Supporting Information

Electroreductive Intramolecular Coupling of Chiral α -Imino Esters: Stereoselective Synthesis of Mixed Ketals of *cis*-2,4-Disubstituted Azetidine-3-ones

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Electrolysis Cell

^1H NMR of **2c**

^1H NMR of **2c and *dl*-**2c** in the Presence of $\text{Eu}(\text{hfc})_3$**

^{13}C NMR of 2c

DEPT of 2c

Results of Calculations

Optimized Structures of Transition States for the intramolecular coupling of 1a

(*R,R,S*)-TS (RHF/AM1)

Z-Matrix orientation:

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-----  
C 0  0.644226 -0.302353 -0.279633  
C 0 -0.579300 -1.238754  0.773788  
C 0 -1.567078 -0.397202 -0.118164  
N 0 -0.528214  0.305923 -0.843185  
O 0 -0.469040 -0.594955  2.037018  
O 0 -0.497025 -2.495560  0.823471  
C 0 -2.495865 -1.308121 -0.934387  
Si 0 -0.579300  1.886124 -1.449203  
C 0  1.534058 -1.112183 -1.106339  
C 0  1.156113 -1.653854 -2.349228  
C 0  2.038330 -2.442642 -3.080200  
C 0  3.316788 -2.716797 -2.593765  
C 0  3.700958 -2.198822 -1.356766  
C 0  2.826340 -1.405975 -0.623520  
C 0 -3.439774 -2.029648  0.006714  
C 0 -3.285141 -0.546417 -1.975464  
C 0 -2.019730  2.830338 -0.793396  
C 0 -0.760895  1.892975 -3.285477  
C 0  0.232819 -1.313446  3.025330  
C 0  0.951874  2.827866 -1.068039  
H 0  1.206161  0.373322  0.406998  
H 0 -2.199188  0.304642  0.495316  
H 0 -1.851639 -2.077393 -1.448563  
H 0  0.143570 -1.467590 -2.736023  
H 0  1.723663 -2.858780 -4.047943  
H 0  4.009232 -3.339691 -3.173370  
H 0  4.701462 -2.421097 -0.959427  
H 0  3.131729 -1.011826  0.356216  
H 0 -4.088882 -1.303513  0.552429  
H 0 -2.843765 -2.615707  0.750854
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H 0	-4.096481	-2.728531	-0.565231
H 0	-2.603851	-0.073608	-2.724457
H 0	-3.899948	0.255157	-1.497864
H 0	-3.975388	-1.237579	-2.518326
H 0	-2.003067	2.863815	0.319778
H 0	-2.980820	2.356140	-1.097855
H 0	-2.024887	3.878693	-1.165878
H 0	-0.177750	2.719452	-3.749542
H 0	-1.824783	2.016678	-3.588654
H 0	-0.396805	0.934647	-3.722214
H 0	1.307907	-1.421402	2.736404
H 0	0.138824	-0.698441	3.955902
H 0	-0.212296	-2.327744	3.176132
H 0	1.103867	2.916962	0.031998
H 0	0.915283	3.856003	-1.492416
H 0	1.850891	2.319427	-1.485031

SCF Energy: -0.17978 hartrees

Only One Imaginary Frequency: -435.0012

(R,S,S)-TS (RHF/AM1)

Z-Matrix orientation:

C 0	0.707520	0.302490	0.650513
C 0	-0.699356	-0.320251	1.685883
C 0	-1.505081	0.346954	0.506531
N 0	-0.330185	0.835693	-0.187515
O 0	-0.703461	0.136612	2.866409
O 0	-0.715988	-1.729156	1.602493
C 0	-2.418564	-0.620605	-0.258530
Si 0	-0.177597	2.260803	-1.090637
C 0	1.654526	-0.679367	0.127411
C 0	1.424545	-1.433762	-1.038452
C 0	2.350327	-2.377716	-1.470642
C 0	3.526550	-2.599258	-0.754150
C 0	3.763474	-1.867905	0.410095

C 0	2.844986	-0.919952	0.845062
C 0	-3.526245	-1.092773	0.662811
C 0	-3.018356	0.006805	-1.497726
C 0	-1.610886	3.392578	-0.845535
C 0	-0.115311	1.902679	-2.900497
C 0	1.359726	3.181900	-0.686127
C 0	-0.283234	-2.408020	2.762894
H 0	1.213135	1.075974	1.276169
H 0	-2.139755	1.190704	0.902802
H 0	-1.799774	-1.511826	-0.563232
H 0	0.491013	-1.288528	-1.601563
H 0	2.151840	-2.957642	-2.383300
H 0	4.254562	-3.343979	-1.098923
H 0	4.683136	-2.042694	0.986252
H 0	3.033859	-0.353577	1.768387
H 0	-4.178467	-0.239258	0.967987
H 0	-3.080368	-1.549286	1.580978
H 0	-4.159424	-1.854950	0.148163
H 0	-2.217636	0.327316	-2.208557
H 0	-3.633850	0.900269	-1.230072
H 0	-3.678879	-0.727081	-2.020981
H 0	-1.756973	3.624939	0.233963
H 0	-2.554260	2.930984	-1.217331
H 0	-1.467606	4.355179	-1.384933
H 0	0.629974	2.548309	-3.416595
H 0	-1.103363	2.072403	-3.384200
H 0	0.171341	0.841736	-3.084442
H 0	1.409698	3.420181	0.401031
H 0	1.420456	4.140121	-1.249039
H 0	2.265854	2.583847	-0.934662
H 0	0.740921	-2.073914	3.058868
H 0	-0.280106	-3.489838	2.477356
H 0	-0.990280	-2.224686	3.609528

