STRATEGIES FOR THE DESIGN OF ORGANIC AZIRIDINATION REAGENTS AND CATALYSTS: TRANSITION STRUCTURES FOR ALKENE AZIRIDINATIONS BY NH TRANSFER

Ilyas Washington[†], Alan Armstrong[‡]* and K. N. Houk[†]*

[†] Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095-1569

[‡]Department of Chemistry, Imperial College of Science, Technology and Medicine, London SW7 2AY, UK

Supporting Information

Transition state (TS) geometries and energies are listed. Calculations were preformed at the B3LYP/6-31G(d) level except where noted.

6a HF=-248.3313983

6	-1.169160	0.552335	0.342685
8	-2.096613	-0.251333	-0.214494
7	-0.207366	-0.353660	-0.271792
1	-1.123716	1.601295	-0.006336
1	-1.060758	0.519726	1.444609
1	-0.128485	-0.141340	-1.268941
6	1.418369	-0.602439	0.385622
6	1.977364	0.506807	-0.230475
1	1.194759	-0.570157	1.449440
1	1.656533	-1.596152	0.016643
1	1.912862	1.492449	0.218452
1	2.413836	0.440240	-1.222360

6a b3lyp/6-31+g(d) HF=-248.3486777

6	-1.170259	0.558768	0.342199
8	-2.107386	-0.254137	-0.205448
7	-0.224280	-0.360022	-0.273731
1	-1.140907	1.598185	-0.026542
1	-1.069617	0.528929	1.441496
1	-0.148496	-0.154112	-1.273980
6	1.449486	-0.605046	0.385151
6	1.982174	0.513432	-0.231547
1	1.219064	-0.581058	1.447361

1	1.672622	-1.594866	-0.002389
1	1.917995	1.495202	0.227600
1	2.409978	0.458041	-1.228660

6a b3lyp/6-311g(d) HF=-248.3943626

6	-1.171187	0.546292	0.346660
8	-2.102873	-0.246464	-0.214980
7	-0.210504	-0.353952	-0.275106
1	-1.128506	1.594236	0.002939
1	-1.069479	0.498525	1.445677
1	-0.132511	-0.136879	-1.267964
6	1.428165	-0.600625	0.383964
6	1.980998	0.507638	-0.229583
1	1.203686	-0.569863	1.444966
1	1.662283	-1.591624	0.013088
1	1.915402	1.490840	0.220306
1	2.417786	0.444308	-1.219675

6a mp2/6-31g(d) MP2=-247.5357903

6	-1.121359	0.613772	0.309857
8	-2.066758	-0.261112	-0.187258
7	-0.270608	-0.400074	-0.257090
1	-1.089966	1.615912	-0.142560
1	-1.025773	0.663165	1.404693
1	-0.137512	-0.180425	-1.254888
6	1.385417	-0.588869	0.400481
6	1.991355	0.482746	-0.241230
1	1.164651	-0.513373	1.462691
1	1.617774	-1.597675	0.071335
1	1.940089	1.485463	0.171085
1	2.426579	0.370445	-1.229311

6a oxygen transfer HF=-624.6756635

6	0.224091	0.804496	0.144537
7	0.408051	1.538282	1.289242
8	-1.129817	0.342800	0.661294
6	-2.446754	-1.207154	-0.034902
6	-2.537112	0.165189	-0.269660
1	-1.859693	-1.844071	-0.685095
6	1.073505	-0.462926	-0.048070
1	-2.297377	0.555562	-1.253393
1	-2.850669	-1.643623	0.871409
1	-3.252919	0.760936	0.288239
9	1.151108	-1.199372	1.075844
9	2.333254	-0.130580	-0.405949
9	0.581195	-1.262882	-1.028432

6	0.142758	1.628754	-1.130373
1	1.139890	2.006255	-1.373401
1	-0.214418	1.042535	-1.981759
1	-0.516838	2.481572	-0.956253
1	0.705252	0.895802	2.032847

