.181920	-2.189583	0.583958
S	0.639430	-2.528713	2.164924
N	1.034338	-1.624886	-0.341200
H	0.769495	-1.734986	-1.316001
C	2.344164	-1.151122	-0.130430
C	4.916105	-0.058133	0.095650
C	2.663156	-0.329144	0.958840
C	3.308369	-1.416107	-1.097718
C	4.585354	-0.868392	-0.977695
C	3.937242	0.204762	1.054870
H	1.910883	-0.092409	1.699854
H	3.065933	-2.046262	-1.948725
H	5.907681	0.373023	0.182220
C	4.282693	1.144428	2.175814
C	5.613079	-1.213674	-2.018228
F	5.350744	0.718018	2.864724
F	6.651145	-0.368320	-1.996492
F	6.101009	-2.449745	-1.837657
F	5.087162	-1.181870	-3.252475
F	4.599696	2.363031	1.697143
F	3.275746	1.305071	3.038584
N	-1.863143	-0.654024	-2.649459
O	-2.776040	-1.415716	-2.421965
O	-0.679697	-0.988651	-2.595378
C	-2.218902	0.923220	-2.885592
C	-2.697905	1.368946	-1.558287
H	-3.397068	0.662593	-1.130347
C	-2.843355	2.782323	-1.178589
C	-3.136039	5.402623	-0.254153
C	-1.805004	3.707660	-1.337843
C	-4.026094	3.183215	-0.547782
C	-4.175642	4.489039	-0.093226
C	-1.951966	5.010327	-0.875649
H	-0.865893	3.399968	-1.784611
H	-4.835776	2.467522	-0.433490
H	-5.100618	4.792504	0.386321

H	-1.135684	5.716123	-0.989437
H	-3.246882	6.419877	0.108103
O	-3.431409	1.108621	-3.318953
C	-1.043399	1.507776	-3.640211
H	-0.105347	1.442669	-3.085937
H	-0.932602	0.977908	-4.589659
H	-1.280862	2.550479	-3.855326
H	-0.608854	0.181014	-0.593000
N	-1.287739	0.744556	-0.080078
H	-1.895508	0.102622	0.468565
C	-0.635383	1.738418	0.684469
C	0.622638	3.794100	2.099876
C	-1.317348	2.406129	1.704716
C	0.669464	2.120006	0.361875
C	1.298982	3.134454	1.076104
C	-0.687710	3.428527	2.405151
H	-2.345507	2.135149	1.929754
H	1.192583	1.607107	-0.442943
H	2.324838	3.398286	0.838587
H	-1.225641	3.942280	3.195683
H	1.113286	4.584873	2.657321

SR epoxide:Catalyst:Aniline, Transition State 22; Energy = -2737.278510; 6-31G(d) basis set.

C	-2.558828	2.881390	-0.150267
C	-1.183238	3.802313	1.738932
C	-2.712851	5.368390	0.506286
C	-2.357767	4.787874	1.874909
C	-3.219885	4.256564	-0.431543
C	-1.130452	3.149472	0.342323
H	-1.263115	3.009199	2.492778
H	-3.472868	6.149938	0.596450
H	-2.104311	5.580981	2.583931
H	-3.030974	4.542640	-1.472946
H	-0.651511	3.839941	-0.356965
H	-3.119049	2.398698	0.667008
H	-0.224944	4.305046	1.905594
H	-1.822833	5.846378	0.080080
H	-3.237196	4.272963	2.282001
H	-4.304651	4.152112	-0.323754
N	-2.624978	1.929152	-1.277298
N	-0.286539	1.965811	0.359976
H	-0.678306	1.114081	0.755764
C	-3.997018	1.821123	-1.774533
H	-4.068680	0.974600	-2.466943
H	-4.330786	2.721961	-2.310177
H	-4.682791	1.651496	-0.936550
C	-1.727396	2.255698	-2.387037
H	-0.688276	2.268545	-2.052887
H	-1.961372	3.224143	-2.855684
H	-1.829905	1.483895	-3.156943
C	1.051748	1.991802	0.139079
S	1.859536	3.356002	-0.426262
N	1.643028	0.794500	0.428216
H	1.036087	0.112946	0.880212
C	2.966538	0.353984	0.289861
C	5.544934	-0.753454	0.109771
C	3.880954	0.854086	-0.642505
C	3.345443	-0.713671	1.113184
C	4.618703	-1.256775	1.015472
C	5.154551	0.299512	-0.708801
H	3.601335	1.659714	-1.306025
H	2.641100	-1.110552	1.839781
H	6.541733	-1.173937	0.041072
C	6.153569	0.888635	-1.666536
C	4.979676	-2.440528	1.868675
F	5.559843	1.425752	-2.740484
F	4.339771	-2.417298	3.046074
F	4.655023	-3.596081	1.269195
F	6.295115	-2.485006	2.120117
F	6.875495	1.860139	-1.088320
F	7.022329	-0.035644	-2.102985
N	-0.975341	-1.911013	1.323222
O	-1.384487	-2.671490	2.158228
O	-0.506886	-0.797035	1.592895

C	-1.121312	-2.364296	-0.225074
C	-2.574616	-2.439955	-0.471799
H	-3.104481	-2.951830	0.324426
C	-3.078191	-2.573482	-1.863901
C	-4.075713	-2.827363	-4.459628
C	-3.778862	-3.721632	-2.236970
C	-2.885280	-1.549923	-2.797880
C	-3.383040	-1.675249	-4.090720
C	-4.270900	-3.849225	-3.532835
H	-3.913392	-4.520081	-1.513564
H	-2.351681	-0.648335	-2.502765
H	-3.228361	-0.875076	-4.808107
H	-4.806507	-4.748473	-3.819227
H	-4.462632	-2.927895	-5.468583
O	-1.091280	-3.663161	-0.365483
C	-0.180724	-1.500763	-1.039686
H	0.847063	-1.664424	-0.701808
H	-0.250153	-1.837897	-2.075086
H	-0.416271	-0.432617	-0.990619
H	-2.889837	0.107528	-0.238858
N	-3.493253	-0.692411	0.011860
H	-4.263609	-0.699423	-0.655902
C	-3.977516	-0.675604	1.354347
C	-4.899102	-0.784347	3.984014
C	-3.336300	0.063524	2.347782
C	-5.076607	-1.474647	1.677359
C	-5.535791	-1.522756	2.988603
C	-3.799646	0.005170	3.658511
H	-2.469946	0.670445	2.103745
H	-5.567993	-2.053756	0.898844
H	-6.392121	-2.143161	3.232118
H	-3.293397	0.580603	4.426628
H	-5.255799	-0.827148	5.007467

SR epoxide:Catalyst:Aniline, Transition State 23; Energy = -2737.304890; 6-31G(d) basis set.

C	-4.922401	0.882556	-0.542683
C	-5.524467	-1.334362	-1.553615
C	-7.327088	0.381551	-1.104792
C	-6.995732	-1.110361	-1.195493
C	-6.386552	1.105562	-0.134353
C	-4.627640	-0.626647	-0.533604
H	-5.310117	-0.930625	-2.552298
H	-7.227098	0.833822	-2.100977
H	-7.203239	-1.587943	-0.228329
H	-6.547296	0.725606	0.883368
H	-4.845041	-1.048394	0.457128
H	-4.816541	1.221299	-1.586182
H	-5.280733	-2.399715	-1.564802
H	-8.367776	0.524329	-0.795620
H	-7.639781	-1.599280	-1.933387
H	-6.612077	2.177577	-0.119287
N	-3.901564	1.621333	0.206593
N	-3.207249	-0.804514	-0.793116
H	-2.721728	0.052439	-1.041341
C	-3.990266	3.060288	0.013437
H	-4.868901	3.514457	0.501186
H	-4.036357	3.283899	-1.056788
H	-3.093435	3.532595	0.422863
C	-3.846897	1.286275	1.621228
H	-3.667476	0.212950	1.747940
H	-4.762256	1.558378	2.173153
H	-3.006297	1.820105	2.073655
C	-2.482948	-1.881382	-0.460945
S	-3.140782	-3.313570	0.150129
N	-1.132622	-1.781537	-0.649135
H	-0.612569	-2.651586	-0.584637
C	-0.397250	-0.601442	-0.893372
C	1.149558	1.691625	-1.319986
C	0.566975	-0.585746	-1.903409
C	-0.583008	0.529992	-0.087552
C	0.180661	1.667277	-0.319872
C	1.338460	0.554578	-2.096575
H	0.747492	-1.474042	-2.497113
H	-1.303171	0.508756	0.725338

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H          1.762058        2.575054       -1.476388
C          2.389203        0.600403       -3.173147
C         -0.042707        2.908889        0.495132
F          3.591649        0.912314       -2.675593
F          1.114946        3.421901        0.948009
F         -0.628788        3.874114       -0.230641
F         -0.823693        2.688634        1.562660
F          2.493435       -0.548193       -3.840140
F          2.091295        1.560228       -4.072545
N          2.298592       -3.229231        0.116196
O          2.319961       -3.855003        1.168457
O          1.383050       -3.270580       -0.677957
C          3.510605       -2.190088       -0.195473
C          3.055485       -0.905618        0.386236
H          1.992750       -0.728197        0.244749
C          3.923222        0.300374        0.430648
C          5.443014        2.647128        0.578356
C          5.163323        0.378593       -0.211666
C          3.436795        1.424898        1.105797
C          4.190682        2.590180        1.185452
C          5.917864        1.544067       -0.128245
H          5.495401       -0.439937       -0.838338
H          2.445530        1.393361        1.548121
H          3.789360        3.454571        1.704815
H          6.874383        1.596346       -0.638239
H          6.035049        3.555212        0.632754
O          3.395133       -1.653593       -1.377715
C          4.775716       -2.918194        0.222198
H          4.669605       -3.412652        1.188112
H          5.000923       -3.667561       -0.541429
H          5.606110       -2.213896        0.272019
H          2.850434       -2.227466        2.456420
N          2.681175       -1.222206        2.383909
H          3.387197       -0.716679        2.916673
C          1.349185       -0.888360        2.782612
C         -1.259860       -0.211830        3.496559
C          1.101530        0.295255        3.482015
C          0.289613       -1.723638        2.419197
C         -1.010757       -1.384125        2.784932
C         -0.202109        0.630477        3.832983
H          1.929316        0.938748        3.769556
H          0.476678       -2.649652        1.881400
H         -1.825934       -2.046318        2.503336
H         -0.386609        1.547733        4.382959
H         -2.271666        0.040300        3.796387

SR epoxide:Catalyst:Aniline, Transition State 24; Energy = -2737.290118; 6-31G(d)
basis set.
C          3.515811       -2.381098       -0.732698
C          2.170144       -4.517038       -1.103242
C          4.566925       -4.632887       -0.353453
C          3.112278       -5.012208       -0.007146
C          4.635690       -3.331689       -1.179127
C          2.166868       -2.972939       -1.179183
H          1.142744       -4.860537       -0.951134
H          5.038104       -5.442355       -0.920187
H          3.020914       -6.094420        0.121943
H          4.520875       -3.553049       -2.247468
H          1.957821       -2.683224       -2.208914
H          3.526968       -2.356222        0.367008
H          2.496369       -4.920197       -2.069135
H          5.145703       -4.513581        0.568400
H          2.821305       -4.562694        0.951396
H          5.617148       -2.862859       -1.058676
N          3.649654       -0.970169       -1.142164
N          1.098538       -2.391240       -0.376588
H          1.259839       -2.325408        0.628542
C          4.788508       -0.330748       -0.486956
H          5.759095       -0.657294       -0.891022
H          4.768627       -0.550215        0.585183
H          4.721115        0.754855       -0.629259
C          3.737074       -0.766940       -2.588069
H          2.830252       -1.114020       -3.087493
H          4.610970       -1.267618       -3.033250
H          3.829876        0.305031       -2.784632
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C	-0.113241	-2.048024	-0.853431
S	-0.552455	-2.182827	-2.467959
N	-0.947606	-1.555536	0.133211
H	-0.650188	-1.734533	1.088324
C	-2.294018	-1.156768	0.019133
C	-4.955538	-0.262047	-0.005745
C	-3.164414	-1.496622	1.053276
C	-2.756704	-0.358613	-1.035154
C	-4.073646	0.075297	-1.030743
C	-4.482628	-1.047086	1.034401
H	-2.819320	-2.124470	1.870122
H	-2.087390	-0.071785	-1.834706
H	-5.984728	0.079163	-0.022517
C	-5.376199	-1.394463	2.191706
C	-4.550135	1.007730	-2.108991
F	-5.128147	-0.609615	3.252684
F	-3.746770	1.005637	-3.176417
F	-5.786920	0.697876	-2.520089
F	-4.602624	2.276732	-1.656672
F	-6.670798	-1.249919	1.885500
F	-5.189081	-2.659427	2.595098
N	2.035657	-0.675154	2.566493
O	0.985627	-1.279412	2.335851
O	3.125874	-1.188523	2.486536
C	1.971761	0.934723	2.889856
C	2.553800	1.548743	1.679091
H	3.439206	1.020423	1.352123
C	2.475718	2.975291	1.340609
C	2.387283	5.619130	0.440698
C	1.280233	3.701399	1.398826
C	3.621860	3.587289	0.820966
C	3.582306	4.905726	0.381476
C	1.237949	5.015151	0.947527
H	0.371747	3.229325	1.756026
H	4.549800	3.023088	0.773925
H	4.479425	5.372955	-0.011535
H	0.302585	5.564195	0.979573
H	2.349273	6.644650	0.086921
O	3.021035	1.349594	3.536078
C	0.582343	1.188666	3.436298
H	0.534245	2.237085	3.733324
H	-0.207449	0.967623	2.714713
H	0.430007	0.573054	4.326257
H	2.190727	0.141133	-0.473654
N	1.484037	0.742448	-0.002747
H	0.784670	0.132737	0.422209
C	0.869453	1.681498	-0.861879
C	-0.323871	3.652654	-2.441314
C	1.638811	2.406436	-1.774410
C	-0.492461	1.959555	-0.731825
C	-1.089745	2.931252	-1.528453
C	1.040858	3.388591	-2.555411
H	2.705330	2.209930	-1.849498
H	-1.081367	1.407835	-0.002339
H	-2.156170	3.115282	-1.437678
H	1.645681	3.951084	-3.259852
H	-0.786168	4.413218	-3.061587

SR epoxide:Catalyst:Aniline, Transition State 25; Energy = -2737.282405; 6-31G(d) basis set.

C	2.115329	3.448274	-0.762461
C	2.318460	1.942192	1.285437
C	4.233335	3.469039	0.699893
C	3.193008	3.111173	1.763058
C	3.551257	3.998193	-0.579440
C	2.071765	2.001194	-0.238959
H	1.360028	1.945397	1.807305
H	4.944431	4.208802	1.080897
H	3.674648	2.852159	2.711536
H	4.160670	3.741225	-1.453707
H	2.875739	1.448556	-0.742475
H	1.438748	4.037282	-0.136138
H	2.802288	0.987991	1.529598
H	4.823154	2.571623	0.466698
H	2.562988	3.987350	1.960404

H	3.499951	5.091974	-0.543416
N	1.571541	3.542270	-2.113412
N	0.874164	1.261668	-0.632258
H	1.053712	0.560548	-1.351404
C	1.359138	4.916810	-2.524835
H	2.296526	5.476118	-2.698637
H	0.779825	5.440751	-1.758202
H	0.785089	4.931373	-3.456999
C	2.287440	2.794833	-3.132469
H	2.397214	1.743472	-2.847534
H	3.291273	3.195170	-3.360254
H	1.705021	2.825820	-4.058884
C	-0.406679	1.573156	-0.348316
S	-0.891703	2.807914	0.686434
N	-1.290844	0.738925	-0.997264
H	-0.857414	0.062910	-1.618329
C	-2.592545	0.359243	-0.638614
C	-5.147740	-0.620338	0.019049
C	-2.920014	-0.987650	-0.849050
C	-3.565824	1.224772	-0.129163
C	-4.819431	0.717492	0.201827
C	-4.182066	-1.462023	-0.521441
H	-2.173792	-1.665578	-1.259399
H	-3.343455	2.273943	0.004473
H	-6.128761	-0.996104	0.285009
C	-4.501422	-2.905288	-0.789208
C	-5.825167	1.649412	0.819362
F	-4.877108	-3.103329	-2.061941
F	-5.748209	2.880396	0.297024
F	-7.081225	1.212469	0.646105
F	-5.632241	1.773159	2.142057
F	-3.436401	-3.692589	-0.571745
F	-5.498641	-3.347540	-0.010912
N	0.717413	-2.128412	-1.771444
O	0.136881	-3.049680	-1.221637
O	0.169034	-1.296038	-2.469109
C	2.288434	-2.012832	-1.621335
C	2.658478	-1.653506	-0.235857
H	2.082217	-0.830409	0.175150
C	4.068394	-1.830500	0.208176
C	6.718712	-2.115559	1.050350
C	4.846718	-0.704904	0.482522
C	4.632536	-3.102914	0.350333
C	5.950324	-3.244702	0.771724
C	6.166207	-0.846177	0.901250
H	4.419957	0.282291	0.341357
H	4.037783	-3.986518	0.131392
H	6.377196	-4.236324	0.880846
H	6.761946	0.037390	1.106808
H	7.746908	-2.226485	1.379309
O	2.741544	-0.815087	-1.937160
C	2.832732	-3.222356	-2.356705
H	2.436162	-4.159397	-1.958850
H	2.559594	-3.129927	-3.411530
H	3.920579	-3.209907	-2.279618
H	2.391632	-3.386979	1.708228
N	1.712429	-2.830315	1.193601
H	1.084276	-3.434746	0.664774
C	1.022876	-1.897222	2.020118
C	-0.216539	0.118672	3.488241
C	-0.239699	-1.436144	1.638506
C	1.672542	-1.344868	3.123429
C	1.043808	-0.343025	3.858674
C	-0.855411	-0.432045	2.378345
H	-0.741889	-1.874536	0.778709
H	2.663935	-1.695886	3.399115
H	1.549342	0.083067	4.719536
H	-1.835397	-0.070982	2.079162
H	-0.696782	0.911929	4.050899

SR epoxide:Catalyst:Aniline, Transition State 26; Energy = -2737.283496; 6-31G(d) basis set.

C	2.452610	2.983885	-0.331656
C	0.876341	3.887183	-2.075494
C	2.537766	5.465486	-1.053800

C	2.019496	4.876158	-2.363790
C	3.159968	4.359672	-0.183515
C	0.982151	3.252072	-0.672854
H	0.874263	3.082451	-2.820321
H	3.279167	6.248011	-1.240029
H	1.676550	5.662319	-3.042292
H	3.130586	4.667580	0.868027
H	0.575644	3.943106	0.069597
H	2.906776	2.451341	-1.183836
H	-0.097856	4.383495	-2.139818
H	1.706129	5.943585	-0.522406
H	2.844646	4.361225	-2.871400
H	4.216168	4.238622	-0.446132
N	2.636591	2.088934	0.829969
N	0.143049	2.064374	-0.605603
H	0.481417	1.243499	-1.101406
C	4.053428	1.999101	1.184742
H	4.190595	1.200226	1.920933
H	4.449661	2.929426	1.618486
H	4.643311	1.756486	0.293685
C	1.855135	2.479901	2.003645
H	0.785247	2.451693	1.783781
H	2.112924	3.483689	2.377084
H	2.058771	1.769358	2.811257
C	-1.177916	2.093039	-0.282809
S	-1.880574	3.371994	0.550425
N	-1.830044	0.970726	-0.708903
H	-1.273131	0.360572	-1.302540
C	-3.089123	0.424136	-0.425667
C	-5.522494	-0.927778	0.006257
C	-3.351821	-0.806627	-1.053448
C	-4.055551	0.972790	0.418277
C	-5.253150	0.285533	0.617115
C	-4.548951	-1.463477	-0.835269
H	-2.606467	-1.253811	-1.707731
H	-3.882633	1.919060	0.911313
H	-6.456909	-1.448170	0.180677
C	-4.832842	-2.754404	-1.551604
C	-6.254927	0.909391	1.549593
F	-5.607462	-2.552581	-2.630033
F	-7.386953	0.197466	1.624645
F	-5.763549	1.015663	2.793373
F	-6.582462	2.148921	1.156954
F	-3.713166	-3.351803	-1.974047
F	-5.486715	-3.617550	-0.761387
N	-0.035066	-1.952156	-0.968857
O	-0.750496	-2.829219	-1.366122
O	0.178125	-0.904127	-1.605197
C	0.618445	-2.112785	0.494321
C	2.074332	-2.280581	0.344232
H	2.355283	-2.921595	-0.485446
C	2.983055	-2.262860	1.514274
C	4.809640	-2.227136	3.629149
C	2.986016	-1.202710	2.426024
C	3.910022	-3.295677	1.662529
C	4.817655	-3.280106	2.718254
C	3.891745	-1.187126	3.481284
H	2.300661	-0.370978	2.288699
H	3.914605	-4.113703	0.948202
H	5.533009	-4.088919	2.825432
H	3.885953	-0.359317	4.184305
H	5.518192	-2.212944	4.451162
O	0.606542	-3.353663	0.896370
C	-0.057639	-1.024963	1.312555
H	-1.144114	-1.135730	1.231692
H	0.217650	-1.177011	2.356979
H	0.235400	-0.019460	0.992124
H	2.218410	-0.514214	-1.376875
N	2.899544	-0.648279	-0.630992
H	2.845367	0.156553	0.011776
C	4.190441	-0.968357	-1.125426
C	6.689504	-1.768694	-2.086055
C	5.306354	-0.938064	-0.283019
C	4.325912	-1.422549	-2.440209
C	5.571755	-1.817503	-2.915975

C	6.548780	-1.330143	-0.771265
H	5.196440	-0.622940	0.750766
H	3.453073	-1.460063	-3.087801
H	5.666583	-2.162360	-3.940686
H	7.410799	-1.299305	-0.112334
H	7.661070	-2.074673	-2.459340

SR epoxide:Catalyst:Aniline, Transition State 27; Energy = -2737.282543; 6-31G(d) basis set.