SCF Energy: -0.17829 hartrees

Only One Imaginary Frequency: -429.4606

(S,R,S)-TS (RHF/AM1)

Z-Matrix orientation:

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-----  
C 0  0.769150 -0.504272 -0.075928  
C 0 -0.390579 -1.366653  1.112961  
C 0 -1.430847 -0.603027  0.211136  
N 0 -0.441650 -0.024826 -0.677521  
C 0  1.741196  0.395309  0.534698  
O 0 -0.330780 -0.720123  2.366837  
O 0 -0.208054 -2.616730  1.155045  
C 0 -2.495956 -1.552628 -0.358963  
Si 0 -0.547104  0.834198 -2.132797  
C 0 -3.206558 -2.256653  0.781265  
C 0 -3.516418 -0.822891 -1.206223  
C 0 -1.883392  2.108368 -2.062500  
C 0 -0.922684 -0.242081 -3.589325  
C 0  0.363663 -1.417557  3.379013  
C 0  1.023483  1.703125 -2.524948  
C 0  3.078003 -0.038422  0.666397  
C 0  4.032593  0.759964  1.284653  
C 0  3.687759  2.015808  1.785049  
C 0  2.367996  2.454453  1.673325  
C 0  1.406265  1.658279  1.061081  
H 0  1.254074 -1.324631 -0.654572  
H 0 -1.962036  0.199722  0.799591  
H 0 -1.977631 -2.331375 -0.985809  
H 0 -3.703827 -1.515747  1.452377  
H 0 -2.467422 -2.846100  1.380096  
H 0 -3.985672 -2.948898  0.379959  
H 0 -3.025436 -0.330032 -2.082291  
H 0 -4.035309 -0.036392 -0.605972  
H 0 -4.285233 -1.536880 -1.589539  
H 0 -1.462173  3.112640 -1.831589  
H 0 -2.628662  1.866241 -1.270050  
H 0 -2.430923  2.184662 -3.028366  
H 0 -0.045670 -0.315491 -4.270905
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H 0	-1.779358	0.148026	-4.182968
H 0	-1.180634	-1.275970	-3.263657
H 0	1.410202	-1.641022	3.058350
H 0	0.358154	-0.727371	4.259583
H 0	-0.159302	-2.375076	3.624557
H 0	0.832962	2.672302	-3.038193
H 0	1.679123	1.093323	-3.186478
H 0	1.599197	1.918091	-1.592712
H 0	3.356949	-1.029968	0.281845
H 0	5.067261	0.400970	1.378906
H 0	4.443893	2.647751	2.266998
H 0	2.084808	3.436111	2.079208
H 0	0.362259	1.999466	1.019333

SCF Energy: -0.17685 hartrees

Only One Imaginary Frequency: -463.1983

(S,S,S)-TS (RHF/AM1)

Z-Matrix orientation:

C 0	0.555084	0.265198	0.613480
C 0	-0.327652	1.733292	-0.153183
C 0	-1.270615	0.561462	-0.613403
N 0	-0.536972	-0.487640	0.065781
C 0	1.924850	0.087585	0.143402
O 0	0.295929	2.484818	-0.950546
O 0	-0.834290	2.390366	0.997787
C 0	-2.750626	0.796829	-0.278763
Si 0	-0.830444	-2.129456	0.353882
C 0	-0.281631	3.661926	1.259521
C 0	-3.197571	2.107407	-0.899384
C 0	-3.638474	-0.319900	-0.784897
C 0	-1.433502	-2.984146	-1.168869
C 0	-2.111450	-2.421402	1.656784
C 0	0.687958	-2.999786	0.914398
C 0	2.991287	0.412659	1.007538

C 0	4.311768	0.306244	0.586868
C 0	4.609009	-0.132523	-0.703354
C 0	3.564835	-0.445450	-1.574463
C 0	2.241470	-0.335648	-1.161957
H 0	0.492950	0.388672	1.718918
H 0	-1.187912	0.448929	-1.734406
H 0	-2.855286	0.877869	0.839371
H 0	-0.577591	4.387329	0.461243
H 0	-0.712128	3.966507	2.246658
H 0	0.833084	3.609421	1.312073
H 0	-3.130859	2.057877	-2.012848
H 0	-2.542770	2.940643	-0.541702
H 0	-4.255051	2.327393	-0.616394
H 0	-3.364426	-1.292038	-0.303925
H 0	-3.534775	-0.433792	-1.891495
H 0	-4.708954	-0.101227	-0.552658
H 0	-0.593079	-3.482071	-1.702972
H 0	-1.900650	-2.262300	-1.877792
H 0	-2.192261	-3.762680	-0.931046
H 0	-1.657593	-2.854843	2.576126
H 0	-2.903336	-3.121902	1.309204
H 0	-2.608078	-1.467056	1.946716
H 0	0.717773	-3.107742	2.021957
H 0	1.601654	-2.434845	0.609924
H 0	0.756973	-4.019470	0.473282
H 0	2.766983	0.766663	2.023682
H 0	5.127609	0.568771	1.275116
H 0	5.651688	-0.220825	-1.032715
H 0	3.790955	-0.773193	-2.599152
H 0	1.428940	-0.544006	-1.872482

SCF Energy: -0.17558 hartrees

Only One Imaginary Frequency: -453.8117

(*R,R,S*)-TS (RHF/PM3)

Z-Matrix orientation:

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-----
C 0  0.825439 -0.029953  0.381226
C 0 -0.507782 -1.060165  1.428207
C 0 -1.449448 -0.083603  0.641205
N 0 -0.386536  0.584152 -0.164154
O 0 -0.320328 -0.577484  2.754608
O 0 -0.458450 -2.296494  1.321579
C 0 -2.486343 -0.801666 -0.239105
Si 0 -0.427063  2.370605 -0.304169
C 0  1.676437 -0.767258 -0.526276
C 0  1.268295 -1.174286 -1.809677
C 0  2.119980 -1.902390 -2.624924
C 0  3.395447 -2.251160 -2.188904
C 0  3.807297 -1.871033 -0.915375
C 0  2.965271 -1.138336 -0.094467
C 0 -3.561478 -1.425323  0.638443
C 0 -3.128204  0.143158 -1.243454
C 0 -2.078262  3.132843  0.267380
C 0 -0.218430  2.793304 -2.147507
C 0  0.704117 -1.179672  3.491898
C 0  0.969100  3.252640  0.637848
H 0  1.386826  0.602478  1.094086
H 0 -1.986908  0.632278  1.313248
H 0 -1.963684 -1.617218 -0.798981
H 0  0.258728 -0.922134 -2.155106
H 0  1.786377 -2.211900 -3.619873
H 0  4.061920 -2.826553 -2.835785
H 0  4.802307 -2.155151 -0.560318
H 0  3.290558 -0.856537  0.913040
H 0 -4.123840 -0.664871  1.197662
H 0 -3.119980 -2.116226  1.368973
H 0 -4.286682 -1.992813  0.040100
H 0 -2.401000  0.488663 -1.992294
H 0 -3.538116  1.043625 -0.753235
H 0 -3.951400 -0.343658 -1.783020
H 0 -2.150528  3.131912  1.358231
H 0 -2.926636  2.555786 -0.127000

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H 0	-2.175415	4.164185	-0.078995
H 0	-0.293106	3.870178	-2.317505
H 0	-0.988754	2.299652	-2.747482
H 0	0.755554	2.457428	-2.513443
H 0	1.668335	-1.119049	2.970413
H 0	0.743851	-0.595184	4.416200
H 0	0.487289	-2.227585	3.729477
H 0	0.918991	3.023346	1.706207
H 0	0.901642	4.336960	0.519791
H 0	1.949936	2.932953	0.274429

SCF Energy: -0.21085 hartrees

Only One Imaginary Frequency: -215.8994

(R,S,S)-TS (RHF/PM3)

Z-Matrix orientation:

C 0	0.816559	0.248734	0.474030
C 0	-0.408295	-0.527573	1.743362
C 0	-1.441498	0.123505	0.744492
N 0	-0.420715	0.652359	-0.207520
O 0	-0.250977	-0.099411	2.910675
O 0	-0.326920	-1.935303	1.623291
C 0	-2.448532	-0.816864	0.063568
Si 0	-0.561188	2.357864	-0.741119
C 0	1.727188	-0.611511	-0.263031
C 0	1.358932	-1.302170	-1.430603
C 0	2.262375	-2.131546	-2.077347
C 0	3.551254	-2.301102	-1.580307
C 0	3.926849	-1.633667	-0.418594
C 0	3.031891	-0.798889	0.232117
C 0	-3.454178	-1.320800	1.088593
C 0	-3.184677	-0.121124	-1.072372
C 0	-2.230621	3.156052	-0.284988
C 0	-0.433350	2.361526	-2.640320
C 0	0.816528	3.489227	-0.081619

C 0	0.667145	-2.564743	2.381775
H 0	1.339188	1.065781	1.007965
H 0	-2.012741	0.941055	1.252884
H 0	-1.897583	-1.690781	-0.363586
H 0	0.340790	-1.187805	-1.821564
H 0	1.959137	-2.661300	-2.985382
H 0	4.259277	-2.956223	-2.093658
H 0	4.935272	-1.769700	-0.016800
H 0	3.331802	-0.284698	1.151779
H 0	-4.057953	-0.500946	1.501465
H 0	-2.949707	-1.813416	1.930038
H 0	-4.148682	-2.046936	0.645248
H 0	-2.508377	0.110077	-1.908005
H 0	-3.629745	0.835342	-0.746262
H 0	-3.996170	-0.746185	-1.468018
H 0	-2.269455	3.388611	0.782730
H 0	-3.061400	2.472931	-0.511078
H 0	-2.388168	4.082733	-0.841309
H 0	-0.552551	3.370850	-3.041916
H 0	-1.205795	1.725983	-3.083282
H 0	0.538773	1.979446	-2.963409
H 0	0.805800	3.510864	1.012177
H 0	0.692719	4.513077	-0.442947
H 0	1.801620	3.135117	-0.398087
H 0	1.662384	-2.155197	2.166031
H 0	0.615479	-3.609024	2.059235
H 0	0.474136	-2.503342	3.459229