C	-3.927791	1.685276	-0.031866
C	-3.493362	3.742183	-1.490453
C	-5.370618	3.767650	0.223415
C	-4.061460	4.422714	-0.243519
C	-5.362685	2.244121	-0.012481
C	-3.275418	2.208845	-1.324416
H	-2.542666	4.206870	-1.766363
H	-6.224340	4.206295	-0.303940
H	-4.223970	5.484820	-0.452994
H	-5.836022	2.018393	-0.977639
H	-3.792375	1.718956	-2.156056
H	-3.368135	2.094576	0.814377
H	-4.178629	3.903056	-2.330731
H	-5.518452	3.979954	1.287259
H	-3.313497	4.369040	0.551818
H	-5.965182	1.740310	0.750116
N	-3.827084	0.216609	0.097812
N	-1.882799	1.799745	-1.521151
H	-1.735787	1.081189	-2.222838
C	-4.124300	-0.187694	1.470443
H	-3.485333	0.368728	2.161411
H	-3.921224	-1.257599	1.589307
H	-5.175698	-0.015710	1.752612
C	-4.714735	-0.504713	-0.811899
H	-4.519260	-0.227699	-1.851487
H	-5.780466	-0.326466	-0.599050
H	-4.535171	-1.579752	-0.715739
C	-0.785087	2.264946	-0.887954
S	-0.816137	3.139452	0.538818
N	0.371417	1.918519	-1.559496
H	0.214090	1.434718	-2.439595
C	1.658582	1.661638	-1.051059
C	4.208843	0.899239	-0.141931
C	2.259813	2.354850	0.006099
C	2.361148	0.626499	-1.678395
C	3.613961	0.248476	-1.214896
C	3.518558	1.956648	0.443724
H	1.750245	3.181845	0.478875
H	1.918122	0.091192	-2.514991
H	5.185765	0.599762	0.220663
C	4.135443	2.650975	1.627375
C	4.238823	-0.975716	-1.821867
F	3.881951	1.989277	2.768756
F	5.531655	-1.095842	-1.495176
F	3.611401	-2.083240	-1.389551
F	4.149648	-0.970903	-3.156272
F	5.469658	2.724311	1.511432
F	3.670344	3.895464	1.780136
N	0.044790	-1.652884	-2.772559
O	-0.445889	-0.519557	-2.839861
O	1.128727	-1.938015	-3.212096
C	-0.783186	-2.793103	-1.977178
C	-0.325260	-2.689504	-0.574940
H	0.747643	-2.531726	-0.499730
C	-0.964749	-3.433884	0.530630
C	-2.084438	-4.723412	2.742527
C	-0.149240	-4.105672	1.443203
C	-2.345302	-3.396247	0.745536
C	-2.903791	-4.042032	1.842927
C	-0.707036	-4.752432	2.542175
H	0.925825	-4.116430	1.288690
H	-2.980518	-2.832664	0.069321
H	-3.977632	-4.007265	2.000414
H	-0.063876	-5.272256	3.244644
H	-2.520310	-5.224449	3.601046
O	-0.179923	-3.946262	-2.010435

C	-2.213574	-2.645511	-2.456092
H	-2.804450	-3.448943	-2.014087
H	-2.632293	-1.673671	-2.187215
H	-2.240219	-2.763689	-3.542855
H	-1.640870	-0.531082	0.200786
N	-0.641563	-0.788406	0.203870
H	-0.164763	-0.189109	-0.468867
C	-0.028966	-0.740462	1.487996
C	1.228042	-0.842451	3.979580
C	1.358642	-0.616826	1.578794
C	-0.783214	-0.949705	2.642561
C	-0.152880	-0.996983	3.881373
C	1.980195	-0.655992	2.822446
H	1.951693	-0.498454	0.676356
H	-1.855145	-1.096081	2.565868
H	-0.748511	-1.157873	4.774498
H	3.056870	-0.533950	2.880875
H	1.714420	-0.872385	4.948893

SR epoxide:Catalyst:Aniline, Transition State 28; Energy = -2737.298566; 6-31G(d) basis set.

C	2.795726	2.820215	0.134144
C	1.307838	4.039659	-1.518761
C	3.581556	4.955443	-1.009969
C	2.145715	5.309211	-1.388964
C	3.624274	4.112929	0.267540
C	1.352766	3.203693	-0.232351
H	1.679116	3.429401	-2.354154
H	4.042735	4.387658	-1.829886
H	1.709788	5.952248	-0.612990
H	3.238054	4.704678	1.108908
H	0.930976	3.806603	0.575944
H	3.219581	2.240739	-0.704320
H	0.259889	4.279192	-1.728208
H	4.182160	5.860615	-0.874524
H	2.119942	5.875456	-2.325307
H	4.663962	3.865132	0.499411
N	2.861596	1.925905	1.312758
N	0.499162	2.030163	-0.366685
H	0.846046	1.306544	-0.993058
C	4.242658	1.668002	1.719973
H	4.257410	0.847535	2.446115
H	4.724504	2.533889	2.196005
H	4.837542	1.366915	0.850828
C	2.078526	2.379623	2.463436
H	1.019224	2.459143	2.205491
H	2.421771	3.346888	2.862432
H	2.174955	1.633624	3.259196
C	-0.834842	2.029855	-0.102753
S	-1.570447	3.210098	0.847281
N	-1.471049	0.945416	-0.633285
H	-0.863505	0.260761	-1.087368
C	-2.786919	0.481047	-0.475226
C	-5.335343	-0.675842	-0.217699
C	-2.954894	-0.906917	-0.587700
C	-3.903351	1.290915	-0.265035
C	-5.158455	0.697687	-0.136840
C	-4.213453	-1.468217	-0.449696
H	-2.087999	-1.540763	-0.761951
H	-3.797651	2.364731	-0.196045
H	-6.318087	-1.119832	-0.107446
C	-4.355365	-2.963162	-0.460231
C	-6.349620	1.598863	0.034142
F	-4.326040	-3.464637	0.789117
F	-6.712247	2.158483	-1.131352
F	-7.416717	0.935686	0.501692
F	-6.092238	2.603507	0.882348
F	-5.520998	-3.346993	-1.000083
F	-3.371007	-3.558171	-1.143158
N	0.872820	-1.806461	-1.415299
O	0.655836	-0.635983	-1.720204
O	0.006706	-2.591993	-1.111607
C	2.425360	-2.267767	-1.483541
C	3.200099	-1.274898	-0.700419
H	2.880326	-0.261434	-0.907751

C	4.648577	-1.499496	-0.441223
C	7.383084	-1.845774	0.027328
C	5.577544	-0.614371	-0.993963
C	5.102099	-2.561269	0.347098
C	6.463312	-2.734558	0.579396
C	6.938405	-0.786189	-0.760926
H	5.225081	0.194265	-1.628217
H	4.386897	-3.254410	0.784285
H	6.804463	-3.562801	1.191959
H	7.651972	-0.096351	-1.199829
H	8.444451	-1.979831	0.209791
O	3.019940	-1.769850	-2.539644
C	2.444005	-3.761904	-1.262368
H	1.960744	-4.061226	-0.331588
H	1.928070	-4.238644	-2.099425
H	3.486798	-4.083448	-1.273668
H	3.358425	-1.403443	1.807052
N	2.593913	-1.042404	1.239024
H	2.589684	-0.005504	1.264894
C	1.327479	-1.569275	1.624429
C	-1.197068	-2.596653	2.207126
C	0.219439	-0.722355	1.642952
C	1.182939	-2.921919	1.934523
C	-0.080999	-3.431561	2.215091
C	-1.036952	-1.237518	1.943165
H	0.357198	0.335578	1.435866
H	2.054785	-3.571647	1.951246
H	-0.192985	-4.487399	2.439858
H	-1.891848	-0.568646	1.974229
H	-2.183889	-2.999370	2.408646

SR epoxide:Catalyst:Aniline, Transition State 29; Energy = -2737.289614; 6-31G(d) basis set.

C	-2.798777	-2.846832	0.156096
C	-1.465621	-3.852153	-1.731570
C	-3.062276	-5.336617	-0.486196
C	-2.666832	-4.805293	-1.862054
C	-3.552054	-4.182813	0.404607
C	-1.385415	-3.178115	-0.345001
H	-1.521834	-3.068378	-2.496350
H	-3.844828	-6.096898	-0.567032
H	-2.426661	-5.622961	-2.547440
H	-3.444547	-4.466719	1.457798
H	-0.912741	-3.861776	0.363687
H	-3.317962	-2.300990	-0.648418
H	-0.522502	-4.385525	-1.891978
H	-2.195486	-5.827936	-0.027979
H	-3.523351	-4.274188	-2.295876
H	-4.621172	-4.018118	0.232181
N	-2.816543	-1.935776	1.318386
N	-0.515449	-2.013286	-0.419967
H	-0.855679	-1.257923	-1.011814
C	-4.186630	-1.705569	1.777781
H	-4.653056	-2.600394	2.214778
H	-4.804254	-1.360012	0.941111
H	-4.182385	-0.926635	2.548260
C	-1.975664	-2.370844	2.434580
H	-2.320359	-3.308911	2.896282
H	-1.994653	-1.592055	3.204426
H	-0.940115	-2.500550	2.109233
C	0.821730	-2.039112	-0.170629
S	1.556304	-3.257395	0.730591
N	1.462982	-0.943884	-0.672467
H	0.859207	-0.246571	-1.111777
C	2.780947	-0.488464	-0.507827
C	5.334482	0.655565	-0.246365
C	3.895620	-1.305840	-0.314650
C	2.953930	0.899931	-0.603705
C	4.215354	1.455030	-0.464581
C	5.152787	-0.718688	-0.182067
H	3.788446	-2.380719	-0.275419
H	2.089449	1.539213	-0.770899
H	6.320888	1.093788	-0.145004
C	6.332210	-1.613411	0.080502
C	4.362853	2.949595	-0.466007

F	6.237067	-2.769623	-0.590598
F	4.327743	3.443875	0.785965
F	5.532775	3.332199	-0.997115
F	3.384386	3.551930	-1.151055
F	7.487438	-1.032297	-0.274418
F	6.433367	-1.925217	1.381837
N	-0.873322	1.839512	-1.408455
O	-0.652001	0.674672	-1.732304
O	-0.009641	2.623758	-1.095339
C	-2.429018	2.295008	-1.464726
C	-3.196519	1.285801	-0.695621
H	-2.872105	0.277626	-0.920333
C	-4.644835	1.496347	-0.425847
C	-7.378637	1.812574	0.067185
C	-5.102528	2.550686	0.370257
C	-5.569059	0.602614	-0.972423
C	-6.929728	0.759655	-0.727432
C	-6.463365	2.709148	0.614360
H	-4.390751	3.248651	0.805240
H	-5.213651	-0.201025	-1.611333
H	-7.639787	0.063377	-1.161816
H	-6.807895	3.531651	1.232748
H	-8.439738	1.935130	0.259014
O	-3.025051	1.810992	-2.526378
C	-2.452264	3.785573	-1.220943
H	-1.969237	4.072303	-0.286069
H	-1.938411	4.276480	-2.051052
H	-3.496014	4.103986	-1.226913
H	-2.575466	-0.011614	1.250908
N	-2.585455	1.026033	1.238981
H	-3.352170	1.373867	1.812323
C	-1.322408	1.556944	1.629042
C	1.195264	2.597706	2.219764
C	-0.206065	0.720500	1.627492
C	-1.188804	2.905216	1.962633
C	0.071475	3.421761	2.246975
C	1.046596	1.242108	1.932314
H	-0.334181	-0.334692	1.401578
H	-2.066766	3.546094	1.994680
H	0.174454	4.474465	2.490058
H	1.907882	0.581108	1.948512
H	2.179135	3.005743	2.424817

SR epoxide:Catalyst:Aniline, Transition State 30; Energy = -2737.285307; 6-31G(d) basis set.

C	-0.883626	-2.982551	-1.325505
C	-2.859693	-3.590952	0.118648
C	-2.654704	-4.625896	-2.148349
C	-3.628657	-4.129053	-1.084527
C	-1.694229	-3.501714	-2.531364
C	-1.862049	-2.476713	-0.253226
H	-2.289211	-4.405928	0.585049
H	-2.087005	-5.480076	-1.756151
H	-4.255578	-3.332736	-1.508604
H	-2.280045	-2.673953	-2.952966
H	-2.412229	-1.613340	-0.648540
H	-0.339120	-3.829533	-0.882265
H	-3.550234	-3.209881	0.877403
H	-3.191723	-4.977387	-3.035300
H	-4.303216	-4.928996	-0.763052
H	-1.012173	-3.839567	-3.317221
N	0.154078	-1.999114	-1.691824
N	-1.130074	-2.064913	0.962999
H	-0.284626	-2.606528	1.144629
C	-0.350412	-0.895645	-2.506512
H	0.443123	-0.151933	-2.629040
H	-1.191463	-0.404902	-2.007337
H	-0.671180	-1.209668	-3.511713
C	1.258297	-2.666030	-2.384863
H	1.749218	-3.366485	-1.703845
H	1.984394	-1.912199	-2.698767
H	0.942685	-3.199955	-3.294159
C	-1.802443	-1.719502	2.089042
S	-1.419469	-2.246195	3.623004
N	-2.902399	-0.900231	1.893549

H	-3.494491	-0.847439	2.714679
C	-2.959627	0.231059	1.059342
C	-3.175843	2.604054	-0.432021
C	-1.814858	0.843547	0.542621
C	-4.212066	0.802194	0.811492
C	-4.308102	1.974892	0.075173
C	-1.938368	2.022090	-0.185772
H	-0.839131	0.406333	0.728059
H	-5.106492	0.324374	1.199226
H	-3.257667	3.524796	-0.997926
C	-0.690630	2.673846	-0.710000
C	-5.657403	2.609900	-0.125954
F	0.325835	2.561232	0.177848
F	-5.712883	3.289999	-1.278182
F	-6.636069	1.695754	-0.141506
F	-5.940492	3.475272	0.858104
F	-0.255323	2.103388	-1.843918
F	-0.862111	3.972780	-0.956390
N	2.719671	-2.680075	0.770489
O	3.590590	-2.970663	-0.025159
O	1.624551	-3.226044	0.794330
C	3.068959	-1.476776	1.833322
C	3.546589	-0.364666	0.992381
H	4.256522	-0.703992	0.248490
C	3.722693	1.016781	1.495100
C	4.090982	3.680257	2.256671
C	2.692095	1.718525	2.131729
C	4.928257	1.669212	1.224988
C	5.116209	2.992325	1.612985
C	2.876750	3.043504	2.510364
H	1.735593	1.236823	2.315021
H	5.719739	1.128737	0.713783
H	6.059706	3.486695	1.405742
H	2.070694	3.580664	2.999807
H	4.233194	4.714394	2.554330
O	4.281410	-1.574633	2.310559
C	1.888090	-1.381280	2.767536
H	1.701715	-2.346383	3.242096
H	2.137179	-0.653456	3.541565
H	0.974680	-1.071599	2.252457
H	1.653543	-0.783980	-0.720743
N	2.201560	0.058533	-0.483517
H	1.559006	0.759594	-0.115662
C	2.979515	0.595317	-1.552152
C	4.652842	1.663095	-3.511619
C	3.861760	-0.237950	-2.246145
C	2.966412	1.967153	-1.807021
C	3.800184	2.493803	-2.788783
C	4.683810	0.298465	-3.232267
H	3.913401	-1.294654	-1.995236
H	2.313518	2.614800	-1.230152
H	3.782069	3.560980	-2.985510
H	5.361093	-0.354630	-3.773099
H	5.298724	2.077885	-4.278311

SR epoxide:Catalyst:Aniline, Transition State 31; Energy = -2737.294733; 6-31G(d) basis set.

C	-5.059487	-0.994515	0.918863
C	-4.778645	0.365482	-1.264878
C	-5.795966	1.495444	0.750959
C	-4.895001	1.673547	-0.473538
C	-5.305287	0.346488	1.643498
C	-4.270567	-0.791877	-0.397617
H	-4.100890	0.484881	-2.119073
H	-5.815871	2.421127	1.337098
H	-5.287926	2.463976	-1.123267
H	-5.996746	0.186684	2.480392
H	-4.313066	-1.735822	-0.948025
H	-4.382664	-1.580237	1.548178
H	-5.757031	0.096983	-1.676595
H	-6.823798	1.318911	0.417173
H	-3.900215	2.009788	-0.145259
H	-4.350098	0.653900	2.089356
N	-6.224010	-1.869998	0.721063
N	-2.870161	-0.512870	-0.091563

H	-2.535907	0.439014	-0.240698
C	-6.440661	-2.730931	1.872860
H	-6.725097	-2.175406	2.786259
H	-5.532418	-3.303090	2.080847
H	-7.246211	-3.437575	1.649527
C	-7.471237	-1.229646	0.344761
H	-7.347920	-0.631519	-0.560181
H	-7.891486	-0.580692	1.135123
H	-8.211348	-2.006725	0.128103
C	-1.932084	-1.431202	0.177901
S	-2.238731	-3.085710	0.291058
N	-0.702587	-0.853399	0.399040
H	-0.709353	0.166619	0.443584
C	0.546755	-1.466934	0.522813
C	3.131350	-2.541102	0.777873
C	1.483521	-0.875245	1.375724
C	0.919453	-2.591186	-0.225503
C	2.196105	-3.114002	-0.078806
C	2.766004	-1.404411	1.484191
H	1.192415	-0.014616	1.971491
H	0.214189	-3.040165	-0.912488
H	4.129202	-2.957126	0.869241
C	3.760908	-0.779112	2.418230
C	2.643724	-4.249179	-0.953387
F	3.534646	0.538695	2.583560
F	3.420101	-5.115008	-0.287164
F	1.621894	-4.929962	-1.476702
F	3.384760	-3.791566	-1.986733
F	3.727705	-1.331297	3.637878
F	5.016092	-0.911086	1.962466
N	-0.883829	1.730041	-2.391381
O	-1.150886	0.560818	-2.238938
O	-0.534770	2.237985	-3.449070
C	-0.910843	2.659826	-1.124002
C	0.435575	2.570995	-0.525490
H	0.825752	1.556849	-0.543905
C	0.995798	3.463613	0.498823
C	2.237647	5.038342	2.444032
C	0.720258	4.835164	0.573900
C	1.921976	2.901251	1.384589
C	2.537305	3.681491	2.357334
C	1.335784	5.612872	1.547234
H	0.043105	5.302288	-0.131203
H	2.171228	1.849500	1.296598
H	3.246131	3.225756	3.040857
H	1.114970	6.673650	1.604285
H	2.711250	5.652792	3.202974
O	-1.311873	2.023050	-0.024464
C	-1.638430	3.924736	-1.531057
H	-1.837173	4.509100	-0.633009
H	-1.074944	4.512380	-2.257523
H	-2.600118	3.647193	-1.972403
H	1.410543	3.003004	-2.919317
N	1.921822	2.923182	-2.040637
H	2.415867	3.787800	-1.832395
C	2.740715	1.766815	-1.962822
C	4.178315	-0.590055	-1.584742
C	3.876767	1.767784	-1.150984
C	2.310911	0.584382	-2.573098
C	3.034798	-0.587844	-2.381712
C	4.593511	0.588029	-0.968455
H	4.192374	2.687430	-0.664770
H	1.415964	0.586828	-3.191985
H	2.701024	-1.507364	-2.850958
H	5.475033	0.591390	-0.335588
H	4.731906	-1.511745	-1.439955

SR epoxide:Catalyst:Aniline, Transition State 32; Energy = -2737.292472; 6-31G(d) basis set.

C	-1.904357	3.025853	-1.270399
C	-0.568110	4.252102	0.439672
C	-2.454005	5.430566	-0.758066
C	-1.098813	5.594679	-0.066373
C	-2.408438	4.357363	-1.852949
C	-0.485949	3.259798	-0.725298

H	-1.237694	3.838111	1.206702
H	-3.203811	5.135909	-0.010899
H	-0.373319	6.015163	-0.775661
H	-1.747007	4.680371	-2.668005
H	0.128550	3.717082	-1.513984
H	-2.555096	2.779559	-0.416127
H	0.422001	4.370503	0.884853
H	-2.786968	6.383517	-1.182200
H	-1.179647	6.305541	0.762174
H	-3.408939	4.227937	-2.278705
N	-1.973650	1.849259	-2.151707
N	0.139310	1.995878	-0.347872
H	-0.386823	1.166658	-0.624604
C	-3.317225	1.638868	-2.675628
H	-3.392691	0.620980	-3.077061
H	-3.578813	2.336940	-3.485766
H	-4.053372	1.762255	-1.873279
C	-1.012233	1.846468	-3.252022
H	0.010274	1.919391	-2.874245
H	-1.184323	2.664153	-3.969820
H	-1.102877	0.896160	-3.786118
C	1.490099	1.846593	-0.262450
S	2.566208	3.129333	-0.415757
N	1.860573	0.546832	-0.067266
H	1.129328	-0.155703	-0.156872
C	3.147811	-0.001844	0.058091
C	5.634778	-1.276844	0.319890
C	4.182210	0.619214	0.764068
C	3.357676	-1.267271	-0.496012
C	4.590090	-1.893485	-0.356755
C	5.410583	-0.021031	0.874282
H	4.025798	1.585820	1.222633
H	2.554495	-1.757611	-1.036702
H	6.598459	-1.764180	0.417971
C	6.542587	0.676070	1.575865
C	4.778242	-3.278905	-0.906674
F	7.341976	-0.197496	2.207641
F	4.455763	-4.217701	-0.003972
F	4.011197	-3.494364	-1.985398
F	6.051493	-3.500950	-1.263225
F	7.314815	1.354538	0.713533
F	6.103469	1.554580	2.486796
N	-0.639335	-1.825372	-0.606767
O	-0.643121	-0.848113	-1.356205
O	0.227315	-2.034110	0.212147
C	-1.912393	-2.830964	-0.646528
C	-2.862703	-2.235618	0.316351
H	-2.370384	-1.881361	1.216911
C	-4.257272	-2.705865	0.475888
C	-6.920071	-3.445930	0.893283
C	-5.129823	-2.846766	-0.610202
C	-4.736363	-2.922374	1.770182
C	-6.060388	-3.298126	1.978105
C	-6.453589	-3.217095	-0.401197
H	-4.782463	-2.652623	-1.620980
H	-4.063128	-2.799677	2.613543
H	-6.419767	-3.469754	2.987405
H	-7.122864	-3.325314	-1.248540
H	-7.953821	-3.735017	1.053542
O	-1.787458	-3.818346	0.190142
C	-2.173541	-3.085839	-2.117750
H	-2.990411	-3.804541	-2.193904
H	-2.416483	-2.171420	-2.663743
H	-1.283014	-3.540666	-2.559915
H	-4.118106	-0.405616	-0.850317
N	-3.325048	-0.301130	-0.220460
H	-2.543922	0.112469	-0.747385
C	-3.671653	0.435316	0.945483
C	-4.317076	1.755998	3.313477
C	-2.667142	1.055863	1.692250
C	-4.993634	0.452251	1.393757
C	-5.310257	1.116983	2.574742
C	-2.996531	1.721188	2.869032
H	-1.635317	1.030124	1.346911
H	-5.764416	-0.058153	0.820497

H	-6.339984	1.133145	2.917047
H	-2.213704	2.210821	3.439644
H	-4.569396	2.275221	4.231886

SR epoxide:Catalyst:Aniline, Transition State 33; Energy = -2737.291303; 6-31G(d) basis set.