SCF Energy: -0.20996 hartrees

Only One Imaginary Frequency: -223.9147

(S,R,S)-TS (RHF/PM3)

Z-Matrix orientation:

C 0	0.799469	-0.339569	-0.008987
C 0	-0.481186	-1.399139	1.118073

C 0	-1.467500	-0.450867	0.351257
N 0	-0.450470	0.254959	-0.484650
C 0	1.763138	0.517044	0.634933
O 0	-0.343597	-0.979889	2.455505
O 0	-0.316116	-2.618240	0.925217
C 0	-2.641800	-1.182144	-0.314758
Si 0	-0.527710	0.579239	-2.239594
C 0	-3.424332	-1.968842	0.730652
C 0	-3.604355	-0.225662	-1.006760
C 0	-1.607498	2.127792	-2.520416
C 0	-1.244247	-0.775162	-3.370010
C 0	0.675583	-1.584427	3.202927
C 0	1.214706	0.983383	-2.889740
C 0	3.044586	-0.000641	0.922714
C 0	3.993988	0.768265	1.574127
C 0	3.705521	2.075821	1.954651
C 0	2.446304	2.601700	1.678513
C 0	1.486282	1.839523	1.033524
H 0	1.248825	-1.095581	-0.677368
H 0	-1.892227	0.331467	1.029556
H 0	-2.234421	-1.900284	-1.069778
H 0	-3.845261	-1.307297	1.499939
H 0	-2.789993	-2.706268	1.240265
H 0	-4.261124	-2.514908	0.274261
H 0	-3.167038	0.210281	-1.925735
H 0	-3.894806	0.606888	-0.351822
H 0	-4.527115	-0.740219	-1.309311
H 0	-1.339340	2.924652	-1.822937
H 0	-2.664474	1.875671	-2.365295
H 0	-1.490921	2.509796	-3.536896
H 0	-1.005341	-0.586349	-4.418884
H 0	-2.336670	-0.800552	-3.263428
H 0	-0.851227	-1.759415	-3.102448
H 0	1.652481	-1.475281	2.714706
H 0	0.664383	-1.033524	4.147842
H 0	0.478119	-2.645767	3.393661
H 0	1.180145	1.245255	-3.950119

H 0	1.882400	0.125275	-2.769287
H 0	1.649521	1.823532	-2.341354
H 0	3.277939	-1.030945	0.633484
H 0	4.979507	0.346222	1.792267
H 0	4.456619	2.680206	2.468475
H 0	2.212479	3.627243	1.980011
H 0	0.497025	2.263718	0.830400

SCF Energy: -0.20527 hartrees

Only One Imaginary Frequency: -237.1077

(S,S,S)-TS (RHF/PM3)

Z-Matrix orientation:

C 0	0.269104	-0.552536	0.002121
C 0	-1.006760	-1.586639	1.434082
C 0	-1.971497	-0.758118	0.540222
N 0	-1.056335	-0.241806	-0.512100
C 0	1.086655	0.494995	0.506607
O 0	-0.781555	-1.380859	2.623886
O 0	-0.723175	-2.881897	0.959167
C 0	-3.247696	-1.514145	0.136810
Si 0	-1.220306	-0.469818	-2.283768
C 0	-0.807678	-3.923981	1.893936
C 0	-3.885666	-2.175644	1.352112
C 0	-4.261215	-0.578506	-0.509048
C 0	-1.757935	1.213531	-2.998123
C 0	-2.468994	-1.749466	-2.950607
C 0	0.466202	-0.917511	-3.053802
C 0	2.448990	0.228134	0.790314
C 0	3.270721	1.202637	1.324615
C 0	2.782089	2.480148	1.587555
C 0	1.445084	2.762375	1.314178
C 0	0.609039	1.796951	0.785294
H 0	0.799561	-1.381393	-0.501923
H 0	-2.276581	0.152695	1.118698

H 0	-2.976028	-2.315964	-0.603577
H 0	-1.829468	-3.983078	2.303879
H 0	-0.589340	-4.818161	1.304337
H 0	-0.086212	-3.832809	2.713120
H 0	-4.135071	-1.438828	2.127121
H 0	-3.215118	-2.923431	1.813156
H 0	-4.813858	-2.696289	1.081085
H 0	-3.936249	-0.276031	-1.520508
H 0	-4.415329	0.333237	0.082687
H 0	-5.239929	-1.065384	-0.621231
H 0	-1.123779	2.013916	-2.606934
H 0	-2.793289	1.444321	-2.732285
H 0	-1.678726	1.219574	-4.087921
H 0	-2.206787	-2.073242	-3.959198
H 0	-3.475952	-1.312424	-2.969055
H 0	-2.504364	-2.629578	-2.296158
H 0	0.350571	-1.626038	-3.876572
H 0	1.102203	-1.373900	-2.280777
H 0	0.979400	-0.030930	-3.432266
H 0	2.845383	-0.772522	0.592178
H 0	4.317535	0.971100	1.543167
H 0	3.435379	3.247375	2.008011
H 0	1.053986	3.762604	1.524017
H 0	-0.440186	2.034958	0.582748

SCF Energy: -0.20003 hartrees

Only One Imaginary Frequency: -211.7153

(R,R,S)-TS (RHF/6-31G*)

Z-Matrix orientation:

C 0	0.843918	-0.056763	0.364395
C 0	-0.595108	-0.863037	1.686554
C 0	-1.440552	-0.093872	0.649094
N 0	-0.389130	0.630585	-0.049500
O 0	-0.341858	-0.016754	2.744324

O 0	-0.617050	-2.062469	1.872620
C 0	-2.268097	-1.053619	-0.228058
Si 0	-0.316895	2.336929	-0.268707
C 0	1.592545	-0.806778	-0.634521
C 0	1.101685	-1.156448	-1.904175
C 0	1.842590	-1.926132	-2.784653
C 0	3.108688	-2.383408	-2.456589
C 0	3.618317	-2.043640	-1.207153
C 0	2.886520	-1.279404	-0.325363
C 0	-3.391708	-1.707520	0.586548
C 0	-2.863663	-0.359436	-1.455002
C 0	-2.015610	3.080124	-0.698654
C 0	0.871460	2.756119	-1.683594
C 0	0.500015	-0.540649	3.724304
C 0	0.277603	3.280060	1.275391
H 0	1.496445	0.553238	0.980621
H 0	-2.136200	0.567322	1.172500
H 0	-1.596893	-1.835449	-0.564880
H 0	0.129547	-0.807831	-2.195419
H 0	1.421677	-2.167664	-3.748352
H 0	3.680450	-2.981979	-3.145355
H 0	4.602142	-2.381577	-0.920853
H 0	3.305527	-1.037704	0.637863
H 0	-4.094452	-0.957367	0.949432
H 0	-2.992279	-2.245407	1.434311
H 0	-3.955048	-2.407242	-0.028397
H 0	-2.098648	0.110611	-2.059204
H 0	-3.580963	0.406265	-1.166061
H 0	-3.390793	-1.079025	-2.078720
H 0	-2.762405	2.866882	0.062454
H 0	-2.397003	2.709091	-1.645386
H 0	-1.935944	4.163681	-0.778030
H 0	0.988205	3.833603	-1.794968
H 0	0.510941	2.358948	-2.628998
H 0	1.854630	2.328781	-1.511154
H 0	1.460236	-0.815964	3.300354
H 0	0.644638	0.240097	4.462814

H 0	0.067368	-1.413559	4.196075
H 0	-0.344757	3.046509	2.135223
H 0	0.245773	4.358032	1.117676
H 0	1.298126	3.016098	1.538544

SCF Energy: -1114.10928 hartrees

Only One Imaginary Frequency: -375.0185

(R,S,S)-TS (RHF/6-31G*)

Z-Matrix orientation:

C 0	0.834534	0.060196	0.452530
C 0	-0.624969	-0.683044	1.736969
C 0	-1.454254	0.069168	0.669205
N 0	-0.371353	0.766907	-0.014130
O 0	-0.480392	-0.212021	2.853027
O 0	-0.618271	-2.042206	1.568314
C 0	-2.323685	-0.826813	-0.236679
Si 0	-0.245056	2.483337	-0.142990
C 0	1.618393	-0.682037	-0.523911
C 0	1.152191	-1.053574	-1.797745
C 0	1.915710	-1.826096	-2.655167
C 0	3.181427	-2.266312	-2.300278
C 0	3.668365	-1.901581	-1.049179
C 0	2.914902	-1.131744	-0.189774
C 0	-3.470200	-1.460724	0.562271
C 0	-2.896820	-0.062912	-1.432800
C 0	-1.905380	3.295853	-0.598251
C 0	0.999771	2.932861	-1.498779
C 0	0.318192	3.313248	1.474289
C 0	0.182922	-2.739883	2.473160
H 0	1.456161	0.643768	1.121948
H 0	-2.121033	0.746277	1.206070
H 0	-1.690887	-1.620758	-0.615173
H 0	0.181259	-0.717941	-2.108582
H 0	1.513626	-2.084824	-3.622543

H 0	3.770996	-2.866714	-2.972244
H 0	4.653198	-2.220428	-0.744690
H 0	3.320007	-0.863419	0.772507
H 0	-4.145279	-0.695831	0.943481
H 0	-3.100266	-2.033203	1.402512
H 0	-4.056763	-2.127762	-0.066788
H 0	-2.111923	0.386292	-2.027466
H 0	-3.570892	0.728195	-1.111374
H 0	-3.464951	-0.733719	-2.074921
H 0	-2.682632	3.083282	0.131836
H 0	-2.268204	2.971405	-1.569168
H 0	-1.786606	4.378098	-0.636780
H 0	1.157043	4.009918	-1.548080
H 0	0.654251	2.600403	-2.474487
H 0	1.961838	2.462097	-1.320831
H 0	-0.234406	2.912766	2.319962
H 0	0.167847	4.392258	1.445100
H 0	1.371445	3.133453	1.671875
H 0	1.207581	-2.389893	2.425186
H 0	0.147125	-3.782471	2.179062
H 0	-0.176315	-2.632462	3.488739