C	-4.014391	-1.627694	-0.219668
C	-3.545703	-3.724185	1.151014
C	-5.593086	-3.612771	-0.295516
C	-5.002433	-4.160395	1.002284
C	-5.480313	-2.088180	-0.314421
C	-3.388900	-2.196830	1.067943
H	-2.946376	-4.180941	0.356487
H	-5.050173	-4.034497	-1.151635
H	-5.591557	-3.787601	1.851790
H	-6.053063	-1.689434	0.533990
H	-3.926894	-1.762336	1.920986
H	-3.465276	-2.067601	-1.056377
H	-3.131794	-4.062202	2.107072
H	-6.641043	-3.912588	-0.399099
H	-5.062954	-5.253100	1.028241
H	-5.934868	-1.680430	-1.224481
N	-3.825068	-0.165589	-0.333190
N	-1.993439	-1.804683	1.295293
H	-1.831471	-1.246249	2.126644
C	-3.928024	0.251678	-1.728895
H	-4.932082	0.091272	-2.155866
H	-3.200757	-0.303489	-2.328466
H	-3.704249	1.321430	-1.807610
C	-4.776568	0.596285	0.472279
H	-4.757789	0.259911	1.513204
H	-5.810381	0.518698	0.101128
H	-4.503596	1.655437	0.460738
C	-0.896641	-2.204093	0.614281
S	-0.905091	-2.789168	-0.957606
N	0.253966	-2.031763	1.359053
H	0.096111	-1.676913	2.298011
C	1.569686	-1.775419	0.923747
C	4.191500	-1.069124	0.198231
C	2.177971	-2.386631	-0.179139
C	2.293597	-0.848487	1.681418
C	3.585649	-0.498831	1.309774
C	3.472691	-2.016923	-0.524997
H	1.646846	-3.130585	-0.754614
H	1.839698	-0.374244	2.548685
H	5.198767	-0.791014	-0.092101
C	4.110478	-2.615087	-1.749146
C	4.250372	0.623639	2.055074
F	3.534885	-3.767493	-2.107263
F	5.572016	0.654315	1.841855
F	3.753977	1.807920	1.656070
F	4.047389	0.537055	3.373809
F	4.025706	-1.782463	-2.799560
F	5.415722	-2.854213	-1.551150
N	-0.021710	1.411381	2.850417
O	1.069685	1.683509	3.282093
O	-0.502727	0.273750	2.875979
C	-0.864868	2.587997	2.115645
C	-0.294555	2.662400	0.755824
H	0.786868	2.554797	0.752719
C	-0.876483	3.485939	-0.324915
C	-1.869817	4.936374	-2.496880
C	-0.020264	4.270360	-1.099959
C	-2.231359	3.416769	-0.659767
C	-2.727966	4.142162	-1.736719
C	-0.515896	4.997351	-2.178512
H	1.036933	4.307624	-0.853708
H	-2.890489	2.765533	-0.095298
H	-3.782702	4.081439	-1.988066
H	0.157740	5.605256	-2.773491
H	-2.256530	5.499917	-3.340059
O	-0.336095	3.761317	2.318842
C	-2.316263	2.302369	2.443804
H	-2.648394	1.357142	2.006951
H	-2.443991	2.264534	3.528925

H	-2.916949	3.127668	2.058624
H	-0.060247	0.181182	0.449248
N	-0.497636	0.832624	-0.201602
H	-1.489159	0.566755	-0.289705
C	0.199931	0.889134	-1.441574
C	1.616448	1.173535	-3.829177
C	-0.482787	1.144511	-2.630218
C	1.593266	0.808751	-1.442194
C	2.295091	0.938677	-2.635858
C	0.227825	1.283759	-3.817827
H	-1.562807	1.246034	-2.619621
H	2.127082	0.653048	-0.508729
H	3.376667	0.849513	-2.628058
H	-0.311100	1.478174	-4.739768
H	2.165380	1.273807	-4.759583

SR epoxide:Catalyst:Aniline, Transition State 34; Energy = -2737.284969; 6-31G(d) basis set.

C	-2.406052	2.866540	0.522006
C	-0.559103	4.369069	-0.387016
C	-1.239364	4.472857	2.066527
C	-0.215662	4.922597	1.003080
C	-2.578230	4.106046	1.423533
C	-1.087543	2.932816	-0.301739
H	0.311425	4.396643	-1.045208
H	-0.863003	3.597008	2.615516
H	-0.187179	6.015288	0.950081
H	-2.952700	4.958782	0.843720
H	-1.267170	2.541759	-1.308639
H	-2.330394	2.001467	1.194703
H	-1.337010	4.983330	-0.856489
H	-1.380483	5.253066	2.819617
H	0.790087	4.600087	1.291447
H	-3.324224	3.894551	2.195520
N	-3.559060	2.554669	-0.343650
N	-0.102589	2.030107	0.301065
H	-0.119033	1.926547	1.310386
C	-4.777572	2.378099	0.442718
H	-5.577022	2.027859	-0.216766
H	-5.122294	3.308197	0.919753
H	-4.606949	1.625917	1.222456
C	-3.794598	3.523751	-1.412121
H	-2.909500	3.627128	-2.043326
H	-4.078595	4.519301	-1.036219
H	-4.610547	3.155688	-2.040138
C	1.013082	1.558212	-0.316169
S	1.448237	1.966692	-1.874734
N	1.667840	0.649334	0.494246
H	1.032683	-0.032618	0.927551
C	2.965131	0.152643	0.307634
C	5.561757	-0.899677	0.142747
C	4.025388	0.963816	-0.102677
C	3.209139	-1.180771	0.647468
C	4.498768	-1.689121	0.566519
C	5.303922	0.425865	-0.189202
H	3.854494	2.004723	-0.348161
H	2.377101	-1.812523	0.946030
H	6.564551	-1.305271	0.074975
C	6.423514	1.291400	-0.693349
C	4.749711	-3.105799	0.996679
F	7.611768	0.899664	-0.208123
F	4.959062	-3.189643	2.321860
F	3.709469	-3.904402	0.718869
F	5.831546	-3.625745	0.399058
F	6.517807	1.255158	-2.030992
F	6.252347	2.577051	-0.349781
N	-0.093007	-1.593572	-1.426459
O	-0.774334	-1.463332	-2.437045
O	1.111821	-1.546638	-1.395685
C	-0.822524	-1.940514	-0.091610
C	-1.767185	-0.888207	0.331855
H	-1.379265	0.115553	0.208375
C	-2.752857	-1.126811	1.413162
C	-4.598999	-1.478344	3.486980
C	-2.713082	-0.308940	2.548764

C	-3.714169	-2.139532	1.338753
C	-4.634355	-2.308762	2.370634
C	-3.629886	-0.479877	3.579384
H	-1.930975	0.440278	2.637421
H	-3.762735	-2.782854	0.466629
H	-5.382832	-3.090963	2.294683
H	-3.581467	0.156354	4.457206
H	-5.317736	-1.613603	4.288956
O	-0.140387	-1.559832	0.991147
C	-1.185867	-3.407358	-0.214966
H	-0.263444	-3.972393	-0.377394
H	-1.628711	-3.733535	0.726396
H	-1.878526	-3.585673	-1.041555
H	-2.413593	-0.319013	-1.970784
N	-3.116387	-0.330833	-1.232675
H	-3.372790	0.636430	-0.973505
C	-4.205391	-1.166868	-1.565711
C	-6.303341	-2.940921	-2.093306
C	-4.017579	-2.233873	-2.452082
C	-5.446435	-0.992995	-0.947084
C	-6.487923	-1.875678	-1.214971
C	-5.064464	-3.112953	-2.709363
H	-3.051185	-2.362853	-2.931450
H	-5.580554	-0.184339	-0.235235
H	-7.447191	-1.731179	-0.727492
H	-4.909946	-3.935950	-3.400253
H	-7.116829	-3.628778	-2.298530

SR epoxide:Catalyst:Aniline, Transition State 35; Energy = -2737.286057; 6-31G(d) basis set.

C	-2.661069	2.846731	-0.963655
C	-1.664959	4.505040	0.631199
C	-3.108704	5.353749	-1.250253
C	-2.926052	5.311696	0.267648
C	-3.376553	3.937601	-1.796032
C	-1.345904	3.433008	-0.427908
H	-1.808324	4.002524	1.594282
H	-3.931288	6.019272	-1.527948
H	-2.858390	6.321681	0.681959
H	-3.055203	3.879620	-2.842699
H	-0.782261	3.881225	-1.250369
H	-3.288369	2.618005	-0.093437
H	-0.790814	5.157359	0.727240
H	-2.202583	5.769734	-1.707482
H	-3.809549	4.843783	0.719585
H	-4.453257	3.737022	-1.781712
N	-2.480332	1.555518	-1.660066
N	-0.488615	2.398867	0.124617
H	-0.927985	1.807764	0.824422
C	-1.519442	1.595394	-2.763057
H	-1.398624	0.581391	-3.158122
H	-0.543441	1.944323	-2.418044
H	-1.847210	2.238461	-3.593991
C	-3.764399	1.048823	-2.141627
H	-4.509645	1.111877	-1.341195
H	-3.651360	0.001298	-2.447581
H	-4.146411	1.610571	-3.007663
C	0.817990	2.228881	-0.147836
S	1.757482	3.326859	-1.002238
N	1.296597	1.024179	0.325067
H	0.608886	0.280037	0.389125
C	2.622045	0.557806	0.211197
C	5.208710	-0.504684	0.106491
C	2.841037	-0.694257	-0.356617
C	3.696456	1.290326	0.720518
C	4.976123	0.757839	0.648817
C	4.128993	-1.222621	-0.387516
H	2.010691	-1.251374	-0.782243
H	3.524683	2.261073	1.170253
H	6.211043	-0.916337	0.074097
C	4.325293	-2.612692	-0.921079
C	6.140705	1.571651	1.140587
F	4.016784	-3.542042	0.003166
F	7.126279	0.789273	1.605950
F	6.666663	2.322718	0.162778

F	5.782936	2.403761	2.127916
F	3.542430	-2.853262	-1.983151
F	5.592436	-2.835702	-1.290262
N	-3.889638	0.899311	1.743537
O	-2.752805	1.309885	1.999341
O	-4.786268	1.606949	1.356242
C	-4.194910	-0.710422	1.880206
C	-3.752736	-1.277621	0.581652
H	-4.096099	-0.670590	-0.246412
C	-3.609402	-2.712453	0.300293
C	-3.211360	-5.379268	-0.433462
C	-2.946059	-3.591221	1.165035
C	-4.057867	-3.182818	-0.939261
C	-3.869055	-4.511393	-1.302253
C	-2.749187	-4.917166	0.797788
H	-2.554151	-3.234039	2.111086
H	-4.568762	-2.499830	-1.613135
H	-4.230195	-4.867476	-2.261515
H	-2.224844	-5.588874	1.469564
H	-3.054468	-6.415248	-0.716698
O	-5.418838	-0.999714	1.573915
C	-3.640998	-1.088431	3.242388
H	-4.142408	-0.483017	4.002204
H	-3.890765	-2.133971	3.427202
H	-2.562117	-0.938781	3.326797
H	-1.894775	0.082124	-0.464151
N	-1.765136	-0.657009	0.259297
H	-1.636834	-0.215731	1.168883
C	-0.810141	-1.657789	-0.023911
C	0.955313	-3.759326	-0.546920
C	-0.708465	-2.180124	-1.316800
C	-0.020616	-2.186243	1.003933
C	0.860408	-3.231247	0.737944
C	0.172254	-3.225653	-1.571289
H	-1.334931	-1.775675	-2.107689
H	-0.101798	-1.778562	2.010127
H	1.482531	-3.624262	1.535581
H	0.248083	-3.626288	-2.577035
H	1.651967	-4.563236	-0.755510

SR epoxide:Catalyst:Aniline, Transition State 36; Energy = -2737.282249; 6-31G(d) basis set.

C	4.024281	-1.518989	0.043708
C	3.640921	-3.746879	-1.171332
C	5.962745	-3.157069	-0.463356
C	4.828704	-4.165445	-0.299034
C	5.550266	-1.794806	0.122267
C	3.445298	-2.210586	-1.204747
H	2.726860	-4.221360	-0.810556
H	6.880209	-3.505071	0.020477
H	5.150731	-5.174585	-0.572950
H	6.105574	-0.996896	-0.383935
H	4.003747	-1.823566	-2.064779
H	3.542493	-1.963202	0.918142
H	3.800143	-4.084648	-2.201392
H	6.192907	-3.057195	-1.532300
H	4.523085	-4.204094	0.754150
H	5.844312	-1.753170	1.176331
N	3.684420	-0.081755	0.095940
N	2.054745	-1.859945	-1.510460
H	1.910062	-1.367514	-2.384961
C	4.073509	0.659570	-1.097546
H	3.442343	0.375634	-1.945491
H	5.129599	0.530800	-1.382558
H	3.918223	1.725996	-0.912295
C	4.257811	0.536645	1.289077
H	3.989872	-0.058242	2.167643
H	3.843749	1.543680	1.411932
H	5.354680	0.625022	1.249513
C	0.951714	-2.210452	-0.814751
S	0.976665	-2.829913	0.742210
N	-0.203616	-1.971202	-1.533711
H	-0.056356	-1.501136	-2.423589
C	-1.509806	-1.760023	-1.049765
C	-4.103814	-1.114555	-0.183288

C	-2.100688	-2.490781	-0.011272
C	-2.243978	-0.755891	-1.685202
C	-3.521135	-0.433018	-1.241879
C	-3.381024	-2.149561	0.406680
H	-1.565707	-3.299062	0.464764
H	-1.813111	-0.205289	-2.518218
H	-5.097813	-0.857687	0.166120
C	-4.005075	-2.879227	1.564496
C	-4.193130	0.757266	-1.866618
F	-5.299544	-3.144524	1.332044
F	-4.112006	0.727637	-3.201441
F	-5.487751	0.835277	-1.533896
F	-3.604781	1.895150	-1.461572
F	-3.391953	-4.038070	1.824454
F	-3.959960	-2.141536	2.686890
N	-0.114353	1.646542	-2.765931
O	0.557905	0.609840	-2.716525
O	-1.162377	1.742157	-3.354434
C	0.412698	2.924522	-1.933651
C	0.061968	2.658862	-0.517946
H	-0.961284	2.312229	-0.412741
C	0.605495	3.459077	0.600168
C	1.574041	4.799377	2.852907
C	1.980709	3.631191	0.782526
C	-0.278240	3.953008	1.561754
C	0.203406	4.624869	2.681230
C	2.463411	4.300653	1.901746
H	2.676521	3.216691	0.059440
H	-1.345658	3.802024	1.429696
H	-0.492308	5.003850	3.422691
H	3.533544	4.426915	2.035019
H	1.951082	5.317913	3.728771
O	-0.454452	3.894257	-1.888530
C	1.790464	3.207942	-2.496350
H	1.659125	3.526999	-3.534538
H	2.224405	4.042152	-1.943341
H	2.448913	2.340899	-2.463380
H	0.193246	0.191055	-0.477837
N	0.652156	0.793737	0.202891
H	1.661790	0.566556	0.180170
C	0.086011	0.662488	1.499340
C	-1.072655	0.605292	4.038884
C	-1.289408	0.466129	1.637820
C	0.877326	0.852402	2.632201
C	0.296373	0.822402	3.894945
C	-1.861704	0.426895	2.905260
H	-1.911006	0.341645	0.754876
H	1.941138	1.033795	2.517922
H	0.919649	0.968651	4.771686
H	-2.927894	0.249030	3.000388
H	-1.520585	0.574881	5.026638

SR epoxide:Catalyst:Aniline, Transition State 37; Energy = -2737.289315; 6-31G(d) basis set.

C	5.712180	-0.720595	-0.015911
C	4.793072	1.564270	-0.638724
C	6.125927	0.245548	-2.328686
C	5.011957	1.276610	-2.127716
C	5.839733	-1.020427	-1.516760
C	4.556407	0.291186	0.179335
H	3.956514	2.259187	-0.501533
H	6.226694	-0.002655	-3.390579
H	5.248367	2.211707	-2.645289
H	6.596417	-1.788948	-1.695186
H	4.445870	0.542809	1.235198
H	5.433359	-1.654416	0.511729
H	5.689603	2.041243	-0.229827
H	7.078984	0.679203	-2.001691
H	4.080521	0.914726	-2.588788
H	4.888930	-1.457492	-1.847616
N	6.950743	-0.173281	0.551120
N	3.289742	-0.318955	-0.216185
H	2.919584	-0.061957	-1.127541
C	6.853901	-0.034247	2.001131
H	6.581606	-0.982949	2.497155

H	6.115204	0.719610	2.279965
H	7.819219	0.296744	2.392496
C	8.110566	-0.994575	0.228274
H	8.333096	-0.954140	-0.840149
H	7.978575	-2.052745	0.520225
H	8.980429	-0.601541	0.760470
C	2.499519	-1.058430	0.579971
S	2.789120	-1.335895	2.207199
N	1.432893	-1.597011	-0.119862
H	1.525303	-1.537983	-1.128006
C	0.122952	-1.857477	0.286212
C	-2.631758	-2.199419	0.789066
C	-0.418723	-1.484410	1.523620
C	-0.722357	-2.428932	-0.677781
C	-2.076901	-2.585811	-0.427042
C	-1.784366	-1.654241	1.748014
H	0.210976	-1.045101	2.286908
H	-0.318859	-2.712308	-1.645993
H	-3.697342	-2.289276	0.968106
C	-2.366993	-1.230203	3.070280
C	-2.963441	-3.170798	-1.494817
F	-3.618578	-0.766732	2.922066
F	-4.198082	-2.661007	-1.438911
F	-2.475825	-2.933052	-2.721399
F	-3.075082	-4.500561	-1.365785
F	-2.420177	-2.242855	3.940945
F	-1.645163	-0.251536	3.641894
N	1.153212	1.954538	-1.538919
O	1.020437	0.744620	-1.765582
O	1.937267	2.659971	-2.117536
C	0.313875	2.604928	-0.330151
C	-1.130723	2.553010	-0.627402
H	-1.372884	2.812787	-1.652053
C	-2.156633	2.849006	0.402299
C	-4.232297	3.314753	2.218083
C	-2.167442	2.206813	1.647186
C	-3.202985	3.711374	0.072694
C	-4.233443	3.948612	0.978853
C	-3.197713	2.440315	2.550879
H	-1.387338	1.498232	1.910078
H	-3.205197	4.198835	-0.897832
H	-5.040048	4.623587	0.711794
H	-3.196499	1.926790	3.506514
H	-5.038428	3.494656	2.922205
O	0.199110	3.900815	-0.438900
C	0.967615	1.997507	0.900316
H	2.044429	2.193413	0.873590
H	0.557560	2.489153	1.782936
H	0.806097	0.917731	0.960859
H	-1.667283	0.192249	-0.007933
N	-1.735394	0.603543	-0.938464
H	-0.974593	0.241143	-1.511818
C	-3.022646	0.420800	-1.508984
C	-5.552567	0.142119	-2.642988
C	-3.151701	0.242639	-2.886705
C	-4.158389	0.468887	-0.695387
C	-5.416865	0.327091	-1.268210
C	-4.417043	0.100592	-3.447814
H	-2.262481	0.200544	-3.510727
H	-4.049446	0.603113	0.378534
H	-6.296607	0.358273	-0.633229
H	-4.511971	-0.049063	-4.518547
H	-6.537318	0.026798	-3.083405

SR epoxide:Catalyst:Aniline, Transition State 38; Energy = -2737.288284; 6-31G(d) basis set.