SCF Energy: -1114.10644 hartrees

Only One Imaginary Frequency: -416.5878

(S,R,S)-TS (RHF/6-31G*)

Z-Matrix orientation:

C 0	0.581757	-0.666718	-0.312607
C 0	-0.624512	-1.364838	1.262985
C 0	-1.606491	-0.612823	0.326400
N 0	-0.635162	0.134949	-0.455292
C 0	1.851974	-0.091095	0.087173
O 0	-0.246124	-0.519257	2.269333
O 0	-0.626648	-2.567139	1.462997
C 0	-2.483383	-1.659576	-0.406296

Si 0	-0.809708	1.491700	-1.501114
C 0	-3.495453	-2.271957	0.572906
C 0	-3.240936	-1.137375	-1.627029
C 0	-2.537827	2.279037	-1.341400
C 0	-0.480484	1.066605	-3.330612
C 0	0.601028	-1.080063	3.230500
C 0	0.371719	2.942368	-1.164169
C 0	3.056396	-0.728134	-0.285645
C 0	4.287170	-0.298615	0.166321
C 0	4.398483	0.803787	1.004181
C 0	3.229187	1.452835	1.377792
C 0	1.991394	1.023239	0.939896
H 0	0.694550	-1.401382	-1.104691
H 0	-2.264420	0.040405	0.904266
H 0	-1.818314	-2.449692	-0.735764
H 0	-4.197250	-1.515518	0.924057
H 0	-2.997055	-2.706757	1.426468
H 0	-4.077896	-3.051514	0.084824
H 0	-2.580475	-0.711472	-2.369461
H 0	-3.975708	-0.385941	-1.351135
H 0	-3.779846	-1.954468	-2.103058
H 0	-2.818375	2.397583	-0.297104
H 0	-3.326050	1.720825	-1.832809
H 0	-2.519043	3.273911	-1.783890
H 0	-0.513474	1.961929	-3.950516
H 0	-1.188690	0.354202	-3.743973
H 0	0.511795	0.634200	-3.436722
H 0	1.472641	-1.527374	2.772278
H 0	0.913513	-0.267853	3.875565
H 0	0.086792	-1.834503	3.814224
H 0	0.168442	3.731079	-1.889450
H 0	1.417007	2.670776	-1.251358
H 0	0.227692	3.364349	-0.173203
H 0	3.004868	-1.582016	-0.940628
H 0	5.175110	-0.824768	-0.148056
H 0	5.359421	1.145126	1.350204
H 0	3.281540	2.310364	2.030609

H 0 1.107300 1.530685 1.271103

SCF Energy: -1114.10012 hartrees

Only One Imaginary Frequency: -467.2859

(S,S,S)-TS (RHF/6-31G*)

Z-Matrix orientation:

C 0 0.962997 -0.418762 -0.081192
C 0 -0.433900 -1.777542 0.788483
C 0 -1.260086 -0.542007 0.407654
N 0 -0.337982 0.108154 -0.509705
C 0 1.807205 0.401688 0.764191
O 0 -0.288025 -2.168198 1.926346
O 0 -0.422897 -2.680984 -0.250427
C 0 -2.699448 -0.846725 -0.059998
Si 0 -0.487183 1.196075 -1.828262
C 0 0.389053 -3.795303 -0.044846
C 0 -3.349457 -1.934692 0.807922
C 0 -3.588562 0.403580 -0.013748
C 0 -0.939850 2.990326 -1.355835
C 0 -1.744049 0.653122 -3.159012
C 0 1.174881 1.309204 -2.729706
C 0 3.170273 0.070969 0.940445
C 0 3.993759 0.781403 1.784775
C 0 3.517334 1.871979 2.506943
C 0 2.184875 2.218307 2.348434
C 0 1.349289 1.510620 1.502396
H 0 1.507919 -0.914063 -0.874146
H 0 -1.337677 0.021744 1.337326
H 0 -2.651413 -1.213989 -1.080017
H 0 0.056015 -4.383179 0.800980
H 0 0.335358 -4.392563 -0.948486
H 0 1.417328 -3.493347 0.125351
H 0 -3.334579 -1.656387 1.857697
H 0 -2.834839 -2.880783 0.712692

H 0	-4.387634	-2.080231	0.514175
H 0	-3.187927	1.228226	-0.587479
H 0	-3.704178	0.746613	1.011795
H 0	-4.581894	0.187714	-0.402390
H 0	-0.148010	3.424957	-0.751083
H 0	-1.860794	3.069122	-0.783875
H 0	-1.055359	3.610764	-2.244629
H 0	-1.525345	-0.358124	-3.494019
H 0	-1.669998	1.309692	-4.025742
H 0	-2.778580	0.670761	-2.830307
H 0	1.469238	0.348633	-3.143906
H 0	1.970398	1.637238	-2.068863
H 0	1.105423	2.019119	-3.553726
H 0	3.569519	-0.769287	0.396027
H 0	5.027252	0.486877	1.882141
H 0	4.162903	2.426941	3.166245
H 0	1.784210	3.059036	2.893417
H 0	0.321854	1.810028	1.406967

SCF Energy: -1114.10117 hartrees

Only One Imaginary Frequency: -344.2473

(R,R,S)-TS (RB3LYP/6-31G*)

Z-Matrix orientation:

C 0	0.862488	-0.091492	0.317596
C 0	-0.640625	-1.116333	1.536407
C 0	-1.453964	-0.163620	0.617600
N 0	-0.375504	0.648148	0.043686
O 0	-0.377350	-0.417404	2.739182
O 0	-0.681976	-2.347275	1.535690
C 0	-2.289398	-0.961243	-0.414429
Si 0	-0.276917	2.383789	0.090729
C 0	1.599808	-0.710037	-0.748291
C 0	1.104950	-0.881042	-2.072600
C 0	1.841293	-1.538116	-3.053207

C 0	3.111862	-2.061310	-2.785172
C 0	3.627029	-1.899734	-1.489975
C 0	2.900787	-1.244064	-0.506454
C 0	-3.418259	-1.737946	0.282471
C 0	-2.862549	-0.064133	-1.517471
C 0	-2.001694	3.182266	-0.029938
C 0	0.778183	3.000549	-1.359879
C 0	0.408844	-1.152557	3.655579
C 0	0.508957	3.042526	1.699173
H 0	1.479248	0.308441	1.126587
H 0	-2.154434	0.432816	1.231674
H 0	-1.607819	-1.688766	-0.871628
H 0	0.128418	-0.471848	-2.312881
H 0	1.416428	-1.640045	-4.052628
H 0	3.682159	-2.576233	-3.555450
H 0	4.616425	-2.290268	-1.248917
H 0	3.325714	-1.134155	0.491211
H 0	-4.113297	-1.050018	0.787125
H 0	-3.005814	-2.425369	1.024536
H 0	-4.002304	-2.317795	-0.445694
H 0	-2.072220	0.507248	-2.013214
H 0	-3.592453	0.649994	-1.110321
H 0	-3.380875	-0.665665	-2.276886
H 0	-2.651154	2.873962	0.798538
H 0	-2.508530	2.918091	-0.964539
H 0	-1.916763	4.277100	0.008392
H 0	1.022629	4.066864	-1.259200
H 0	0.260147	2.858261	-2.315842
H 0	1.716797	2.437820	-1.412277
H 0	1.419434	-1.325439	3.257004
H 0	0.476456	-0.548218	4.566681
H 0	-0.040680	-2.126602	3.880066
H 0	0.017517	2.596008	2.571533
H 0	0.426544	4.135651	1.773758
H 0	1.572189	2.782654	1.758652

SCF Energy: -1120.09371 hartrees

Only One Imaginary Frequency: -129.8217

(*R,S,S*)-TS (RB3LYP/6-31G*)

Z-Matrix orientation:

```
-----  
C 0  0.872360  0.160904  0.323486  
C 0 -0.485931 -0.553970  1.789444  
C 0 -1.418106  0.074783  0.710159  
N 0 -0.402496  0.767197 -0.102173  
O 0 -0.273758  0.020874  2.866516  
O 0 -0.457718 -1.959641  1.722565  
C 0 -2.299927 -0.922836 -0.082413  
Si 0 -0.361954  2.502258 -0.283829  
C 0  1.622253 -0.657486 -0.591461  
C 0  1.095764 -1.185760 -1.803741  
C 0  1.839508 -2.032410 -2.619492  
C 0  3.148590 -2.402420 -2.287857  
C 0  3.696625 -1.885071 -1.104340  
C 0  2.963394 -1.036728 -0.286697  
C 0 -3.359055 -1.563019  0.829391  
C 0 -2.973831 -0.258621 -1.290024  
C 0 -2.096802  3.202927 -0.639282  
C 0  0.771942  2.949875 -1.735703  
C 0  0.276077  3.367981  1.291718  
C 0  0.391479 -2.549286  2.688600  
H 0  1.481903  0.765808  0.999283  
H 0 -2.094100  0.774628  1.234177  
H 0 -1.636551 -1.714203 -0.449844  
H 0  0.088150 -0.901611 -2.091843  
H 0  1.389938 -2.409500 -3.538956  
H 0  3.724670 -3.066055 -2.929214  
H 0  4.718018 -2.143829 -0.822845  
H 0  3.416077 -0.644363  0.623900  
H 0 -4.036118 -0.799011  1.238754  
H 0 -2.889313 -2.089081  1.664291  
H 0 -3.974976 -2.282364  0.271835
```

H 0	-2.231918	0.211365	-1.942169
H 0	-3.685318	0.516479	-0.971939
H 0	-3.534286	-0.998123	-1.878906
H 0	-2.794739	2.996643	0.181290
H 0	-2.525864	2.779816	-1.554367
H 0	-2.047775	4.293594	-0.762787
H 0	0.955688	4.031830	-1.783356
H 0	0.337097	2.635269	-2.691879
H 0	1.738159	2.443893	-1.632904
H 0	-0.064621	2.807739	2.170975
H 0	-0.077805	4.404877	1.370926
H 0	1.371857	3.385727	1.328003
H 0	1.433762	-2.241425	2.531052
H 0	0.308960	-3.632782	2.553482
H 0	0.099243	-2.270569	3.707764