C	-1.107137	2.729805	0.957850
C	-0.193302	3.924273	-1.138282
C	-1.800593	5.120726	0.327748
C	-1.343278	4.923423	-1.111831
C	-2.220261	3.794313	0.961123
C	-0.595699	2.585438	-0.499555
H	0.667307	4.331909	-0.600189
H	-0.978525	5.555362	0.911609
H	-2.181907	4.548521	-1.715335

H	-3.095084	3.389535	0.427206
H	-1.451518	2.199361	-1.071462
H	-0.279940	3.083716	1.592800
H	0.131264	3.718253	-2.163791
H	-2.637979	5.823972	0.381890
H	-1.027449	5.872972	-1.555466
H	-2.533933	3.992481	1.988219
N	-1.623417	1.436497	1.494463
N	0.442302	1.577168	-0.723545
H	0.183381	0.861200	-1.398592
C	-2.457430	1.621198	2.688873
H	-2.760982	0.634543	3.050972
H	-3.363225	2.181147	2.458325
H	-1.918183	2.134063	3.502160
C	-0.542765	0.504273	1.862309
H	-0.072671	0.066766	0.983353
H	-0.967949	-0.312383	2.452864
H	0.232789	0.997167	2.467306
C	1.697636	1.526860	-0.235411
S	2.385006	2.672639	0.784920
N	2.334253	0.372880	-0.630083
H	1.719225	-0.368464	-0.961598
C	3.637886	-0.052653	-0.331064
C	6.211871	-1.056825	0.159175
C	4.743121	0.803066	-0.373541
C	3.828145	-1.408511	-0.059395
C	5.108403	-1.898783	0.175132
C	6.008543	0.292578	-0.116191
H	4.611253	1.850349	-0.610250
H	2.972183	-2.077270	-0.022357
H	7.207240	-1.441293	0.349980
C	7.187142	1.225613	-0.099358
C	5.289046	-3.373255	0.400477
F	7.428304	1.694857	1.133973
F	5.316032	-4.047493	-0.760302
F	6.434849	-3.644228	1.039599
F	4.286073	-3.889172	1.124990
F	8.307703	0.610284	-0.507305
F	6.996082	2.287155	-0.894077
N	-0.882337	-1.444083	-1.495079
O	0.155562	-1.664374	-0.906658
O	-1.045375	-0.483655	-2.244009
C	-2.146894	-2.448454	-1.203786
C	-2.833201	-1.840812	-0.044018
H	-2.130401	-1.471953	0.695615
C	-4.151177	-2.258532	0.453298
C	-6.668910	-2.835663	1.519079
C	-4.336488	-2.327132	1.838010
C	-5.244742	-2.471977	-0.394383
C	-6.495895	-2.758882	0.137996
C	-5.587234	-2.621744	2.370132
H	-3.489076	-2.155702	2.497240
H	-5.131238	-2.370641	-1.467859
H	-7.340831	-2.908124	-0.526282
H	-5.717492	-2.680632	3.445857
H	-7.648439	-3.056818	1.931322
O	-1.812981	-3.422729	-0.415693
C	-2.741666	-2.722228	-2.570443
H	-3.537893	-3.456909	-2.446847
H	-3.129699	-1.821697	-3.050324
H	-1.971206	-3.164585	-3.207759
H	-2.895612	0.304520	-1.447415
N	-3.339120	0.191137	-0.536859
H	-2.775363	0.679638	0.192349
C	-4.709165	0.525361	-0.546158
C	-7.471510	0.962881	-0.534912
C	-5.389430	0.696973	0.663625
C	-5.417889	0.582358	-1.749556
C	-6.791659	0.801813	-1.739984
C	-6.762205	0.912298	0.664306
H	-4.842065	0.622649	1.598660
H	-4.889181	0.450198	-2.690863
H	-7.331556	0.845810	-2.680768
H	-7.282048	1.032791	1.609735
H	-8.543648	1.128776	-0.529908

SR epoxide:Catalyst:Aniline, Transition State 39; Energy = -2737.296280; 6-31G(d) basis set.

C	4.605500	-0.322601	-0.155704
C	4.900477	0.526633	-2.521597
C	6.855435	0.534143	-0.929266
C	6.197914	1.231511	-2.121529
C	5.888973	0.419702	0.254680
C	3.956902	0.440148	-1.319366
H	5.116391	-0.488517	-2.881756
H	7.172749	-0.473769	-1.230081
H	5.970917	2.272294	-1.855164
H	5.631154	1.424113	0.616546
H	3.720283	1.461841	-1.003957
H	4.907370	-1.312599	-0.537037
H	4.391645	1.064510	-3.327714
H	7.758467	1.071620	-0.622913
H	6.883887	1.264201	-2.973692
H	6.374912	-0.106801	1.082142
N	3.634956	-0.595804	0.911609
N	2.686393	-0.186442	-1.664122
H	2.639515	-1.195606	-1.569709
C	4.193181	-1.446251	1.955418
H	3.391486	-1.762983	2.624713
H	4.963638	-0.941350	2.559659
H	4.635479	-2.339278	1.502927
C	3.011861	0.587309	1.493239
H	2.513871	1.178715	0.716751
H	3.719942	1.241538	2.027141
H	2.246888	0.259649	2.204943
C	1.587529	0.469189	-2.038347
S	1.526627	2.116471	-2.382314
N	0.430005	-0.283132	-2.126525
H	-0.312166	0.188927	-2.636947
C	0.009686	-1.359359	-1.323419
C	-1.119103	-3.366757	0.292651
C	-1.209068	-1.959338	-1.677701
C	0.659695	-1.765980	-0.154664
C	0.082939	-2.768002	0.626749
C	-1.761086	-2.936851	-0.869957
H	-1.729578	-1.630545	-2.571796
H	1.588176	-1.308053	0.189848
H	-1.560157	-4.130060	0.923860
C	-3.118424	-3.500552	-1.186079
C	0.789675	-3.130027	1.903595
F	-3.124728	-4.837118	-1.114547
F	1.989462	-3.680160	1.661772
F	1.007811	-2.039783	2.658214
F	0.088090	-3.996828	2.641187
F	-4.031580	-3.059320	-0.303378
F	-3.543233	-3.152013	-2.406558
N	-1.418894	4.372189	1.427344
O	-1.803713	5.043744	2.360137
O	-0.245129	4.314156	1.075673
C	-2.540868	3.610690	0.542611
C	-1.842022	2.768834	-0.451291
H	-1.023054	3.294000	-0.926481
C	-2.560000	1.788228	-1.305486
C	-3.827353	-0.029974	-3.023340
C	-2.291249	1.801389	-2.680742
C	-3.456138	0.838912	-0.799235
C	-4.085638	-0.062815	-1.654104
C	-2.923079	0.900065	-3.535785
H	-1.594412	2.535256	-3.075904
H	-3.656416	0.793705	0.265291
H	-4.772615	-0.798015	-1.248232
H	-2.718971	0.935469	-4.601421
H	-4.322176	-0.733468	-3.685792
O	-2.957664	4.368188	-0.448561
C	-3.567698	3.106579	1.536809
H	-4.392684	2.670340	0.972898
H	-3.158631	2.375010	2.241059
H	-3.948239	3.966095	2.090566
H	0.270391	2.222245	0.511713
N	-0.491216	1.546640	0.449077

H	-0.279661	0.853478	-0.264749
C	-0.831723	0.973167	1.704118
C	-1.613442	-0.092777	4.160810
C	-0.474981	1.621958	2.888990
C	-1.579698	-0.205474	1.747921
C	-1.964245	-0.734857	2.975076
C	-0.868894	1.084062	4.110780
H	0.105188	2.540237	2.848166
H	-1.858765	-0.702770	0.822482
H	-2.536957	-1.657471	2.999720
H	-0.588596	1.591080	5.028392
H	-1.914697	-0.507865	5.116672

SR epoxide:Catalyst:Aniline, Transition State 40; Energy = -2737.294369; 6-31G(d) basis set.

C	4.927344	-1.481014	-0.053661
C	3.968981	0.587330	1.065471
C	6.447710	0.407216	0.722685
C	5.342234	0.942392	1.634001
C	6.302924	-1.101733	0.512707
C	3.828815	-0.928118	0.875184
H	3.845666	1.068214	0.084368
H	7.433918	0.632583	1.141680
H	5.444588	0.501108	2.634491
H	6.452214	-1.610923	1.474384
H	3.896880	-1.415024	1.854610
H	4.817129	-0.974042	-1.024393
H	3.164936	0.940997	1.722185
H	6.390181	0.915948	-0.249333
H	5.428437	2.027184	1.753422
H	7.066713	-1.481606	-0.171989
N	4.860982	-2.917232	-0.323529
N	2.520974	-1.262110	0.318671
H	2.473495	-1.331734	-0.697606
C	4.661884	-3.754555	0.845377
H	3.634884	-3.697323	1.250825
H	5.360876	-3.481908	1.640331
H	4.855808	-4.797174	0.573806
C	3.991735	-3.332829	-1.410089
H	4.045855	-2.615044	-2.233962
H	2.931491	-3.442034	-1.117064
H	4.322154	-4.308260	-1.784752
C	1.396834	-1.446006	1.031492
S	1.320978	-1.273711	2.699680
N	0.319691	-1.776775	0.231791
H	0.548900	-2.060603	-0.718146
C	-1.054326	-1.784860	0.515114
C	-3.858832	-1.741284	0.787489
C	-1.657607	-1.002548	1.505765
C	-1.869562	-2.536095	-0.344411
C	-3.247760	-2.512908	-0.198146
C	-3.045412	-0.986354	1.619611
H	-1.058527	-0.414512	2.189048
H	-1.419847	-3.136897	-1.129062
H	-4.938514	-1.718444	0.886525
C	-3.663209	-0.103951	2.670191
C	-4.119176	-3.265833	-1.166247
F	-2.968535	1.036508	2.817394
F	-5.146043	-3.854658	-0.538241
F	-4.642269	-2.439460	-2.083011
F	-3.440024	-4.214571	-1.820390
F	-4.921695	0.230879	2.350825
F	-3.700138	-0.698024	3.868174
N	1.625735	0.136293	-2.477821
O	1.458678	-1.074757	-2.463772
O	2.647880	0.670120	-2.075567
C	0.333039	1.071257	-2.916342
C	-0.542748	0.979934	-1.718759
H	-0.639245	-0.046973	-1.389222
C	-1.707095	1.840610	-1.474904
C	-3.936796	3.372723	-0.786156
C	-1.678831	3.231397	-1.631278
C	-2.860899	1.228662	-0.969223
C	-3.969656	1.988218	-0.619349
C	-2.796618	3.989567	-1.296651

H	-0.776442	3.726961	-1.974397
H	-2.885875	0.146571	-0.875243
H	-4.852832	1.502405	-0.216306
H	-2.767379	5.067781	-1.414760
H	-4.800377	3.971602	-0.514450
O	-0.545223	0.407213	-3.593260
C	0.931646	2.342463	-3.482288
H	0.107614	2.947203	-3.863739
H	1.502563	2.910145	-2.746455
H	1.580912	2.084376	-4.322851
H	0.045435	0.850849	0.739922
N	0.550582	1.395040	0.040675
H	1.471045	0.970505	-0.091620
C	0.652240	2.759767	0.421624
C	0.764111	5.472732	1.028142
C	1.714273	3.531701	-0.052837
C	-0.351892	3.336278	1.199691
C	-0.289056	4.692394	1.501523
C	1.764659	4.888009	0.253680
H	2.491464	3.063900	-0.652780
H	-1.181227	2.724997	1.549811
H	-1.070814	5.140043	2.106669
H	2.592341	5.487575	-0.111458
H	0.808115	6.530372	1.265727

SR epoxide:Catalyst:Aniline, Transition State 41; Energy = -2737.303289; 6-31G(d) basis set.

C	4.843328	-0.481237	0.063980
C	4.870310	-0.854552	-2.448582
C	6.974925	-1.193665	-1.111697
C	6.397165	-0.763496	-2.460354
C	6.379249	-0.362527	0.027801
C	4.294454	-0.016413	-1.298926
H	4.556617	-1.895709	-2.328872
H	6.743445	-2.253873	-0.942454
H	6.702071	0.271525	-2.669984
H	6.668353	0.689682	-0.104352
H	4.645823	1.012195	-1.456147
H	4.587704	-1.541980	0.173483
H	4.449612	-0.490977	-3.392213
H	8.066345	-1.101757	-1.114413
H	6.800803	-1.383354	-3.267691
H	6.795808	-0.690384	0.986456
N	4.186281	0.204008	1.181606
N	2.839647	0.114427	-1.351186
H	2.511855	1.067159	-1.463238
C	4.326550	1.652239	1.186154
H	3.872457	2.096331	0.295307
H	5.372114	1.997007	1.263363
H	3.784638	2.051718	2.050177
C	4.579493	-0.344824	2.469069
H	5.599882	-0.060045	2.778154
H	4.524571	-1.437871	2.435365
H	3.884097	0.008355	3.238585
C	1.892704	-0.824332	-1.202193
S	2.198508	-2.462861	-0.950508
N	0.625831	-0.293936	-1.318116
H	0.532311	0.669575	-1.654107
C	-0.612100	-0.946369	-1.205568
C	-3.191855	-2.035667	-0.964655
C	-1.654479	-0.490880	-2.018176
C	-0.871120	-1.933059	-0.246297
C	-2.151535	-2.462036	-0.143310
C	-2.927181	-1.035087	-1.889461
H	-1.471835	0.306193	-2.731054
H	-0.087264	-2.260646	0.421944
H	-4.187151	-2.456238	-0.867774
C	-4.051367	-0.447311	-2.692914
C	-2.479533	-3.393805	0.985896
F	-5.054148	-1.322114	-2.861541
F	-1.395768	-3.969163	1.516435
F	-3.099333	-2.724580	1.982423
F	-3.317822	-4.368653	0.606258
F	-4.569909	0.631922	-2.085157
F	-3.646463	-0.054142	-3.908317

N	1.193604	3.194455	-0.258106
O	1.586401	3.603040	0.821577
O	1.926742	2.876413	-1.174659
C	-0.375604	3.154830	-0.549193
C	-1.021003	2.150126	0.326680
H	-0.465740	1.219502	0.360110
C	-2.469963	2.042351	0.574586
C	-5.177095	1.664276	1.181442
C	-2.971223	0.763366	0.845063
C	-3.338563	3.140353	0.647409
C	-4.683611	2.946760	0.938367
C	-4.315354	0.572639	1.145529
H	-2.296812	-0.086202	0.829227
H	-2.971657	4.147978	0.496558
H	-5.349859	3.802195	0.982277
H	-4.677259	-0.430817	1.348514
H	-6.229449	1.522435	1.406301
O	-0.670611	2.359543	-1.555765
C	-0.737960	4.627440	-0.651624
H	-1.750599	4.706361	-1.045435
H	-0.654194	5.142050	0.308294
H	-0.063523	5.096008	-1.373926
H	-1.181392	2.690819	2.935547
N	-0.435196	2.283372	2.377207
H	0.375856	2.898678	2.344110
C	-0.133162	0.940256	2.717088
C	0.345732	-1.781043	3.107799
C	-1.056110	0.164343	3.420977
C	1.025194	0.352753	2.196301
C	1.262527	-1.002358	2.401279
C	-0.812532	-1.193840	3.611999
H	-1.966372	0.620815	3.801326
H	1.741733	0.934490	1.617775
H	2.155463	-1.440719	1.966429
H	-1.539474	-1.795257	4.147996
H	0.522778	-2.842531	3.245700

SR epoxide:Catalyst:Aniline, Transition State 42; Energy = -2737.292383; 6-31G(d) basis set.

C	2.448321	2.961291	-0.360290
C	0.739375	4.071268	-1.868694
C	3.009139	5.098152	-1.628562
C	1.527090	5.378975	-1.862690
C	3.227627	4.292489	-0.345245
C	0.962261	3.284582	-0.570439
H	1.049580	3.449535	-2.720307
H	3.408180	4.529088	-2.479593
H	1.144521	6.025733	-1.062034
H	2.910367	4.888047	0.522023
H	0.620373	3.905529	0.262678
H	2.805270	2.382409	-1.230741
H	-0.334296	4.259870	-1.971691
H	3.578392	6.031845	-1.577871
H	1.377860	5.914730	-2.805394
H	4.296303	4.095306	-0.225828
N	2.672833	2.093611	0.819215
N	0.134296	2.084966	-0.555976
H	0.488102	1.276523	-1.060674
C	4.096423	1.978256	1.134295
H	4.516462	2.892529	1.579378
H	4.662747	1.744354	0.225895
H	4.238610	1.162535	1.850985
C	1.939239	2.509090	2.015685
H	0.860475	2.436399	1.857300
H	2.185643	3.534576	2.334289
H	2.207986	1.837092	2.836948
C	-1.185140	2.092450	-0.228595
S	-1.891920	3.348810	0.634936
N	-1.830823	0.976139	-0.679124
H	-1.268197	0.378534	-1.280064
C	-3.089381	0.420051	-0.412457
C	-5.521440	-0.946429	-0.019893
C	-4.065446	0.954009	0.429896
C	-3.342008	-0.803280	-1.058848
C	-4.538423	-1.467354	-0.859765

C	-5.262214	0.259707	0.609023
H	-3.900451	1.894282	0.936958
H	-2.589344	-1.239154	-1.712286
H	-6.455217	-1.472775	0.139530
C	-6.275466	0.869020	1.538679
C	-4.811625	-2.750362	-1.594200
F	-6.614021	2.106684	1.149227
F	-5.463418	-3.627537	-0.817805
F	-5.583559	-2.539107	-2.672831
F	-3.686962	-3.335685	-2.020108
F	-7.400427	0.145083	1.604568
F	-5.791919	0.975443	2.785447
N	-0.034221	-1.939529	-0.951645
O	-0.745578	-2.817790	-1.353426
O	0.176655	-0.888471	-1.583971
C	0.620070	-2.103413	0.510518
C	2.075009	-2.276369	0.356484
H	2.351044	-2.921989	-0.471208
C	2.986777	-2.256685	1.524229
C	4.820286	-2.218930	3.632980
C	3.907699	-3.294406	1.676310
C	2.998598	-1.190803	2.429543
C	3.908295	-1.174273	3.481482
C	4.818712	-3.277921	2.729050
H	3.904700	-4.116946	0.967188
H	2.317198	-0.355755	2.290460
H	3.910347	-0.342172	4.179409
H	5.529191	-4.090603	2.839310
H	5.531652	-2.203738	4.452540
O	0.604291	-3.344061	0.913069
C	-0.048918	-1.013588	1.331778
H	-1.136080	-1.119645	1.254292
H	0.229366	-1.168316	2.375012
H	0.247221	-0.008862	1.012094
H	2.213006	-0.512358	-1.366948
N	2.901843	-0.652888	-0.629234
H	2.861295	0.150343	0.015815
C	4.184122	-0.984608	-1.138480
C	6.663944	-1.807916	-2.128843
C	4.300726	-1.434177	-2.456643
C	5.309006	-0.970500	-0.307645
C	6.541853	-1.373946	-0.810703
C	5.537104	-1.840610	-2.947204
H	3.420769	-1.459160	-3.095167
H	5.213694	-0.658792	0.728563
H	7.411025	-1.355459	-0.160773
H	5.617403	-2.181774	-3.974380
H	7.628128	-2.122783	-2.513702

SR epoxide:Catalyst:Aniline, Transition State 43; Energy = -2737.268959; 6-31G(d) basis set.

C	-5.878894	-0.067161	-0.413951
C	-4.753010	-2.317909	-0.073358
C	-7.136192	-2.013044	0.699087
C	-6.204419	-2.810075	-0.214807
C	-7.189779	-0.532943	0.265711
C	-4.699828	-0.810973	0.244844
H	-4.211698	-2.505819	-1.002673
H	-8.143154	-2.440844	0.697567
H	-6.255735	-3.879573	0.009398
H	-7.400093	0.094613	1.139208
H	-4.799218	-0.695389	1.330721
H	-5.901174	-0.381763	-1.461226
H	-4.238390	-2.859192	0.728942
H	-6.770383	-2.090774	1.731112
H	-6.534138	-2.691679	-1.254130
H	-8.016560	-0.381363	-0.436691
N	-5.655040	1.374932	-0.451599
N	-3.387869	-0.218902	-0.042460
H	-3.034938	0.369894	0.703179
C	-6.533297	2.045538	-1.393635
H	-6.221051	3.089599	-1.498587
H	-7.593687	2.040821	-1.084619
H	-6.451486	1.563462	-2.372290
C	-5.667202	2.043024	0.836735

H	-5.015209	1.525474	1.548424
H	-6.668392	2.120301	1.294094
H	-5.282730	3.060383	0.711566
C	-2.871171	0.035297	-1.256287
S	-3.464257	-0.508581	-2.732361
N	-1.731113	0.810529	-1.271287
H	-1.479186	1.116232	-2.203186
C	-0.894719	1.208978	-0.221135
C	0.863106	2.059548	1.802995
C	-0.243092	2.444047	-0.317739
C	-0.635106	0.383275	0.881640
C	0.216185	0.827974	1.885431
C	0.637687	2.846672	0.678620
H	-0.427963	3.087707	-1.172515
H	-1.073745	-0.606831	0.940828
H	1.525363	2.396992	2.593839
C	1.404121	4.132574	0.515039
C	0.536604	-0.075946	3.045673
F	0.736559	5.013966	-0.238905
F	0.591076	0.602910	4.195394
F	-0.353540	-1.060421	3.184959
F	1.747276	-0.652625	2.879584
F	1.654044	4.706373	1.698043
F	2.584950	3.912037	-0.078224
N	5.568220	-2.054031	0.240187
O	6.576957	-2.205727	-0.414621
O	5.553975	-1.520874	1.345135
C	4.185078	-2.664768	-0.332957
C	3.075079	-2.056766	0.435280
H	3.266373	-2.081459	1.499130
C	1.664319	-2.246609	0.011484
C	-0.996639	-2.699970	-0.722706
C	1.192136	-1.819531	-1.235499
C	0.785950	-2.884124	0.893364
C	-0.535008	-3.122642	0.523186
C	-0.134848	-2.037248	-1.596233
H	1.866179	-1.321412	-1.925215
H	1.153100	-3.214347	1.860485
H	-1.202329	-3.637974	1.207509
H	-0.504886	-1.700787	-2.560539
H	-2.025788	-2.877980	-1.019167
O	3.906810	-3.822217	0.222211
C	4.291517	-2.599703	-1.842294
H	5.132235	-3.222910	-2.150699
H	3.375178	-3.021714	-2.257730
H	4.442429	-1.582084	-2.216366
H	3.885655	0.027698	1.260209
N	3.242371	-0.032613	0.471055
H	2.321138	0.297182	0.751821
C	3.736501	0.658459	-0.673026
C	4.693492	1.887398	-2.986085
C	5.111329	0.827938	-0.851701
C	2.841850	1.118285	-1.640791
C	3.322910	1.729521	-2.793666
C	5.580778	1.439950	-2.009706
H	5.806148	0.487866	-0.088993
H	1.773251	0.993410	-1.483720
H	2.622438	2.086299	-3.542151
H	6.649871	1.567066	-2.144770
H	5.066854	2.362738	-3.886781

SR epoxide:Catalyst:Aniline, Transition State 44; Energy = -2737.299266; 6-31G(d) basis set.

C	2.450791	3.694427	-0.108552
C	0.947137	3.965508	-0.273490
N	0.242422	2.750008	-0.653360
H	0.720742	2.173381	-1.344813
C	-1.028294	2.450282	-0.316205
S	-1.848239	3.214934	0.941190
N	-1.545692	1.433730	-1.079946
H	-0.911044	1.065150	-1.786616
C	-2.592421	0.542642	-0.780357
C	-4.514356	-1.421144	-0.181896
C	-3.787532	0.903835	-0.152335
C	-2.398033	-0.787893	-1.162738

C	-3.343297	-1.753345	-0.852501
C	-4.721951	-0.085477	0.144683
H	-3.980110	1.935383	0.106808
H	-1.487584	-1.069592	-1.683584
H	-5.252529	-2.176573	0.061137
C	-5.968913	0.305248	0.888886
C	-3.017446	-3.182259	-1.179929
F	-5.768638	0.303711	2.216174
F	-4.100237	-3.968600	-1.146931
F	-2.129725	-3.690671	-0.306781
F	-2.463721	-3.296974	-2.396632
F	-6.382667	1.534897	0.556705
F	-6.978477	-0.543261	0.645116
C	3.272782	-1.538668	-0.735783
H	3.383143	-0.645346	1.638127
N	2.623838	-0.524522	0.971396
H	2.551233	0.466321	0.691829
C	1.389214	-1.006669	1.495073
C	-1.066757	-2.003845	2.342662
C	1.314898	-2.294089	2.031207
C	0.248012	-0.211349	1.399304
C	-0.978213	-0.710437	1.833501
C	0.082429	-2.787568	2.446321
H	2.211940	-2.904506	2.101170
H	0.338008	0.797524	1.001977
H	-1.859507	-0.077468	1.779835
H	0.019448	-3.792609	2.851468
H	-2.025439	-2.396454	2.665241
O	2.936783	-2.131281	-2.529020
C	2.099529	-1.741660	-1.598820
C	4.015736	-2.658585	-0.102887
C	5.439155	-4.681617	1.215762
C	3.744093	-4.004250	-0.369549
C	5.051964	-2.343693	0.785420
C	5.752073	-3.344203	1.449216
C	4.447317	-5.005456	0.293273
H	3.026816	-4.264461	-1.137718
H	5.324180	-1.302591	0.947928
H	6.547713	-3.079732	2.138070
H	4.225934	-6.045231	0.075246
H	5.982590	-5.466659	1.731569
H	3.844943	-0.659470	-1.001798
C	0.867946	-2.565939	-1.279899
H	0.176733	-2.049251	-0.610492
H	1.165286	-3.494695	-0.793009
H	0.364591	-2.802639	-2.220689
N	1.509080	-0.243655	-1.950005
O	0.442378	-0.182318	-2.542437
O	2.173255	0.745469	-1.686838
H	0.528610	4.297915	0.680257
H	2.837940	3.354530	-1.082588
N	2.726528	2.586484	0.831234
C	3.154419	5.020106	0.245466
H	4.232050	4.855970	0.335619
H	2.798630	5.368939	1.224548
C	0.685838	5.059904	-1.318527
H	1.031782	4.701402	-2.298118
H	-0.397107	5.208313	-1.388622
C	2.895924	6.108562	-0.798959
H	3.317799	5.791841	-1.762696
H	3.416467	7.027774	-0.511215
C	1.399566	6.361523	-0.963127
H	1.214403	7.115221	-1.735078
H	0.989787	6.756738	-0.024071
C	2.130298	2.751809	2.154916
H	1.041957	2.830281	2.079685
H	2.516269	3.625863	2.703324
H	2.354504	1.859129	2.749782
C	4.160163	2.340781	0.943072
H	4.590459	2.221558	-0.056893
H	4.331389	1.417611	1.507910
H	4.705988	3.137412	1.470438

SR epoxide:Catalyst:Aniline, Transition State 45; Energy = -2737.300228; 6-31G(d) basis set.

C	2.263008	4.537765	-0.451202
C	2.113429	3.258280	0.381530
N	1.053302	2.424728	-0.165212
H	1.226648	2.033509	-1.090256
C	-0.190096	2.297250	0.340683
S	-0.685420	2.939526	1.810739
N	-1.011128	1.552941	-0.481821
H	-0.766011	1.522171	-1.471007
C	-2.303914	1.074877	-0.184729
C	-4.827537	-0.060151	0.253975
C	-2.581634	0.432970	1.028383
C	-3.281434	1.137450	-1.171537
C	-4.535715	0.572361	-0.943137
C	-3.832278	-0.126354	1.229813
H	-1.814414	0.350104	1.787877
H	-3.062655	1.612522	-2.123282
H	-5.801179	-0.507063	0.423584
C	-4.131286	-0.879542	2.494966
C	-5.579092	0.697220	-2.017227
F	-5.189988	-0.366085	3.137401
F	-6.049922	1.950955	-2.099828
F	-6.625855	-0.108119	-1.796341
F	-5.078230	0.392946	-3.223490
H	2.492651	4.262085	-1.490358
F	-4.434279	-2.164311	2.227649
F	-3.099531	-0.882774	3.344486
C	2.313645	-1.301742	-1.673205
H	1.999814	-0.106589	0.510009
N	1.290595	-0.729648	0.074873
H	0.551285	-0.124618	-0.286224
C	0.726564	-1.693139	0.946274
C	-0.401875	-3.639913	2.598935
C	1.485604	-2.265788	1.968541
C	-0.589776	-2.115353	0.736019
C	-1.153707	-3.075830	1.569212
C	0.917947	-3.235708	2.789287
H	2.519264	-1.959688	2.107573
H	-1.167860	-1.672599	-0.073389
H	-2.187246	-3.371616	1.419813
H	1.511876	-3.673872	3.585173
H	-0.843016	-4.387326	3.249663
O	2.323582	-1.401075	-3.591533
C	1.336735	-1.562622	-2.752303
C	3.201452	-2.367655	-1.165818
C	4.954930	-4.315750	-0.197362
C	4.585126	-2.163391	-1.214421
C	2.703528	-3.562603	-0.634172
C	3.579834	-4.529009	-0.148164
C	5.458764	-3.132278	-0.736144
H	4.969083	-1.248600	-1.656990
H	1.632903	-3.730195	-0.576979
H	3.184015	-5.447878	0.272085
H	6.530212	-2.968021	-0.787767
H	5.635236	-5.072696	0.180207
H	2.702558	-0.291655	-1.704267
C	0.467993	-2.797321	-2.845271
H	-0.205858	-2.908545	-1.993175
H	1.136871	-3.657016	-2.906207
H	-0.121626	-2.749468	-3.763735
N	0.317357	-0.291161	-2.714543
O	-0.875759	-0.470724	-2.562436
O	0.819120	0.826784	-2.764857
H	1.298616	5.056380	-0.457275
H	1.800212	3.537861	1.390746
C	3.439019	2.480388	0.450800
H	3.724806	2.223728	-0.583140
C	4.532689	3.401883	1.020098
H	4.275101	3.679647	2.050828
H	5.485482	2.864399	1.059996
C	3.368652	5.437144	0.099805
H	3.474359	6.327272	-0.528205
H	3.086108	5.784295	1.102457
C	4.689016	4.672918	0.181461
H	5.474641	5.304920	0.607607
H	5.014356	4.400139	-0.831788

N	3.291778	1.188717	1.150514
C	4.530087	0.415434	1.127326
H	5.285051	0.786761	1.836901
H	4.959898	0.437706	0.121499
H	4.316614	-0.629590	1.378992
C	2.786730	1.295478	2.520243
H	1.792930	1.750353	2.530429
H	3.455467	1.868004	3.181216
H	2.693445	0.286722	2.934673

SR epoxide:Catalyst:Aniline, Transition State 46; Energy = -2737.301088; 6-31G(d) basis set.

N	-2.261333	-1.937225	-0.492410
H	-1.644564	-1.197344	-0.817872
C	-1.914859	-3.204622	-0.729186
S	-2.945623	-4.525295	-0.634709
N	-0.585694	-3.389670	-1.091744
H	-0.431467	-4.312759	-1.480811
C	0.538919	-2.846706	-0.443452
C	2.898275	-1.998390	0.840402
C	0.469780	-2.130430	0.756543
C	1.793677	-3.104265	-1.009242
C	2.948957	-2.680159	-0.369694
C	1.648894	-1.732241	1.381232
H	-0.487647	-1.886428	1.205856
H	1.857159	-3.631575	-1.957190
H	3.803407	-1.660763	1.329083
C	1.543825	-1.045554	2.712707
C	4.271674	-2.967452	-1.023608
F	2.701993	-0.508674	3.106885
F	5.280091	-2.319462	-0.427642
F	4.266870	-2.601409	-2.316921
F	4.561880	-4.276094	-0.997049
F	0.631860	-0.047712	2.687258
F	1.139030	-1.888452	3.673088
C	-0.665434	3.219655	-0.461972
H	0.130871	1.690943	1.359846
N	0.144410	1.498986	0.359521
H	-0.540274	0.760861	0.176223
C	1.454582	1.155540	-0.073819
C	4.032344	0.635965	-1.005589
C	2.561114	1.574303	0.666507
C	1.633857	0.465376	-1.274933
C	2.921467	0.214944	-1.736878
C	3.845623	1.311144	0.198377
H	2.414334	2.112349	1.600091
H	0.764766	0.130626	-1.833436
H	3.056748	-0.331583	-2.664637
H	4.701526	1.638155	0.780359
H	5.033592	0.424263	-1.366267
O	-1.767664	4.186683	-1.740530
C	-1.115923	3.071274	-1.872894
C	0.406914	4.152129	-0.060386
C	2.406344	5.886179	0.839649
C	0.202077	4.943402	1.075861
C	1.634091	4.222143	-0.730111
C	2.624680	5.090987	-0.282587
C	1.193633	5.808767	1.522824
H	-0.749841	4.888448	1.597584
H	1.831993	3.576435	-1.579140
H	3.573771	5.135860	-0.806820
H	1.019345	6.424922	2.398899
H	3.181987	6.562283	1.185292
H	-1.505334	3.137170	0.219838
C	-0.228376	2.882143	-3.090266
H	0.393078	1.987617	-3.037246
H	0.395827	3.770659	-3.190566
H	-0.875110	2.828459	-3.970963
N	-2.096082	1.782121	-1.878069
O	-3.285703	1.977035	-1.895484
O	-1.579194	0.662823	-1.829379
C	-3.588129	-1.513919	-0.066309
H	-3.983757	-2.325107	0.555412
C	-3.506842	-0.223878	0.762497
H	-3.243761	0.590665	0.072964

C	-4.530709	-1.317500	-1.259226
H	-4.129436	-0.511245	-1.885503
H	-4.543514	-2.238687	-1.849787
C	-5.934618	-0.962982	-0.767020
H	-6.345447	-1.815927	-0.209523
H	-6.598339	-0.790885	-1.620375
C	-4.916014	0.084234	1.299016
H	-5.255102	-0.735498	1.947320
H	-4.895817	0.992942	1.909122
C	-5.900447	0.269317	0.138194
H	-6.900102	0.486652	0.528761
H	-5.588263	1.140281	-0.452737
N	-2.417981	-0.269794	1.754256
C	-2.504275	-1.391587	2.685628
H	-3.396903	-1.349709	3.330475
H	-1.620042	-1.378234	3.331381
H	-2.511531	-2.343101	2.145279
C	-2.321336	0.976928	2.501403
H	-2.325520	1.825667	1.807090
H	-1.389323	0.985876	3.073774
H	-3.148193	1.126942	3.213257

SR epoxide:Catalyst:Aniline, Transition State 47; Energy = -2737.285581; 6-31G(d) basis set.

C	-1.503876	-2.566233	0.305862
C	-0.356188	-3.905504	-1.537705
C	-2.732822	-4.404057	-0.957556
C	-1.408101	-5.004007	-1.423801
C	-2.528161	-3.706922	0.384728
C	-0.156277	-3.096831	-0.242808
H	-0.665252	-3.202517	-2.325533
H	-3.095831	-3.687826	-1.708522
H	-1.079874	-5.762630	-0.701059
H	-2.176788	-4.462477	1.098323
H	0.348042	-3.706393	0.512483
H	-1.864027	-1.847637	-0.447277
H	0.617414	-4.308377	-1.835630
H	-3.499630	-5.179008	-0.857130
H	-1.521902	-5.508687	-2.388489
H	-3.470379	-3.305560	0.775359
N	-1.485328	-1.829639	1.587811
N	0.729009	-1.986009	-0.567686
H	0.323265	-1.290631	-1.193568
C	-1.430005	-2.669698	2.783820
H	-0.527685	-3.301598	2.815163
H	-2.314185	-3.301976	2.866195
H	-1.407776	-2.015348	3.659373
C	-0.487240	-0.768806	1.725306
H	-0.440080	-0.157655	0.824070
H	0.524203	-1.146160	1.937039
H	-0.787425	-0.124641	2.560667
C	1.989913	-1.800655	-0.139549
S	2.797979	-2.878945	0.871106
N	2.506201	-0.608765	-0.581631
H	1.822594	0.039559	-0.967868
C	3.756042	-0.029114	-0.317470
C	6.196235	1.293350	0.105367
C	4.948374	-0.757841	-0.272286
C	3.793898	1.359435	-0.168188
C	5.006715	2.006706	0.034737
C	6.145503	-0.088361	-0.050532
H	4.936951	-1.830040	-0.413405
H	2.869617	1.930087	-0.201411
H	7.139966	1.800127	0.271800
C	7.417057	-0.882860	0.062241
C	5.024367	3.505841	0.131107
F	7.362238	-2.016941	-0.648245
F	5.073028	4.078153	-1.082064
F	3.923666	3.975542	0.737315
F	6.086441	3.948440	0.817302
F	8.475778	-0.182356	-0.372432
F	7.672976	-1.226308	1.333549
N	-0.989226	1.027673	-1.200429
O	0.199699	1.228945	-0.997037
O	-1.404984	0.012445	-1.730641

C	-2.054847	2.232488	-0.858533
C	-3.391442	1.620369	-0.687303
H	-3.576412	0.832073	-1.405530
C	-4.561722	2.432759	-0.271976
C	-6.876778	3.797917	0.499711
C	-4.584028	3.170999	0.916392
C	-5.714928	2.371953	-1.058266
C	-6.864908	3.056425	-0.678855
C	-5.735553	3.852137	1.298194
H	-3.708590	3.201832	1.558878
H	-5.703463	1.783240	-1.970917
H	-7.752955	3.004071	-1.300179
H	-5.742476	4.422482	2.221495
H	-7.774509	4.328963	0.799966
O	-2.493753	2.748176	-1.974983
C	-1.366111	3.101582	0.166923
H	-0.440324	3.491615	-0.257629
H	-1.135586	2.554558	1.086918
H	-2.026195	3.942042	0.384548
H	-2.827091	-0.459717	0.992065
N	-3.581860	0.236143	0.849145
H	-3.643348	0.790260	1.702878
C	-4.819333	-0.426580	0.585241
C	-7.238289	-1.640168	-0.086448
C	-5.978688	-0.102070	1.288465
C	-4.873886	-1.337804	-0.471298
C	-6.079903	-1.950983	-0.795812
C	-7.183423	-0.710666	0.949835
H	-5.938117	0.634052	2.087516
H	-3.971195	-1.555162	-1.038369
H	-6.112339	-2.666875	-1.611264
H	-8.082987	-0.454221	1.500218
H	-8.179259	-2.114691	-0.344158

SR epoxide:Catalyst:Aniline, Transition State 48; Energy = -2737.310785; 6-31G(d) basis set.

N	-1.933657	-1.813382	0.155424
C	-0.679747	-2.119259	-0.255012
S	-0.359311	-2.771238	-1.775754
N	0.259232	-1.782863	0.685764
C	1.653823	-1.670923	0.566929
C	2.449988	-2.447834	-0.273821
C	3.816742	-2.179107	-0.354378
C	4.418586	-1.186216	0.401162
C	3.616820	-0.452149	1.274527
C	2.256843	-0.684298	1.366402
C	4.627416	-2.934773	-1.367602
F	4.504645	-2.387612	-2.590420
C	4.262881	0.607097	2.120118
F	5.110858	1.360447	1.397319
F	4.236486	-4.211587	-1.472950
F	5.934864	-2.933252	-1.070005
F	4.985560	0.071552	3.117026
F	3.369154	1.433329	2.679382
H	-2.102831	-1.698172	1.157259
H	-0.112782	-1.158188	1.405260
H	2.014747	-3.233517	-0.874110
H	5.480737	-0.984330	0.315733
H	1.637536	-0.068076	2.012225
N	-2.888785	1.115254	1.421870
O	-3.645162	1.693744	0.651019
O	-3.221800	0.234071	2.180511
C	-1.372377	1.570687	1.476001
C	-0.759222	1.278759	0.165266
H	-1.206052	0.404513	-0.299211
O	-0.607672	0.588246	1.928244
C	0.617870	1.576846	-0.258250
C	3.247949	1.928952	-1.138908
C	1.426179	2.561509	0.317640
C	1.134301	0.789079	-1.297265
C	2.442179	0.959996	-1.735043
C	2.735753	2.730177	-0.119944
H	1.047661	3.192009	1.112043
H	0.518364	0.004322	-1.735736
H	2.840295	0.311285	-2.509423

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H          3.365165        3.477954        0.351299
H          4.279097        2.050477       -1.455931
C         -1.407861        2.887498        2.226525
H         -0.390777        3.201078        2.455782
H         -1.919725        3.667519        1.660936
H         -1.924590        2.718299        3.175949
N         -1.722406        2.437199       -1.389102
H         -1.432094        1.972065       -2.247028
H         -2.705532        2.254604       -1.197079
C         -1.404256        3.816983       -1.367415
C         -0.717812        6.516388       -1.197271
C         -0.202614        4.266931       -1.920405
C         -2.261375        4.717244       -0.728776
C         -1.913991        6.061635       -0.645556
C          0.131544        5.614798       -1.835058
H          0.465665        3.560858       -2.407310
H         -3.196526        4.356759       -0.306797
H         -2.586698        6.756566       -0.152891
H          1.065045        5.958916       -2.269005
H         -0.451755        7.566228       -1.134013
C         -3.141721       -2.105828       -0.604095
C         -3.407183       -1.084184       -1.715622
H         -3.025250       -3.093702       -1.070154
C         -4.665758       -1.475533       -2.494994
H         -3.549305       -0.098008       -1.248078
H         -2.537761       -1.030845       -2.378305
C         -5.875181       -1.614375       -1.565391
H         -4.869868       -0.737257       -3.277463
H         -4.482644       -2.432345       -3.002062
C         -5.584271       -2.575831       -0.407123
H         -6.124848       -0.627633       -1.151990
H         -6.750327       -1.953883       -2.129268
C         -4.338314       -2.112017        0.362603
H         -6.445128       -2.623268        0.269222
H         -5.423915       -3.588710       -0.800251
H         -4.507461       -1.069557        0.669169
N         -4.009548       -2.824851        1.595863
C         -4.955165       -2.556169        2.666435
H         -5.948986       -3.003768        2.493817
H         -5.069905       -1.475613        2.785191
H         -4.562270       -2.966356        3.601874
C         -3.796833       -4.253788        1.423779
H         -3.436724       -4.673089        2.367867
H         -4.712311       -4.798862        1.138330
H         -3.031315       -4.436113        0.663366

SR epoxide:Catalyst:Aniline, Transition State 49; Energy = -2737.309910; 6-31G(d)
basis set.
N         -2.252194       -1.550705        0.186752
C         -1.073622       -2.098680       -0.171615
S         -0.863986       -2.970425       -1.601206
N         -0.087783       -1.856060        0.753982
C          1.308056       -1.881129        0.616929
C          2.023404       -2.754892       -0.201089
C          3.409061       -2.616517       -0.291035
C          4.105539       -1.662808        0.433345
C          3.379514       -0.827235        1.281828
C          2.004582       -0.927811        1.379092
C          4.137904       -3.472589       -1.286492
F          4.021832       -2.969232       -2.529288
C          4.116924        0.203267        2.086899
F          5.055042        0.821108        1.347978
F          3.653830       -4.720298       -1.327038
F          5.449196       -3.552969       -1.019386
F          4.753926       -0.344148        3.133335
F          3.301012        1.150566        2.572822
H         -2.259688       -0.893650        0.970114
H         -0.377795       -1.204133        1.480000
H          1.510792       -3.513722       -0.774996
H          5.181417       -1.564488        0.339247
H          1.445399       -0.233356        2.000254
N         -2.784374        2.042098        1.377417
O         -3.198313        3.167697        1.147146
O         -3.483508        1.057372        1.491343
C         -1.221028        1.842592        1.467731
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C	-0.779519	1.491630	0.097638
H	-1.476653	0.821592	-0.397794
O	-0.908271	0.596760	1.792176
C	0.604655	1.446072	-0.376592
C	3.210971	1.220267	-1.352701
C	1.605883	2.312930	0.081601
C	0.915137	0.496686	-1.361679
C	2.214126	0.376341	-1.841180
C	2.902826	2.193874	-0.403720
H	1.375311	3.093096	0.797670
H	0.143402	-0.181368	-1.723800
H	2.452849	-0.395886	-2.566057
H	3.677341	2.855824	-0.031093
H	4.231804	1.116396	-1.707975
C	-0.685553	2.962997	2.337029
H	0.348921	2.726771	2.588108
H	-0.744675	3.937007	1.850055
H	-1.260323	2.988372	3.266765
N	-1.487060	3.046160	-1.271656
H	-1.516407	2.561444	-2.166594
H	-2.434968	3.251917	-0.959398
C	-0.666064	4.201378	-1.305755
C	1.043143	6.404421	-1.249550
C	0.462418	4.228961	-2.127281
C	-0.940899	5.274504	-0.454177
C	-0.084221	6.370541	-0.430491
C	1.309757	5.331852	-2.097409
H	0.681792	3.380767	-2.771596
H	-1.823977	5.242478	0.179157
H	-0.304198	7.204113	0.228941
H	2.185902	5.346807	-2.737859
H	1.707041	7.262159	-1.228670
C	-3.507651	-1.715442	-0.532391
C	-3.743048	-0.549191	-1.500818
H	-3.412238	-2.635254	-1.118598
C	-5.051083	-0.729427	-2.270896
H	-3.789369	0.383687	-0.918567
H	-2.884967	-0.484907	-2.182218
C	-6.222545	-0.885471	-1.299751
H	-5.215858	0.119618	-2.942778
H	-4.975994	-1.625861	-2.900902
C	-5.981989	-2.047399	-0.333078
H	-6.340228	0.043998	-0.725682
H	-7.156755	-1.041165	-1.849475
C	-4.678771	-1.872649	0.459777
H	-6.804475	-2.143016	0.381829
H	-5.941930	-2.984530	-0.904871
H	-4.767021	-0.935722	1.026133
N	-4.525845	-2.940385	1.447124
C	-4.087460	-4.215702	0.908021
H	-3.026886	-4.217478	0.597322
H	-4.697417	-4.500295	0.046287
H	-4.213102	-4.987507	1.674496
C	-3.764936	-2.596227	2.636555
H	-4.024862	-3.291592	3.443102
H	-2.671369	-2.649646	2.496154
H	-4.022092	-1.584169	2.963634

SR epoxide:Catalyst:Aniline, Transition State 50; Energy = -2737.299770; 6-31G(d) basis set.