SCF Energy: -1120.09084 hartrees

Only One Imaginary Frequency: -158.3714

(*S,R,S*)-TS (RB3LYP/6-31G*)

Z-Matrix orientation:

C 0	0.615356	-0.597931	-0.402039
C 0	-0.563995	-1.443848	1.182816
C 0	-1.586655	-0.663483	0.289169
N 0	-0.638290	0.148132	-0.476135
C 0	1.855972	-0.045746	0.062958
O 0	-0.218430	-0.612640	2.257751
O 0	-0.513367	-2.674194	1.311371
C 0	-2.452835	-1.701294	-0.482239
Si 0	-0.870209	1.563690	-1.456680
C 0	-3.409622	-2.406906	0.494415
C 0	-3.251800	-1.133728	-1.659470
C 0	-2.613770	2.290985	-1.203262
C 0	-0.583817	1.227249	-3.315338
C 0	0.650162	-1.226929	3.195755

C 0	0.303406	3.006241	-1.056534
C 0	3.089890	-0.665054	-0.301331
C 0	4.310562	-0.242981	0.207306
C 0	4.388200	0.837204	1.098450
C 0	3.193436	1.470184	1.465485
C 0	1.964005	1.048737	0.970673
H 0	0.729309	-1.364304	-1.177063
H 0	-2.263550	-0.042618	0.905380
H 0	-1.757553	-2.457123	-0.868225
H 0	-4.109070	-1.686142	0.943985
H 0	-2.845367	-2.895218	1.291595
H 0	-4.010330	-3.166946	-0.024765
H 0	-2.611557	-0.625443	-2.385025
H 0	-4.017029	-0.422073	-1.321854
H 0	-3.773590	-1.944168	-2.187454
H 0	-2.842865	2.381897	-0.134186
H 0	-3.410034	1.701019	-1.665817
H 0	-2.652390	3.301483	-1.632874
H 0	-0.593674	2.159988	-3.895828
H 0	-1.332138	0.554077	-3.749908
H 0	0.398514	0.759766	-3.456223
H 0	1.580414	-1.557175	2.720520
H 0	0.878220	-0.462875	3.945755
H 0	0.175446	-2.093964	3.671814
H 0	0.127625	3.822495	-1.772476
H 0	1.357819	2.721298	-1.110733
H 0	0.127029	3.400436	-0.048889
H 0	3.059174	-1.501434	-0.998917
H 0	5.221664	-0.754822	-0.104706
H 0	5.346024	1.175278	1.488419
H 0	3.221176	2.310165	2.160690
H 0	1.052887	1.535370	1.298798

SCF Energy: -1120.08793 hartrees

Only One Imaginary Frequency: -199.4081

(S,S,S)-TS (RB3LYP/6-31G*)

Z-Matrix orientation:

C 0	0.988113	-0.424744	-0.126160
C 0	-0.588379	-1.837952	0.676437
C 0	-1.280350	-0.495239	0.359726
N 0	-0.301254	0.139847	-0.523193
C 0	1.846237	0.254776	0.789795
O 0	-0.493408	-2.329575	1.796967
O 0	-0.601273	-2.659317	-0.466583
C 0	-2.748810	-0.626953	-0.126556
Si 0	-0.386719	1.336777	-1.773865
C 0	0.067825	-3.891815	-0.280579
C 0	-3.493210	-1.730682	0.646912
C 0	-3.523163	0.693878	0.023743
C 0	-0.677872	3.128265	-1.170135
C 0	-1.713364	0.987854	-3.106964
C 0	1.271225	1.348251	-2.691849
C 0	3.195557	-0.177002	0.985275
C 0	4.041245	0.426483	1.903229
C 0	3.610977	1.507278	2.689957
C 0	2.295624	1.955826	2.516724
C 0	1.437454	1.358215	1.600082
H 0	1.479126	-1.034393	-0.885925
H 0	-1.312546	0.016098	1.338348
H 0	-2.723053	-0.913681	-1.185379
H 0	-0.340118	-4.451340	0.568985
H 0	-0.064713	-4.461000	-1.206879
H 0	1.140121	-3.728470	-0.101303
H 0	-3.446136	-1.553452	1.728439
H 0	-3.055725	-2.713196	0.453857
H 0	-4.552017	-1.758240	0.353836
H 0	-3.051178	1.526047	-0.505051
H 0	-3.591568	0.974838	1.083374
H 0	-4.548523	0.595900	-0.359787
H 0	0.144974	3.431503	-0.511795
H 0	-1.608505	3.243515	-0.600739

H 0	-0.717331	3.834122	-2.012192
H 0	-1.569427	-0.011597	-3.535278
H 0	-1.621155	1.717880	-3.923828
H 0	-2.742157	1.042770	-2.735031
H 0	1.477798	0.373108	-3.147919
H 0	2.100052	1.577698	-2.015137
H 0	1.257202	2.101593	-3.492203
H 0	3.559418	-1.013245	0.388351
H 0	5.061783	0.055374	2.007828
H 0	4.277054	1.979492	3.408752
H 0	1.930038	2.794525	3.110977
H 0	0.422882	1.732529	1.491791

SCF Energy: -1120.08559 hartrees

Only One Imaginary Frequency: -72.7583