N	-2.331649	-1.336650	0.345770
C	-1.209087	-1.970112	-0.045972
S	-1.115563	-2.869700	-1.471072
N	-0.177387	-1.791952	0.843352
C	1.205966	-1.940554	0.669163
C	1.818653	-2.885924	-0.152570
C	3.208102	-2.872609	-0.280897
C	4.005625	-1.973849	0.408526
C	3.379758	-1.064144	1.260663
C	2.004530	-1.040745	1.395628
C	3.830725	-3.804594	-1.280290
F	3.728159	-3.309781	-2.527666
C	4.228500	-0.091043	2.026578
F	5.190887	0.434951	1.248640
F	3.235047	-5.003712	-1.288868

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F          5.135878       -3.999846       -1.044514
F          4.851229       -0.678601        3.059805
F          3.513329        0.928485        2.524009
H         -2.267006       -0.678902        1.126071
H         -0.390399       -1.106957        1.565610
H          1.225436       -3.604214       -0.700458
H          5.083037       -1.972558        0.285147
H          1.526110       -0.289790        2.018606
N         -2.550401        2.301114        1.436623
O         -2.888753        3.440540        1.155208
O         -3.315338        1.377652        1.617312
C         -1.002418        1.996524        1.506659
C         -0.611783        1.578242        0.140277
H         -1.365108        0.947649       -0.323360
O         -0.767908        0.741440        1.859963
C          0.756602        1.416911       -0.356554
C          3.317043        0.974670       -1.379831
C          1.831348        2.208409        0.069295
C          0.972354        0.432042       -1.332055
C          2.247593        0.204707       -1.835920
C          3.105200        1.981121       -0.438869
H          1.676962        3.012952        0.778685
H          0.142825       -0.189328       -1.667511
H          2.410246       -0.593459       -2.553742
H          3.936337        2.585228       -0.090753
H          4.319165        0.786681       -1.753307
C         -0.379401        3.102800        2.335044
H          0.640291        2.805049        2.580706
H         -0.380481        4.063629        1.819031
H         -0.937409        3.194311        3.270887
N         -1.220015        3.134206       -1.265918
H         -1.268908        2.629334       -2.148912
H         -2.157564        3.397291       -0.965890
C         -0.340165        4.244888       -1.321957
C          1.472991        6.364027       -1.312163
C          0.794819        4.194582       -2.133544
C         -0.568848        5.353620       -0.502804
C          0.339275        6.407422       -0.502340
C          1.694223        5.255986       -2.126772
H          0.976835        3.319674       -2.753255
H         -1.455960        5.381108        0.124803
H          0.154830        7.268921        0.131608
H          2.574667        5.210840       -2.759860
H          2.177170        7.189273       -1.309831
C         -3.613075       -1.390263       -0.346795
C         -3.754224       -0.194184       -1.298352
H         -3.609228       -2.310452       -0.939041
C         -5.007514       -0.312244       -2.181809
H         -3.806076        0.717911       -0.687778
H         -2.849606       -0.131434       -1.916261
C         -6.133909       -1.075315       -1.460134
H         -5.349625        0.691539       -2.455270
H         -4.755840       -0.825836       -3.115204
C         -6.059236       -0.858812        0.054450
H         -7.109777       -0.756691       -1.839726
H         -6.048107       -2.143313       -1.686854
C         -4.771757       -1.433023        0.686268
H         -6.094253        0.219025        0.254572
H         -6.919874       -1.298239        0.568241
H         -4.486684       -0.772196        1.515419
N         -5.013880       -2.740759        1.300953
C         -5.542004       -3.761644        0.413809
H         -4.857972       -4.036156       -0.410130
H         -6.496260       -3.445381       -0.014222
H         -5.727595       -4.667290        0.999473
C         -3.880346       -3.258494        2.050717
H         -4.222147       -4.084758        2.683381
H         -3.061544       -3.636279        1.414398
H         -3.476161       -2.474621        2.699182

SR epoxide:Catalyst:Aniline, Transition State 51; Energy = -2737.301574; 6-31G(d)
basis set.
N         -1.997090       -1.784200        0.125011
C         -0.749848       -2.087327       -0.298942
S         -0.444466       -2.696521       -1.840326
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N	0.196455	-1.786096	0.647583
C	1.592926	-1.703124	0.536408
C	2.374249	-2.472897	-0.324631
C	3.747931	-2.237105	-0.388378
C	4.370545	-1.285978	0.403162
C	3.582189	-0.558836	1.294465
C	2.215900	-0.757393	1.369562
C	4.544592	-2.977716	-1.423430
F	5.851297	-3.012650	-1.124927
C	4.249027	0.454459	2.179483
F	5.139361	1.192844	1.493425
F	4.435112	-2.389960	-2.628846
F	4.127416	-4.242125	-1.569448
F	4.929487	-0.131602	3.177778
F	3.374483	1.299646	2.740991
H	-2.160743	-1.655955	1.127734
H	-0.164266	-1.169095	1.379000
H	1.922341	-3.226252	-0.953524
H	5.438077	-1.109393	0.330318
H	1.608011	-0.143904	2.028844
N	-2.885772	1.153311	1.303377
O	-3.593249	1.676810	0.450429
O	-3.270686	0.338977	2.109856
C	-1.365598	1.592178	1.410834
C	-0.705522	1.299903	0.123733
H	-1.146473	0.435672	-0.363922
O	-0.630017	0.599774	1.890159
C	0.692078	1.575581	-0.246037
C	3.351392	1.897625	-1.047520
C	1.504923	2.524493	0.380393
C	1.221663	0.803499	-1.290514
C	2.543471	0.960083	-1.689612
C	2.828843	2.678594	-0.018398
H	1.120301	3.135675	1.186675
H	0.602811	0.041512	-1.763837
H	2.949988	0.323182	-2.469431
H	3.460752	3.398363	0.491564
H	4.392525	2.007543	-1.334755
C	-1.418626	2.906177	2.164845
H	-0.408514	3.229962	2.409746
H	-1.928402	3.684542	1.594817
H	-1.948154	2.727267	3.105313
N	-1.576995	2.489909	-1.455942
H	-1.237267	2.041869	-2.304600
H	-2.569509	2.305078	-1.323438
C	-1.259291	3.868434	-1.389745
C	-0.582658	6.563086	-1.130196
C	-0.026408	4.326075	-1.861990
C	-2.152905	4.758769	-0.788333
C	-1.810381	6.100790	-0.659933
C	0.302765	5.671672	-1.732313
H	0.668467	3.628208	-2.322938
H	-3.112470	4.392542	-0.430841
H	-2.511063	6.788046	-0.196353
H	1.260512	6.022212	-2.103818
H	-0.320158	7.611153	-1.032290
C	-3.219077	-2.073266	-0.615427
C	-3.484649	-1.056447	-1.746091
H	-3.122149	-3.075587	-1.053340
C	-4.983735	-0.948320	-2.085526
H	-3.110434	-0.078899	-1.416337
H	-2.905921	-1.351318	-2.624822
C	-5.687665	-2.280908	-1.820223
H	-5.451928	-0.168258	-1.472291
H	-5.107846	-0.644360	-3.129322
C	-5.652449	-2.616848	-0.316132
H	-6.722012	-2.253847	-2.175841
H	-5.181557	-3.067624	-2.393192
C	-4.397248	-2.038479	0.372548
H	-6.540627	-2.207788	0.177825
H	-5.685113	-3.703644	-0.179871
H	-4.582833	-0.979091	0.597366
N	-4.030988	-2.634695	1.657272
C	-5.010259	-2.354758	2.694027
H	-5.967487	-2.881009	2.536979

H	-5.199126	-1.278595	2.730719
H	-4.608531	-2.668465	3.662452
C	-3.703027	-4.051350	1.605524
H	-3.299943	-4.351671	2.577364
H	-4.568328	-4.698602	1.387222
H	-2.932440	-4.236596	0.850951

SR epoxide:Catalyst:Aniline, Transition State 52; Energy = -2737.303805; 6-31G(d) basis set.

N	-2.279191	-1.540670	0.104333
C	-1.099343	-2.089569	-0.243269
S	-0.875766	-2.943109	-1.681812
N	-0.128123	-1.874010	0.702995
C	1.269658	-1.921812	0.594895
C	1.986438	-2.799004	-0.219180
C	3.375701	-2.688171	-0.273762
C	4.073677	-1.758051	0.480562
C	3.344979	-0.917810	1.321060
C	1.965960	-0.991996	1.384590
C	4.120992	-3.536554	-1.263676
F	4.166911	-2.939426	-2.469425
C	4.082919	0.088554	2.155814
F	5.052582	0.693571	1.447955
F	3.544307	-4.730940	-1.442283
F	5.390667	-3.748811	-0.888173
F	4.680696	-0.482579	3.212656
F	3.274597	1.048241	2.630407
H	-2.299771	-0.901047	0.902241
H	-0.422348	-1.229851	1.434147
H	1.472614	-3.539221	-0.815403
H	5.153604	-1.681437	0.414157
H	1.405475	-0.294171	2.000754
N	-2.731587	2.109705	1.344297
O	-3.093519	3.257674	1.133799
O	-3.473648	1.154477	1.426209
C	-1.179924	1.842517	1.452156
C	-0.729032	1.506762	0.081133
H	-1.438529	0.868513	-0.438156
O	-0.921637	0.578474	1.752753
C	0.661164	1.428364	-0.371388
C	3.276555	1.145790	-1.308539
C	1.676827	2.264997	0.111189
C	0.963219	0.481895	-1.361773
C	2.266457	0.332623	-1.821334
C	2.977890	2.118002	-0.355148
H	1.454543	3.044559	0.830575
H	0.180172	-0.171692	-1.743922
H	2.497323	-0.437415	-2.551025
H	3.762249	2.757956	0.034857
H	4.299795	1.019349	-1.649313
C	-0.611366	2.919084	2.355446
H	0.411161	2.637557	2.609061
H	-0.629449	3.907422	1.894731
H	-1.194097	2.940891	3.280336
N	-1.363632	3.112889	-1.262241
H	-1.400101	2.648993	-2.167778
H	-2.307012	3.343567	-0.953639
C	-0.504699	4.240670	-1.264843
C	1.275399	6.384271	-1.149701
C	0.627991	4.250411	-2.080873
C	-0.748515	5.301879	-0.389235
C	0.143506	6.368245	-0.336309
C	1.510872	5.323766	-2.021606
H	0.822463	3.411015	-2.744386
H	-1.635427	5.283837	0.239194
H	-0.052342	7.193046	0.341504
H	2.389999	5.325096	-2.658129
H	1.966888	7.219031	-1.105975
C	-3.530067	-1.686508	-0.633754
C	-3.698871	-0.460605	-1.548175
H	-3.439624	-2.582710	-1.255619
C	-5.022159	-0.454452	-2.306880
H	-3.652376	0.439237	-0.917504
H	-2.840425	-0.439663	-2.231352
C	-6.176198	-0.533728	-1.310231

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H         -5.095156        0.445907       -2.926285
H         -5.063169       -1.316497       -2.985661
C         -6.031476       -1.789570       -0.454588
H         -6.164743        0.358092       -0.668202
H         -7.139859       -0.543500       -1.830088
C         -4.711593       -1.852754        0.335267
H         -6.869329       -1.876654        0.244425
H         -6.066574       -2.679534       -1.096172
H         -4.672296       -0.990234        1.027806
N         -4.715218       -3.114293        1.096982
C         -3.467248       -3.833713        1.297969
H         -2.757519       -3.326000        1.975191
H         -2.962966       -4.027367        0.348275
H         -3.712969       -4.803943        1.742441
C         -5.391182       -2.941558        2.370947
H         -5.566610       -3.919461        2.829968
H         -4.804234       -2.328527        3.080191
H         -6.361440       -2.458073        2.230270

SR epoxide:Catalyst:Aniline, Transition State 53; Energy = -2737.299462; 6-31G(d)
basis set.
N         -2.339599       -1.316894        0.303590
C         -1.208529       -1.924985       -0.098582
S         -1.081224       -2.732290       -1.578458
N         -0.189738       -1.782686        0.810853
C          1.192259       -1.961264        0.662349
C          1.796125       -2.909712       -0.163421
C          3.187126       -2.932811       -0.262901
C          3.993993       -2.066853        0.458170
C          3.375934       -1.154591        1.312370
C          1.998870       -1.096401        1.420876
C          3.814420       -3.859241       -1.264462
F          3.855485       -3.292328       -2.484816
C          4.236283       -0.217180        2.109340
F          5.222760        0.299976        1.355577
F          3.132845       -5.004375       -1.390419
F          5.077644       -4.170583       -0.939331
F          4.829927       -0.839461        3.139567
F          3.539409        0.809922        2.616255
H         -2.304390       -0.726829        1.136122
H         -0.405673       -1.114278        1.547823
H          1.194808       -3.601832       -0.735329
H          5.073568       -2.093508        0.357126
H          1.527961       -0.343816        2.047647
N         -2.521378        2.291286        1.366029
O         -2.857302        3.412580        1.014999
O         -3.288450        1.379817        1.589402
C         -0.972960        1.996230        1.486408
C         -0.536798        1.564789        0.138032
H         -1.272452        0.923891       -0.340203
O         -0.740816        0.749772        1.865682
C          0.847574        1.404000       -0.313603
C          3.437840        0.967273       -1.263614
C          1.912553        2.179185        0.163035
C          1.089518        0.439318       -1.302717
C          2.378800        0.215275       -1.771000
C          3.201132        1.953624       -0.307592
H          1.741424        2.968781        0.884925
H          0.267998       -0.170496       -1.676920
H          2.559437       -0.568136       -2.500718
H          4.024139        2.543913        0.081273
H          4.450528        0.780385       -1.607894
C         -0.391057        3.123179        2.318648
H          0.616683        2.835046        2.618111
H         -0.371225        4.072360        1.781633
H         -0.990940        3.233547        3.226169
N         -1.094698        3.093975       -1.312991
H         -1.106868        2.575458       -2.189282
H         -2.043214        3.357072       -1.050136
C         -0.214331        4.204595       -1.349482
C          1.595351        6.326393       -1.298682
C          0.955088        4.141588       -2.109866
C         -0.478737        5.327178       -0.560475
C          0.427710        6.382277       -0.539514
C          1.852504        5.204264       -2.082916
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H	1.165021	3.255941	-2.705185
H	-1.391970	5.363940	0.027951
H	0.215578	7.254408	0.070825
H	2.759856	5.148818	-2.675953
H	2.298202	7.152595	-1.280481
C	-3.595199	-1.330167	-0.430053
C	-3.714735	-0.139782	-1.388403
H	-3.588968	-2.244589	-1.028143
C	-4.924132	-0.318015	-2.327221
H	-3.820787	0.775814	-0.789663
H	-2.786956	-0.058152	-1.967238
C	-6.037668	-1.150462	-1.663762
H	-5.313514	0.666737	-2.606604
H	-4.603509	-0.806823	-3.252841
C	-6.078115	-0.893795	-0.155697
H	-7.005285	-0.915847	-2.118459
H	-5.862027	-2.216993	-1.847234
C	-4.774634	-1.345989	0.557692
H	-6.226316	0.179346	0.016562
H	-6.937112	-1.398213	0.301429
H	-4.548543	-0.603609	1.332018
N	-4.838450	-2.629833	1.260012
C	-5.598904	-2.540367	2.494057
H	-6.677248	-2.354476	2.337013
H	-5.199941	-1.734581	3.117274
H	-5.502409	-3.480563	3.045911
C	-5.314151	-3.742186	0.454676
H	-5.226246	-4.662754	1.039449
H	-6.370639	-3.640736	0.146087
H	-4.701205	-3.864032	-0.442481

SR epoxide:Catalyst:Aniline, Transition State 54; Energy = -2737.303805; 6-31G(d) basis set.

N	-2.274898	-1.542551	0.106589
C	-1.094791	-2.092502	-0.238447
S	-0.869729	-2.950179	-1.674232
N	-0.124042	-1.874218	0.707815
C	1.273741	-1.920731	0.598689
C	1.991407	-2.800516	-0.210531
C	3.381005	-2.685931	-0.268991
C	4.077839	-1.750333	0.478108
C	3.347951	-0.908556	1.317269
C	1.969735	-0.985567	1.383395
C	4.115191	-3.548802	-1.254598
F	4.017648	-3.046317	-2.499221
C	4.085012	0.102250	2.147295
F	5.052400	0.706903	1.436019
F	3.621358	-4.792632	-1.299409
F	5.422407	-3.639599	-0.971691
F	4.685655	-0.464130	3.205114
F	3.275459	1.061834	2.620127
H	-2.296020	-0.900627	0.902660
H	-0.418474	-1.227872	1.436967
H	1.478694	-3.545916	-0.801756
H	5.157030	-1.670250	0.408334
H	1.408569	-0.286549	1.997593
N	-2.729898	2.112943	1.347628
O	-3.090842	3.262368	1.143506
O	-3.472732	1.157816	1.423946
C	-1.178468	1.843539	1.452734
C	-0.731169	1.508134	0.080372
H	-1.442372	0.870623	-0.437414
O	-0.921373	0.578968	1.752199
C	0.657774	1.428859	-0.375542
C	3.270319	1.145335	-1.319922
C	1.674345	2.267435	0.101744
C	0.957402	0.479616	-1.363996
C	2.259324	0.329612	-1.826929
C	2.973959	2.120181	-0.368501
H	1.453694	3.048819	0.819697
H	0.173629	-0.175403	-1.742089
H	2.488059	-0.442974	-2.554621
H	3.759056	2.761948	0.017002
H	4.292601	1.019065	-1.663630
C	-0.605762	2.918552	2.355091

H	0.417709	2.636171	2.604037
H	-0.625278	3.907538	1.895881
H	-1.184784	2.939299	3.282326
N	-1.368312	3.116115	-1.259670
H	-1.406986	2.652708	-2.165378
H	-2.310992	3.346922	-0.949055
C	-0.509278	4.243873	-1.263932
C	1.271686	6.386933	-1.152080
C	0.620786	4.254287	-2.083579
C	-0.750138	5.304243	-0.386485
C	0.142304	6.370328	-0.335204
C	1.504132	5.327360	-2.025916
H	0.812948	3.415569	-2.748614
H	-1.634987	5.285736	0.244816
H	-0.051205	7.194419	0.344140
H	2.381266	5.329174	-2.665182
H	1.963556	7.221440	-1.109547
C	-3.524960	-1.689663	-0.632674
C	-3.692801	-0.465249	-1.549294
H	-3.433782	-2.586872	-1.252961
C	-5.015040	-0.460486	-2.309841
H	-3.647499	0.435584	-0.919915
H	-2.833466	-0.445139	-2.231388
C	-6.170412	-0.538121	-1.314617
H	-5.087225	0.438829	-2.930865
H	-5.055055	-1.323667	-2.987232
C	-6.026621	-1.792375	-0.456500
H	-6.159966	0.354882	-0.674212
H	-7.133369	-0.548996	-1.835754
C	-4.707718	-1.854107	0.335140
H	-6.865340	-1.878272	0.241622
H	-6.060851	-2.683495	-1.096518
H	-4.669227	-0.990275	1.026118
N	-4.712402	-3.114210	1.099158
C	-3.464816	-3.833594	1.302617
H	-2.755725	-3.325008	1.979842
H	-2.959532	-4.028726	0.353760
H	-3.711236	-4.803119	1.748238
C	-5.389715	-2.939064	2.372057
H	-5.565661	-3.916101	2.832722
H	-4.803532	-2.324701	3.080778
H	-6.359818	-2.455833	2.229408

SR epoxide:Catalyst:Aniline, Transition State 55; Energy = -2737.310943; 6-31G(d) basis set.

N	-2.205766	-1.636183	1.039446
C	-1.080292	-2.173631	0.530625
S	-1.018785	-3.189274	-0.819178
N	0.032101	-1.778784	1.237493
C	1.392914	-1.801781	0.908258
C	2.017291	-2.730682	0.073831
C	3.376960	-2.589270	-0.202410
C	4.143018	-1.574373	0.348166
C	3.514625	-0.679892	1.213462
C	2.165837	-0.785621	1.496351
C	3.994510	-3.517031	-1.208951
F	5.322524	-3.618729	-1.051618
C	4.330303	0.423305	1.822393
F	3.568366	1.382500	2.368022
F	3.783131	-3.078152	-2.463260
F	3.481809	-4.751996	-1.138147
F	5.116718	1.011108	0.902956
F	5.145081	-0.031212	2.786913
H	-2.085630	-0.897907	1.734312
H	-0.170022	-1.065026	1.934443
H	1.452719	-3.538492	-0.367841
H	5.196617	-1.475499	0.110741
H	1.681064	-0.052485	2.135335
N	-1.775187	3.089044	-0.778488
H	-2.292456	2.567598	-1.481471
H	-2.425889	3.568367	-0.156487
C	-0.778531	3.921826	-1.335324
C	1.366996	5.424042	-2.304017
C	-0.104190	3.516204	-2.489986
C	-0.388093	5.089607	-0.676337

C	0.681993	5.834534	-1.162973
C	0.964051	4.265825	-2.967051
H	-0.401581	2.599713	-2.992998
H	-0.927080	5.417371	0.208916
H	0.977691	6.742214	-0.646321
H	1.488318	3.937283	-3.858907
H	2.203407	6.005089	-2.677761
C	-3.598266	-1.927599	0.691445
C	-3.965757	-3.383822	1.014639
H	-4.174493	-1.280238	1.365247
C	-5.437504	-3.673456	0.720627
H	-3.335605	-4.047859	0.414495
H	-3.732373	-3.574069	2.067573
C	-5.771907	-3.332520	-0.731256
H	-5.655945	-4.725254	0.932422
H	-6.074805	-3.074567	1.386334
C	-5.457937	-1.861328	-1.007458
H	-5.178436	-3.968891	-1.401164
H	-6.826735	-3.537312	-0.942821
C	-3.974473	-1.546011	-0.753330
H	-5.715264	-1.597601	-2.040613
H	-6.089045	-1.244077	-0.353730
H	-3.378433	-2.183660	-1.411144
N	-3.583579	-0.156376	-1.063126
C	-3.292748	-0.003072	-2.481528
H	-2.510649	-0.709087	-2.774812
H	-2.928020	1.011773	-2.683278
H	-4.174059	-0.161558	-3.126840
C	-4.562490	0.835828	-0.632902
H	-4.127228	1.839380	-0.698139
H	-5.478678	0.835229	-1.245357
H	-4.838367	0.676447	0.412413
H	-0.321660	-0.263530	-1.351991
C	0.500569	0.415438	-1.127748
C	2.600761	2.139635	-0.519633
C	0.337974	1.387059	-0.130580
C	1.716061	0.282656	-1.791564
C	2.766823	1.144185	-1.483871
C	1.395880	2.260359	0.159408
H	1.848310	-0.506464	-2.525446
H	3.721595	1.037727	-1.990187
H	1.276422	3.046646	0.895270
H	3.418853	2.812593	-0.285684
C	-0.974370	1.452224	0.506800
H	-1.734763	0.779275	0.099361
O	-0.829256	0.669327	2.266251
C	-1.261656	1.864841	1.896894
C	-0.726663	3.088303	2.613005
H	-0.941458	4.011800	2.073922
H	0.349126	2.967226	2.739563
H	-1.178572	3.142738	3.607093
N	-2.840949	1.944066	1.997365
O	-3.430875	0.941965	2.338085
O	-3.378800	2.999306	1.695149

SR epoxide:Catalyst:Aniline, Transition State 1; Energy = -2738.170651; TZVP basis set.

C	-4.118058	0.793701	-0.328993
C	-4.163266	-1.614946	0.401126
C	-6.161791	-0.632824	-0.757679
C	-5.683771	-1.650569	0.275809
C	-5.650928	0.772657	-0.433962
C	-3.692030	-0.203358	0.753523
H	-3.709091	-1.903493	-0.553665
H	-5.792194	-0.926582	-1.746065
H	-6.128573	-1.418811	1.249246
H	-6.085450	1.107798	0.513761
H	-4.131580	0.075553	1.712931
H	-3.707993	0.429393	-1.280478
H	-3.805570	-2.307954	1.165286
H	-7.252127	-0.629199	-0.814978
H	-6.013388	-2.655284	0.005325
H	-5.979631	1.470888	-1.205456
N	-3.506851	2.111675	-0.118038
N	-2.250279	-0.151748	0.913053

H	-1.715968	-0.234734	0.042206
C	-3.806472	3.033586	-1.202835
H	-4.853879	3.368768	-1.208898
H	-3.588293	2.555634	-2.159139
H	-3.173440	3.915604	-1.111252
C	-3.790297	2.717775	1.174695
H	-3.431258	2.082395	1.986219
H	-4.858645	2.924151	1.335762
H	-3.253443	3.665869	1.235612
C	-1.609187	-0.306032	2.058783
S	-2.307330	-0.703962	3.539981
N	-0.230403	-0.133527	1.990368
H	0.238776	-0.501536	2.806644
C	0.470413	0.869928	1.317145
C	2.046905	2.877967	0.130326
C	1.861218	0.889361	1.491019
C	-0.126546	1.857987	0.530012
C	0.674665	2.836007	-0.046445
C	2.623626	1.886547	0.914752
H	2.335427	0.120679	2.090692
H	-1.200901	1.888687	0.363492
H	2.647024	3.656238	-0.319288
C	4.118122	1.857109	1.078704
C	-0.011871	3.877761	-0.888332
F	4.490218	1.317219	2.245471
F	0.845854	4.778958	-1.381321
F	-0.651153	3.330300	-1.929548
F	-0.930613	4.555826	-0.182117
F	4.708468	1.134012	0.110415
F	4.652292	3.082842	1.018723
N	-1.385671	-3.228345	-0.478188
O	-2.111564	-4.147381	-0.779996
O	-1.107430	-2.921550	0.661573
C	-0.757902	-2.330046	-1.644607
C	0.560117	-1.845746	-1.200067
H	0.558783	-1.472876	-0.185170
C	1.548566	-1.300633	-2.151984
C	3.483959	-0.229098	-3.844567
C	2.057342	-2.059693	-3.208302
C	2.018595	-0.006190	-1.953013
C	2.977608	0.531397	-2.799626
C	3.023309	-1.526524	-4.047231
H	1.707231	-3.072100	-3.370581
H	1.611665	0.580165	-1.142048
H	3.331438	1.541327	-2.635519
H	3.417568	-2.121741	-4.860636
H	4.237557	0.184995	-4.502037
O	-1.147566	-1.058399	-1.565984
C	-0.990259	-3.048359	-2.947304
H	-0.564555	-2.441092	-3.742813
H	-0.551051	-4.046232	-2.957051
H	-2.063072	-3.137142	-3.108225
H	1.072483	-4.181458	-0.148485
N	1.708440	-3.444855	-0.439158
H	2.308614	-3.785921	-1.182729
C	2.446956	-2.921006	0.657864
C	3.871060	-1.860946	2.795525
C	3.670936	-2.295828	0.432307
C	1.908467	-2.973150	1.941116
C	2.630399	-2.452037	3.006959
C	4.381850	-1.776732	1.505635
H	4.067523	-2.229955	-0.575054
H	0.936438	-3.425516	2.100216
H	2.218389	-2.512400	4.006577
H	5.336580	-1.298711	1.330170
H	4.431694	-1.456567	3.627987

SR epoxide:Catalyst:Aniline, Transition State 2; Energy = -2738.168277; TZVP basis set.

C	-5.022657	0.803733	-0.505172
C	-5.493436	-1.408958	-1.586052
C	-7.386574	0.187404	-1.117566
C	-6.975512	-1.278937	-1.239732
C	-6.501222	0.932379	-0.115875
C	-4.648744	-0.682883	-0.538631

H	-5.294394	-0.965543	-2.567270
H	-7.296600	0.668241	-2.097494
H	-7.164761	-1.790215	-0.289991
H	-6.654601	0.516808	0.885086
H	-4.849109	-1.141691	0.434597
H	-4.917473	1.184117	-1.530374
H	-5.190344	-2.454948	-1.622938
H	-8.434061	0.266930	-0.820826
H	-7.580684	-1.781960	-1.995800
H	-6.784797	1.985875	-0.077884
N	-4.062686	1.572207	0.293651
N	-3.219692	-0.787386	-0.791859
H	-2.775867	0.081223	-1.064336
C	-4.266822	3.008297	0.183093
H	-5.171436	3.358104	0.700987
H	-4.342621	3.287542	-0.868897
H	-3.410724	3.527625	0.614733
C	-3.980743	1.159381	1.685995
H	-3.689032	0.108693	1.754327
H	-4.921624	1.298933	2.237775
H	-3.209978	1.751910	2.179734
C	-2.454258	-1.835942	-0.479260
S	-3.053638	-3.291340	0.141734
N	-1.113154	-1.698881	-0.695753
H	-0.571171	-2.553398	-0.639511
C	-0.406996	-0.496675	-0.898643
C	1.076434	1.841646	-1.255847
C	0.566767	-0.432992	-1.893124
C	-0.631566	0.607250	-0.072026
C	0.105010	1.764002	-0.266513
C	1.300688	0.732204	-2.056339
H	0.770725	-1.300656	-2.505702
H	-1.370155	0.554784	0.718724
H	1.653023	2.748666	-1.395550
C	2.341545	0.843341	-3.140607
C	-0.127477	2.969468	0.601390
F	3.551698	1.125124	-2.645702
F	0.991640	3.338795	1.250764
F	-0.513235	4.032211	-0.119034
F	-1.064718	2.761881	1.531021
F	2.440059	-0.258760	-3.876967
F	2.036562	1.853281	-3.981190
N	2.309595	-3.280124	0.024738
O	2.355026	-3.962248	1.031953
O	1.366495	-3.251359	-0.728490
C	3.559258	-2.258812	-0.291834
C	3.139931	-0.977019	0.313290
H	2.079868	-0.780189	0.203082
C	4.012745	0.213865	0.385289
C	5.524590	2.551983	0.582934
C	5.291224	0.272816	-0.169092
C	3.488860	1.350961	1.002662
C	4.239885	2.510928	1.110744
C	6.039599	1.435995	-0.065287
H	5.671358	-0.555897	-0.746769
H	2.475835	1.328320	1.384043
H	3.813672	3.383760	1.588490
H	7.024432	1.476125	-0.512286
H	6.113555	3.457323	0.655219
O	3.435512	-1.705459	-1.461363
C	4.794371	-3.045254	0.090181
H	4.730997	-3.444662	1.099509
H	4.899899	-3.873030	-0.611729
H	5.673052	-2.412939	0.011261
H	2.910855	-2.342219	2.413196
N	2.770616	-1.335932	2.346020
H	3.494982	-0.849165	2.864569
C	1.456581	-0.953140	2.743195
C	-1.119019	-0.172559	3.448074
C	1.253975	0.241253	3.432034
C	0.367622	-1.745597	2.386161
C	-0.915287	-1.355790	2.748891
C	-0.031929	0.626714	3.781541
H	2.103285	0.853466	3.713302
H	0.515599	-2.681521	1.858688

H	-1.752506	-1.986236	2.470403
H	-0.180984	1.551682	4.323674
H	-2.118127	0.121761	3.740570

SR epoxide:Catalyst:Aniline, Transition State 3, TS-SR; Energy = -2738.177802; TZVP basis set.

N	-2.130523	-1.652441	0.135587
C	-0.909563	-2.028303	-0.275209
S	-0.638058	-2.718859	-1.795716
N	0.060214	-1.749315	0.652490
C	1.454093	-1.768707	0.537292
C	2.175338	-2.644312	-0.266342
C	3.561612	-2.531661	-0.316962
C	4.252376	-1.594814	0.426944
C	3.517877	-0.755765	1.259706
C	2.143526	-0.834436	1.323822
C	4.305463	-3.437733	-1.259280
F	3.851580	-4.696051	-1.210570
C	4.261976	0.239772	2.104635
F	5.164961	0.925962	1.384564
F	5.617325	-3.477682	-0.996067
F	4.177924	-3.032296	-2.534528
F	4.946114	-0.361099	3.091509
F	3.453238	1.135566	2.680740
H	-2.251135	-1.343846	1.097461
H	-0.257402	-1.104283	1.374154
H	1.665394	-3.391508	-0.853049
H	5.330188	-1.520206	0.371509
H	1.579548	-0.154063	1.951570
N	-2.855943	1.768956	1.424860
O	-3.414349	2.761978	0.992506
O	-3.417969	0.761374	1.768522
C	-1.261778	1.807131	1.514809
C	-0.768286	1.475205	0.160244
H	-1.382703	0.726029	-0.326267
O	-0.773244	0.641166	1.888043
C	0.614296	1.563324	-0.301663
C	3.226088	1.580948	-1.270184
C	1.550075	2.458582	0.220476
C	0.992145	0.705016	-1.339597
C	2.291320	0.710714	-1.820804
C	2.851838	2.456191	-0.256964
H	1.269632	3.161576	0.990873
H	0.273222	0.000880	-1.747697
H	2.576135	0.021848	-2.606135
H	3.577365	3.139409	0.164813
H	4.248274	1.575071	-1.627368
C	-0.933172	3.035801	2.336115
H	0.099379	2.957832	2.665900
H	-1.086126	3.956054	1.776928
H	-1.566432	3.042983	3.223815
N	-1.584310	2.923570	-1.301388
H	-1.504675	2.413424	-2.174786
H	-2.557317	3.015268	-1.026585
C	-0.897718	4.159071	-1.314296
C	0.527132	6.548529	-1.222005
C	0.282086	4.295003	-2.042221
C	-1.363911	5.218955	-0.538348
C	-0.649804	6.407325	-0.495376
C	0.985402	5.490054	-1.996448
H	0.649438	3.463330	-2.633638
H	-2.285685	5.104649	0.020909
H	-1.019612	7.228873	0.104795
H	1.900631	5.589039	-2.566017
H	1.079384	7.478304	-1.188328
C	-3.363432	-1.882124	-0.599713
C	-3.642240	-0.775777	-1.619508
H	-3.251187	-2.822939	-1.144877
C	-4.914079	-1.091449	-2.404949
H	-3.764387	0.171965	-1.078865
H	-2.782782	-0.684419	-2.287314
C	-6.101721	-1.297631	-1.465267
H	-5.125906	-0.291700	-3.117075
H	-4.749001	-2.002716	-2.989052
C	-5.796759	-2.361651	-0.408358

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H         -6.328848       -0.352017       -0.961547
H         -6.990501       -1.576065       -2.034697
C         -4.536047       -1.984962        0.383536
H         -6.643468       -2.465940        0.273260
H         -5.650008       -3.330537       -0.896449
H         -4.695049       -0.984560        0.800506
N         -4.198053       -2.832760        1.524122
C         -5.154342       -2.714859        2.610490
H         -6.128163       -3.176314        2.386421
H         -5.314925       -1.661108        2.843127
H         -4.750854       -3.203218        3.498801
C         -3.943316       -4.224097        1.189402
H         -3.592900       -4.742178        2.082983
H         -4.836218       -4.751363        0.821463
H         -3.158718       -4.297651        0.434945

SR epoxide:Catalyst:Aniline, Transition State 4; "TS-SR1"; Energy = -2738.176944; TZVP
basis set.
N         -2.131358       -1.685416        0.176123
C         -0.917830       -2.128534       -0.192799
S         -0.657485       -2.999084       -1.617305
N          0.058675       -1.778377        0.704994
C          1.450628       -1.752893        0.568358
C          2.198493       -2.625606       -0.214840
C          3.578042       -2.457334       -0.286759
C          4.238782       -1.467854        0.415546
C          3.479829       -0.630593        1.227274
C          2.110958       -0.763562        1.310824
C          4.348907       -3.359825       -1.211127
F          4.210555       -2.980949       -2.493664
C          4.188171        0.427664        2.025133
F          5.066602        1.110942        1.273230
F          3.932419       -4.629130       -1.139122
F          5.661134       -3.355181       -0.946830
F          4.890141       -0.100629        3.039503
F          3.346012        1.321059        2.557806
H         -2.190995       -1.048666        0.969757
H         -0.263560       -1.114860        1.405077
H          1.712378       -3.413407       -0.767714
H          5.311883       -1.351132        0.343579
H          1.527924       -0.084427        1.922436
N         -2.939800        1.951174        1.453271
O         -3.403097        3.065886        1.312059
O         -3.589339        0.935117        1.491259
C         -1.353923        1.813084        1.511145
C         -0.942379        1.499027        0.123754
H         -1.626733        0.815411       -0.363278
O         -0.990092        0.579712        1.815239
C          0.417941        1.524535       -0.395490
C          2.988438        1.428767       -1.459916
C          1.392663        2.426563        0.041609
C          0.734422        0.605464       -1.402319
C          2.015556        0.551179       -1.926880
C          2.672940        2.369614       -0.485583
H          1.153105        3.183396        0.774733
H         -0.016825       -0.097818       -1.748864
H          2.255925       -0.185872       -2.682638
H          3.427302        3.061860       -0.135353
H          3.995391        1.379926       -1.855372
C         -0.845839        2.945941        2.372294
H          0.197404        2.747092        2.605939
H         -0.950017        3.913757        1.887851
H         -1.406732        2.949956        3.307073
N         -1.782641        3.066988       -1.225122
H         -1.826934        2.575224       -2.111629
H         -2.720306        3.252472       -0.881382
C         -0.981747        4.231319       -1.284213
C          0.689619        6.455678       -1.288984
C          0.103919        4.284227       -2.154201
C         -1.232646        5.291338       -0.415205
C         -0.395607        6.397769       -0.421637
C          0.931444        5.397728       -2.156262
H          0.303642        3.448854       -2.816408
H         -2.084807        5.243782        0.253560
H         -0.597377        7.221253        0.251421
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H          1.773361        5.432461       -2.835748
H          1.337801        7.321930       -1.292260
C         -3.374850       -1.952047       -0.533135
C         -3.690424       -0.824087       -1.519226
H         -3.222694       -2.871842       -1.100607
C         -4.983946       -1.106170       -2.277658
H         -3.798479        0.111044       -0.954971
H         -2.843651       -0.718298       -2.203932
C         -6.135720       -1.313025       -1.296837
H         -5.204678       -0.287454       -2.965357
H         -4.853836       -2.008165       -2.884524
C         -5.816834       -2.432704       -0.307350
H         -6.308085       -0.382621       -0.744852
H         -7.058241       -1.541046       -1.834090
C         -4.523658       -2.162774        0.469887
H         -6.624076       -2.558988        0.414952
H         -5.722936       -3.376716       -0.853988
H         -4.662141       -1.226212        1.019586
N         -4.294776       -3.204485        1.470667
C         -3.755239       -4.447903        0.948826
H         -2.697333       -4.367218        0.650979
H         -4.329180       -4.784189        0.085424
H         -3.829748       -5.218478        1.718158
C         -3.576869       -2.787877        2.664034
H         -3.784331       -3.493799        3.471742
H         -2.484884       -2.752528        2.531057
H         -3.919425       -1.801929        2.980638

SR epoxide:Catalyst:Aniline, Transition State 5; "TS-SR2",   Energy = -2738.177021;
TZVP basis set.
N         -2.128710       -1.746133        1.046694
C         -0.981772       -2.202502        0.518990
S         -0.879219       -3.220067       -0.828605
N          0.114768       -1.724336        1.196228
C          1.472070       -1.718809        0.867326
C          2.121551       -2.657348        0.070250
C          3.478721       -2.502022       -0.193235
C          4.219652       -1.460760        0.331052
C          3.566028       -0.555918        1.161355
C          2.220355       -0.674762        1.431825
C          4.126355       -3.486779       -1.127693
F          5.462950       -3.444708       -1.063828
C          4.366068        0.563940        1.764062
F          3.598059        1.493011        2.345577
F          3.791750       -3.243169       -2.406843
F          3.755437       -4.746334       -0.868570
F          5.113906        1.191229        0.840614
F          5.218622        0.119791        2.700638
H         -2.044697       -1.013669        1.748087
H         -0.114740       -0.990621        1.862016
H          1.576008       -3.487655       -0.347252
H          5.273483       -1.355306        0.111062
H          1.719967        0.054003        2.059004
N         -1.946820        3.176608       -0.744788
H         -2.491588        2.682681       -1.441666
H         -2.563686        3.646667       -0.087782
C         -0.947699        3.994959       -1.309143
C          1.188670        5.471932       -2.316803
C         -0.319563        3.600649       -2.489187
C         -0.512975        5.137919       -0.642302
C          0.551757        5.870548       -1.148366
C          0.741908        4.338816       -2.987565
H         -0.652608        2.704608       -3.000588
H         -1.013941        5.457698        0.264140
H          0.881742        6.759507       -0.626046
H          1.228253        4.020693       -3.900891
H          2.020034        6.044084       -2.706666
C         -3.506291       -2.093752        0.690715
C         -3.819331       -3.562669        0.999290
H         -4.109896       -1.475482        1.362799
C         -5.277976       -3.897652        0.699380
H         -3.167662       -4.196040        0.395203
H         -3.583593       -3.753894        2.047954
C         -5.621792       -3.556670       -0.747974
H         -5.459994       -4.954937        0.900445
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H         -5.933597       -3.327923        1.367204
C         -5.356686       -2.075992       -1.011315
H         -5.008474       -4.165578       -1.420005
H         -6.666107       -3.793725       -0.960482
C         -3.887431       -1.719014       -0.750923
H         -5.614987       -1.813689       -2.040793
H         -6.007089       -1.486445       -0.356965
H         -3.273179       -2.332461       -1.408459
N         -3.538427       -0.318166       -1.047464
C         -3.229949       -0.135039       -2.457366
H         -2.449906       -0.836631       -2.755924
H         -2.853636        0.877388       -2.629126
H         -4.103263       -0.275833       -3.112188
C         -4.545029        0.640341       -0.609415
H         -4.131920        1.651688       -0.627878
H         -5.442345        0.639843       -1.243661
H         -4.844810        0.438759        0.418252
H         -0.461374       -0.223375       -1.366103
C          0.352701        0.466090       -1.161423
C          2.431218        2.223164       -0.603525
C          0.198577        1.431775       -0.161347
C          1.548792        0.358532       -1.855369
C          2.587818        1.237595       -1.574680
C          1.246328        2.320653        0.104789
H          1.670134       -0.415795       -2.602273
H          3.525447        1.155089       -2.110473
H          1.133272        3.099002        0.845165
H          3.238732        2.912886       -0.395830
C         -1.088608        1.467194        0.510147
H         -1.846537        0.790434        0.110208
O         -0.891541        0.664991        2.271669
C         -1.336199        1.854159        1.916076
C         -0.800945        3.077255        2.624289
H         -1.036788        3.995810        2.092120
H          0.275069        2.966819        2.731565
H         -1.236067        3.123450        3.622904
N         -2.928402        1.918647        2.061343
O         -3.497798        0.915384        2.407177
O         -3.479842        2.968288        1.783245

PRC-RS; Energy = -2738.206837; TZVP basis set.
C          4.232900       -1.776749        0.026399
C          3.481716       -4.007306        0.934411
C          5.879625       -3.684225        0.267375
C          4.729237       -4.682204        0.371262
C          5.476540       -2.463047       -0.559706
C          3.093213       -2.796532        0.083839
H          3.666547       -3.673202        1.960879
H          6.163558       -3.356513        1.273186
H          4.502536       -5.081303       -0.622888
H          5.267220       -2.773512       -1.588891
H          2.875555       -3.151581       -0.924348
H          4.467413       -1.479291        1.057856
H          2.637621       -4.699278        0.956726
H          6.759450       -4.158088       -0.171895
H          5.011592       -5.529892        0.997960
H          6.303083       -1.751320       -0.597794
N          3.816600       -0.543611       -0.648816
N          1.883473       -2.165858        0.593356
H          2.018380       -1.364276        1.203799
C          4.850742        0.479308       -0.621428
H          5.659664        0.294983       -1.342913
H          5.280221        0.544518        0.378283
H          4.399416        1.444185       -0.860534
C          3.299964       -0.718011       -1.998221
H          2.461802       -1.416596       -2.005809
H          4.057348       -1.070852       -2.713263
H          2.929121        0.247846       -2.351952
C          0.633221       -2.540574        0.275100
S          0.301126       -3.645493       -0.955585
N         -0.318827       -1.920589        1.046513
H          0.060466       -1.268222        1.722233
C         -1.683979       -1.704164        0.812658
C         -4.381261       -1.025661        0.429053
C         -2.519163       -2.547861        0.088576
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C         -2.218112       -0.540173        1.379479
C         -3.542227       -0.213118        1.183675
C         -3.849176       -2.185689       -0.099752
H         -2.135782       -3.463331       -0.331983
H         -1.571634        0.122915        1.941004
H         -5.416712       -0.758457        0.266080
C         -4.703767       -3.074160       -0.962208
C         -4.111436        1.033664        1.800028
F         -4.451070       -2.880102       -2.267603
F         -3.161788        1.862874        2.253469
F         -4.858746        1.724466        0.927524
F         -4.909210        0.751333        2.842633
F         -4.487354       -4.371838       -0.717758
F         -6.010987       -2.847779       -0.783618
N          2.652775        3.236398       -1.485226
H          2.994374        2.985430       -2.402612
H          3.403724        3.539642       -0.879207
C          1.548878        4.094853       -1.493675
C         -0.740745        5.707317       -1.430705
C          1.330681        4.974636       -0.431326
C          0.614891        4.040735       -2.531061
C         -0.513709        4.843020       -2.497003
C          0.191996        5.768846       -0.402650
H          2.066432        5.034450        0.362899
H          0.770659        3.351732       -3.353454
H         -1.230418        4.782482       -3.306678
H          0.039846        6.448285        0.427540
H         -1.625147        6.330131       -1.407680
N          2.955045        1.967689        1.819474
O          3.428239        3.064581        1.605246
O          3.569980        0.992192        2.165876
C          1.449639        1.845771        1.622549
O          1.040410        0.532178        1.684806
C          1.125208        1.168146        0.359924
H          1.982702        0.771000       -0.180862
C          0.713463        2.880862        2.421199
H          0.839493        3.869794        1.988198
H          1.094768        2.881970        3.443160
H         -0.341542        2.618155        2.442033
C         -0.135836        1.287371       -0.413805
C         -2.544009        1.229952       -1.812645
C         -0.399992        0.263471       -1.323626
C         -1.063974        2.312147       -0.249209
C         -2.262793        2.280310       -0.947281
C         -1.604629        0.224532       -2.010667
H          0.330763       -0.524715       -1.473072
H         -0.847859        3.158320        0.388312
H         -2.976487        3.083481       -0.815531
H         -1.809607       -0.594383       -2.688956
H         -3.489357        1.200190       -2.340176

CP from RS; Energy = -2738.239972; TZVP basis set.
C          3.259393       -2.746782       -0.299614
C          1.763909       -4.488342        0.760159
C          4.058567       -5.136480        0.001301
C          2.626176       -5.616385        0.205029
C          4.099332       -3.894752       -0.888805
C          1.817493       -3.250410       -0.140721
H          2.110456       -4.212764        1.763031
H          4.500425       -4.894266        0.973783
H          2.211968       -5.945749       -0.753360
H          3.720980       -4.148771       -1.884526
H          1.429010       -3.527474       -1.119768
H          3.657536       -2.534737        0.699510
H          0.720641       -4.799515        0.845425
H          4.670351       -5.926721       -0.437523
H          2.598004       -6.474912        0.878132
H          5.133508       -3.570993       -1.007707
N          3.345296       -1.474736       -1.043602
N          0.917309       -2.226608        0.381032
H          1.187070       -1.836810        1.279602
C          4.729858       -1.025372       -1.171814
H          5.314883       -1.626624       -1.878913
H          5.220194       -1.052557       -0.197217
H          4.754609        0.005250       -1.537793
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C          2.705014       -1.503978       -2.356134
H          1.653230       -1.776658       -2.269087
H          3.191505       -2.198008       -3.055663
H          2.756591       -0.503589       -2.793779
C         -0.364806       -2.067296       -0.015787
S         -0.991575       -2.802799       -1.401237
N         -1.075218       -1.208692        0.772825
H         -0.550655       -0.649836        1.447435
C         -2.383751       -0.735252        0.552044
C         -4.960687        0.306414        0.222778
C         -3.437155       -1.576167        0.215806
C         -2.625744        0.624143        0.752705
C         -3.904089        1.127340        0.595158
C         -4.707681       -1.042028        0.042725
H         -3.267095       -2.635542        0.092988
H         -1.810593        1.279358        1.030368
H         -5.957370        0.707083        0.094848
C         -5.815885       -1.979834       -0.351594
C         -4.168780        2.594310        0.789653
F         -5.647100       -2.452336       -1.595067
F         -3.159513        3.219027        1.405685
F         -4.368599        3.227382       -0.378682
F         -5.271629        2.803561        1.524283
F         -5.873364       -3.047168        0.458285
F         -7.016357       -1.390397       -0.315039
N          2.904198        1.395916        0.092623
H          3.099934        0.661264       -0.588094
H          3.799513        0.710181        1.295937
C          3.287640        2.681321       -0.440640
C          4.114165        5.137842       -1.458827
C          4.065840        3.533256        0.334527
C          2.942290        3.053015       -1.738566
C          3.355447        4.277713       -2.243839
C          4.472734        4.761744       -0.171272
H          4.366133        3.223750        1.327856
H          2.344966        2.383188       -2.346113
H          3.082664        4.559881       -3.252557
H          5.079961        5.418057        0.438719
H          4.433874        6.093319       -1.854180
N          3.249433       -0.706628        2.397797
O          4.214331        0.167048        2.061497
O          3.566908       -1.422524        3.277471
C          1.154942        1.462968        1.926746
O          0.286523        0.802686        2.459848
C          1.487489        1.153367        0.466556
H          1.400586        0.071008        0.383354
C          1.867829        2.551806        2.669453
H          2.864807        2.197430        2.944179
H          1.313842        2.790847        3.573680
H          2.001254        3.435998        2.046434
C          0.430023        1.746964       -0.443373
C         -1.595877        2.710919       -2.100033
C         -0.077354        0.956583       -1.472087
C         -0.075355        3.032184       -0.259959
C         -1.086468        3.510225       -1.083892
C         -1.085273        1.433589       -2.298272
H          0.301912       -0.049846       -1.613268
H          0.305139        3.665942        0.532852
H         -1.488095        4.502161       -0.921282
H         -1.484755        0.796879       -3.077401
H         -2.397391        3.079743       -2.727013

PRC-SR; Energy = -2738.205562; TZVP basis set.
N         -1.490903       -2.172342        0.287158
C         -0.255763       -2.094137       -0.221227
S          0.096069       -2.482895       -1.824931
N          0.661707       -1.623416        0.690390
C          2.018319       -1.312728        0.512705
C          2.868652       -2.015767       -0.333087
C          4.195440       -1.617347       -0.447121
C          4.707653       -0.558231        0.278211
C          3.855750        0.104851        1.153627
C          2.529729       -0.259136        1.276269
C          5.070373       -2.358015       -1.421575
F          4.787243       -2.026287       -2.690802
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C          4.419528        1.221989        1.986471
F          5.104942        2.101660        1.240650
F          4.910239       -3.684548       -1.326868
F          6.369729       -2.100048       -1.232163
F          5.276420        0.762863        2.912499
F          3.472632        1.906570        2.638290
H         -1.621660       -2.115108        1.293016
H          0.259474       -1.225716        1.532250
H          2.501012       -2.856008       -0.900385
H          5.742612       -0.260098        0.177121
H          1.876477        0.283310        1.949328
N         -3.053682        1.148614        1.450821
O         -4.018160        1.802812        1.133092
O         -3.077396       -0.021171        1.760379
C         -1.691583        1.845353        1.411462
C         -0.769772        1.147001        0.497892
H         -1.200980        0.282610        0.001984
O         -0.713503        1.015344        1.932680
C          0.418517        1.725426       -0.170350
C          2.732342        2.605249       -1.447598
C          1.251809        2.652849        0.451693
C          0.770666        1.214475       -1.417368
C          1.923849        1.651911       -2.054930
C          2.395673        3.100578       -0.192532
H          1.040782        2.988003        1.458617
H          0.163215        0.437519       -1.869230
H          2.198870        1.232602       -3.014266
H          3.042424        3.815826        0.299198
H          3.635763        2.944154       -1.938440
C         -1.771341        3.290889        1.780196
H         -0.869198        3.804210        1.462007
H         -2.616116        3.753707        1.276133
H         -1.888597        3.384916        2.860600
N         -2.504034        2.033386       -1.897415
H         -1.779237        1.787314       -2.557516
H         -3.395780        1.645035       -2.171046
C         -2.540892        3.390429       -1.558442
C         -2.580942        6.060203       -0.704666
C         -1.373337        4.158930       -1.575006
C         -3.731855        3.981295       -1.128072
C         -3.747236        5.302313       -0.707611
C         -1.399007        5.478946       -1.148031
H         -0.445189        3.716306       -1.918165
H         -4.640560        3.391872       -1.108105
H         -4.680093        5.741250       -0.375920
H         -0.482807        6.056597       -1.165435
H         -2.596550        7.090083       -0.373613
C         -2.669737       -2.621219       -0.438327
C         -3.246338       -1.540343       -1.355481
H         -2.375899       -3.474686       -1.057174
C         -4.448106       -2.096178       -2.118585
H         -3.552182       -0.687653       -0.738781
H         -2.471167       -1.199158       -2.043348
C         -5.510159       -2.634607       -1.159974
H         -4.874604       -1.323287       -2.761184
H         -4.107698       -2.902904       -2.776235
C         -4.916843       -3.661412       -0.192216
H         -5.925708       -1.802273       -0.582201
H         -6.336011       -3.078237       -1.719258
C         -3.738870       -3.048013        0.576076
H         -5.681232       -4.000128        0.510218
H         -4.576436       -4.538437       -0.751999
H         -4.097547       -2.133216        1.060387
N         -3.157640       -3.854129        1.649889
C         -4.057949       -4.010403        2.779937
H         -4.916011       -4.664117        2.563937
H         -4.434803       -3.033472        3.085811
H         -3.510918       -4.444770        3.618027
C         -2.626759       -5.137792        1.217720
H         -2.116185       -5.609300        2.058318
H         -3.405900       -5.828799        0.864382
H         -1.896043       -4.998348        0.419941

CP from SR; Energy = -2738.239321; TZVP basis set.
N         -1.571940       -2.014049        0.142792
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C	-0.299034	-2.107385	-0.289502
S	0.104741	-2.757112	-1.791275
N	0.583050	-1.578433	0.616484
C	1.961625	-1.365788	0.520135
C	2.834093	-2.137682	-0.239745
C	4.184963	-1.807778	-0.266541
C	4.699065	-0.749783	0.457981
C	3.819516	-0.013907	1.244774
C	2.473688	-0.308854	1.283425
C	5.085509	-2.619932	-1.156756
F	4.895213	-2.322152	-2.452589
C	4.373032	1.125804	2.052818
F	5.089437	1.970299	1.292150
F	4.862898	-3.934299	-1.029277
F	6.381137	-2.409106	-0.896112
F	5.200178	0.694543	3.017815
F	3.417556	1.846724	2.649554
H	-1.727487	-1.921181	1.144149
H	0.138701	-0.983932	1.314887
H	2.466291	-2.974869	-0.810947
H	5.752322	-0.505460	0.421914
H	1.801046	0.289753	1.885609
N	-4.363325	0.833798	0.936663
O	-4.581157	1.945682	0.210963
O	-5.337501	0.439506	1.466980
C	-1.253661	1.528715	1.494032
C	-1.147150	1.501653	-0.034604
H	-1.447769	0.482601	-0.294417
O	-0.815811	0.571890	2.098439
C	0.299718	1.679604	-0.456265
C	2.926746	2.011424	-1.334130
C	1.122516	2.639154	0.131110
C	0.803546	0.891686	-1.486605
C	2.113768	1.049450	-1.920796
C	2.427966	2.807486	-0.309162
H	0.749463	3.267653	0.932291
H	0.179458	0.126716	-1.937123
H	2.498212	0.409232	-2.705176
H	3.059953	3.552901	0.156199
H	3.951349	2.132200	-1.662812
C	-1.831177	2.702236	2.223661
H	-1.348871	3.626410	1.901229
H	-2.892810	2.801125	1.994311
H	-1.700184	2.554856	3.292364
N	-2.117690	2.375859	-0.760077
H	-2.204210	1.963066	-1.686763
H	-3.663025	2.156699	-0.183314
C	-1.794976	3.779141	-0.945682
C	-1.276821	6.487186	-1.335924
C	-0.833937	4.181589	-1.870911
C	-2.516506	4.737361	-0.242922
C	-2.251410	6.088038	-0.431485
C	-0.576281	5.531663	-2.061961
H	-0.286356	3.437653	-2.436927
H	-3.299394	4.428482	0.437998
H	-2.819006	6.826613	0.119622
H	0.173274	5.835512	-2.781165
H	-1.073274	7.539600	-1.485644
C	-2.732125	-2.516645	-0.576362
C	-3.198043	-1.559055	-1.674874
H	-2.462378	-3.468508	-1.045051
C	-4.413179	-2.137197	-2.398395
H	-3.462997	-0.602251	-1.208726
H	-2.376099	-1.383034	-2.370449
C	-5.542929	-2.443814	-1.415739
H	-4.755712	-1.442956	-3.167734
H	-4.114982	-3.057942	-2.910533
C	-5.062812	-3.358237	-0.286579
H	-5.907364	-1.505980	-0.982303
H	-6.385948	-2.900712	-1.937211
C	-3.866271	-2.726528	0.434925
H	-5.872425	-3.532900	0.424923
H	-4.774405	-4.330185	-0.699577
H	-4.174612	-1.732178	0.775470
N	-3.381923	-3.407082	1.636370

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C         -4.335501       -3.345454        2.732555
H         -5.216304       -3.984904        2.574298
H         -4.674716       -2.317200        2.865568
H         -3.847362       -3.670371        3.652500
C         -2.922666       -4.769573        1.413347
H         -2.485692       -5.148959        2.337763
H         -3.731535       -5.452415        1.115869
H         -2.147851       -4.790172        0.645834

RS epoxide:Catalyst:Aniline most stable ternary complex, T-RS; Energy = -2737.356951;
TZVP basis set.
N          2.223744       -0.850170       -0.622323
C          1.046832       -1.183156       -1.170182
S          0.844066       -2.534364       -2.155911
C          3.509140       -1.443165       -0.937881
C          4.593412       -0.360113       -0.874660
C          5.941642       -0.984577       -1.260979
C          6.288453       -2.157219       -0.341768
C          5.189976       -3.217492       -0.357041
C          3.841316       -2.601566        0.003752
N          4.204893        0.839238       -1.635451
C          3.868286        0.587103       -3.032290
N          0.069192       -0.268468       -0.865108
C         -1.321205       -0.369907       -0.911158
C         -2.006847       -1.587075       -0.958082
C         -3.386245       -1.589580       -0.888677
C         -4.125156       -0.418844       -0.767686
C         -3.433000        0.777126       -0.721388
C         -2.048132        0.815523       -0.801752
C         -4.135427       -2.893397       -0.901802
F         -3.326409       -3.955282       -0.930463
C         -4.170945        2.080285       -0.588788
F         -3.659587        2.838949        0.394734
C          5.187523        1.910113       -1.521099
F         -4.916256       -3.022782        0.186900
F         -4.952683       -2.987666       -1.961882
F         -4.108633        2.812140       -1.709859
F         -5.467925        1.901317       -0.310545
H          2.239989       -0.031530       -0.023561
H          0.428232        0.622218       -0.524638
H          3.861989       -2.223058        1.032042
H          3.038515       -3.337995       -0.065270
H          5.124810       -3.659518       -1.356638
H          5.430380       -4.027578        0.333584
H          7.244185       -2.591870       -0.639956
H          6.414171       -1.784198        0.680443
H          5.896792       -1.335778       -2.296825
H          6.727875       -0.229729       -1.208178
H          3.445818       -1.841716       -1.953193
H          4.666993       -0.031966        0.172517
H          4.746698        2.841800       -1.881040
H          5.463044        2.044307       -0.473461
H          6.101714        1.723519       -2.099902
H          4.699581        0.154555       -3.605346
H          3.602234        1.535824       -3.500744
H          3.005887       -0.077136       -3.106710
H         -1.461559       -2.514005       -1.025095
H         -5.204588       -0.443826       -0.701584
H         -1.531856        1.770366       -0.770642
N          1.431214        2.071961        3.768474
O          1.322168        2.415994        4.919230
O          1.708563        2.804048        2.843094
C          1.161595        0.609322        3.463288
C          0.262366        0.400920        2.307096
H         -0.089590        1.300110        1.800674
O          1.679262        0.233701        2.236119
C         -0.592971       -0.811398        2.218630
C         -2.234384       -3.049019        2.107156
C         -1.960804       -0.682583        2.446778
C         -0.049255       -2.053905        1.910936
C         -0.874029       -3.170573        1.851327
C         -2.777990       -1.803393        2.400223
H         -2.383885        0.293201        2.659640
H          1.011865       -2.138261        1.704703
H         -0.452894       -4.134575        1.595799
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H	-3.841364	-1.703470	2.576218
H	-2.875221	-3.920126	2.057861
C	1.298325	-0.283944	4.651877
H	0.580133	-0.006080	5.419650
H	2.304561	-0.211988	5.063558
H	1.108832	-1.306098	4.331993
N	1.827986	2.188067	-0.184394
H	2.619458	1.907066	-0.768231
H	2.096351	2.466385	0.751575
C	0.858357	2.990638	-0.790610
C	-1.258352	4.386428	-1.979496
C	0.606435	2.865226	-2.160101
C	0.044236	3.829705	-0.024002
C	-1.004610	4.517205	-0.619314
C	-0.441708	3.560834	-2.744505
H	1.224456	2.199741	-2.753438
H	0.241786	3.935075	1.036913
H	-1.633392	5.154932	-0.010761
H	-0.628720	3.445778	-3.804782
H	-2.085024	4.913900	-2.435330

SR epoxide:Catalyst:Aniline most stable ternary complex, T-SR; Energy = -2737.355237; TZVP basis set.

C	4.525724	-0.169838	-0.941166
C	3.717131	-2.349705	0.030930
C	6.172550	-1.990285	-0.335081
C	5.046112	-3.019863	-0.304882
C	5.854691	-0.848858	-1.302189
C	3.412624	-1.225462	-0.960534
H	3.755378	-1.919482	1.037580
H	6.308867	-1.577401	0.670174
H	4.966330	-3.502702	-1.284399
H	5.798216	-1.240327	-2.323239
H	3.341177	-1.664815	-1.958517
H	4.606890	0.199912	0.091024
H	2.895456	-3.068121	-0.002706
H	7.115862	-2.462354	-0.615536
H	5.264646	-3.805516	0.420411
H	6.661802	-0.115090	-1.280371
N	4.175069	1.006736	-1.756094
N	2.135933	-0.594474	-0.669979
H	2.173860	0.268585	-0.127404
C	3.790471	0.705591	-3.130088
H	3.551286	1.641976	-3.636120
H	2.899984	0.076355	-3.152836
H	4.588103	0.211385	-3.701565
C	5.210484	2.033013	-1.718927
H	5.526180	2.198606	-0.686730
H	4.802568	2.968320	-2.107517
H	6.096275	1.777483	-2.314927
C	0.956307	-0.953360	-1.197209
S	0.751470	-2.347883	-2.118321
N	-0.025508	-0.030342	-0.919606
H	0.321792	0.871613	-0.612834
C	-1.419937	-0.104871	-0.920569
C	-4.221337	-0.070958	-0.712180
C	-2.159383	-1.253723	-1.211622
C	-2.093374	1.055862	-0.534010
C	-3.475529	1.060336	-0.432793
C	-3.536883	-1.215385	-1.097900
H	-1.659170	-2.160578	-1.507392
H	-1.533035	1.956544	-0.300203
H	-5.299308	-0.067127	-0.622531
C	-4.343484	-2.451470	-1.389211
C	-4.156748	2.336966	-0.024321
F	-5.127106	-2.289372	-2.467142
F	-3.546990	2.913064	1.022441
F	-4.158237	3.243112	-1.014329
F	-5.433588	2.139118	0.323240
F	-3.582352	-3.525335	-1.613968
F	-5.165129	-2.755512	-0.369154
N	2.325254	0.825915	2.921104
O	2.103598	1.992477	3.136504
O	3.343851	0.388278	2.428863
C	1.241725	-0.186864	3.240188

C	0.041866	-0.023772	2.404731
H	0.033044	0.821992	1.715614
C	-0.833553	-1.186115	2.088934
C	-2.488730	-3.334238	1.487082
C	-0.310425	-2.313644	1.465212
C	-2.190148	-1.125625	2.397478
C	-3.014466	-2.201668	2.099809
C	-1.139474	-3.386767	1.162650
H	0.742962	-2.349302	1.206013
H	-2.592702	-0.240750	2.876722
H	-4.069874	-2.154354	2.336024
H	-0.729869	-4.255485	0.663278
H	-3.136300	-4.168348	1.247991
O	0.118740	0.401417	3.774544
C	1.782943	-1.454483	3.822635
H	2.455427	-1.943655	3.121816
H	2.321279	-1.235255	4.745140
H	0.944967	-2.111542	4.043158
H	2.916364	2.107923	-0.541681
N	2.240080	2.301045	0.201586
H	2.682188	2.600624	1.061853
C	1.150025	3.090356	-0.189926
C	-1.110274	4.543843	-0.975806
C	0.799755	3.181330	-1.540530
C	0.345262	3.718084	0.766237
C	-0.767774	4.445368	0.368753
C	-0.322201	3.903797	-1.924907
H	1.417706	2.684969	-2.282232
H	0.605094	3.634081	1.815429
H	-1.379953	4.929492	1.118925
H	-0.579977	3.964912	-2.974692
H	-1.985436	5.102816	-1.277471