6b conformation 1 HF=-287.6343539

6	1.028377	-.085917	-.445365
7	1.699172	-1.065636	.265833
8	-.271945	-.653031	.072097
6	1.320773	1.331139	.007166
1	1.649967	-1.933580	-.280023
1	.599368	2.052772	-.391938
1	2.313521	1.616331	-.357794
1	1.332789	1.381922	1.099936
6	-2.267440	.018469	-.486504
6	-1.525749	.239339	.680617
1	-2.175721	.683041	-1.338928
1	-2.836536	-.894083	-.619995
1	-1.133907	1.232722	.877937
1	-1.780430	-.314427	1.580052
1	.976541	-.159178	-1.542350

6b conformation 2 HF=-287.6540839

1	-2.827941	-.718320	.855071
6	.999585	-.077756	.445285
7	-.173475	-.674141	-.211790
6	-1.621036	.184202	-.695865
6	-2.209253	.124238	.561919
1	-1.204127	1.123401	-1.046722
1	-.455881	-1.510325	.301228
1	-2.002794	-.446793	-1.494043
1	-1.985225	.864409	1.322748
8	1.676905	-1.100144	-.118693
1	.931680	-.086842	1.551247
6	1.334585	1.320134	-.061406
1	1.318008	1.334215	-1.155851
1	.653380	2.085367	.332036
1	2.348699	1.570122	.266762

6b oxygen transfer HF=-287.6365039

6	.992199	-.085100	.377961
7	1.631167	-1.192047	-.168463
8	-.235106	-.473482	-.359363
6	1.433190	1.327218	.029964
1	1.973369	-.911323	-1.098093

1	1.491805	1.443977	-1.057689
1	2.421947	1.524488	.460498
1	.737074	2.076899	.421590
6	-2.197215	.600327	-.266489
6	-1.694328	-.508229	.423167
1	-2.001316	1.609202	.080200
1	-2.667034	.487331	-1.236978
1	-1.438254	-.401591	1.476921
1	-2.065616	-1.496663	.165467
1	.807624	-.205426	1.454612

6c HF=-326.973957991

C	0.470000	1.125717	-0.137253
O	1.191666	1.869781	0.737747
N	0.352051	0.191696	1.003235
C	1.283173	0.516205	-1.283859
C	-0.837097	1.768951	-0.612305
H	-0.324158	0.555588	1.676239
H	2.188385	0.047226	-0.887619
H	1.588470	1.323822	-1.956863
H	0.713150	-0.214996	-1.870148
H	-0.600311	2.620071	-1.260880
H	-1.400208	2.150497	0.245880
H	-1.468933	1.074921	-1.177948
C	0.196426	-1.533585	0.936400
C	-1.192215	-1.532822	0.831528
H	0.794540	-1.773392	0.062225
H	0.657257	-1.845184	1.870285
H	-1.681503	-1.418045	-0.129471
H	-1.823914	-1.534882	1.714340

6c oxygen transfer HF=–326.953866

C	-0.517883	1.042847	-0.392960
N	-1.372421	1.581573	0.553146
O	-0.112534	0.015015	0.676483
C	0.733566	1.812195	-0.805527
C	-1.251953	0.403351	-1.562912
H	-0.814392	2.196716	1.158539
H	1.274216	2.155029	0.082000
H	0.452118	2.685608	-1.405930
H	1.411148	1.194489	-1.404968
H	-0.605026	-0.263855	-2.142990
H	-1.600861	1.194443	-2.235718
H	-2.126495	-0.145477	-1.204407
C	1.360367	-1.596481	0.608215
C	-0.033585	-1.625153	0.479797
H	1.996948	-1.438736	-0.255569

H	1.829742	-1.586777	1.585037
H	-0.467728	-1.841156	-0.492004
H	-0.633392	-1.983963	1.311905

6d HF=-624.6942683

1	3.569572	.395916	.636948
6	-.235438	.812481	-.162853
7	1.072289	.505860	-.768932
6	2.169590	-.871552	-.411976
6	2.702030	-.253295	.705950
1	1.449951	-1.674011	-.298777
1	1.632481	1.360757	-.748483
1	2.743526	-.912378	-1.333119
1	2.219132	-.344880	1.672486
6	-1.019755	-.500889	.063473
8	-.519729	1.420474	-1.324151
6	-.265191	1.689048	1.091043
1	.343413	2.580296	.911850
1	-1.295176	2.011941	1.270230
1	.095990	1.170918	1.983909
9	-2.309667	-.233437	.332264
9	-.972304	-1.320351	-.997903
9	-.519640	-1.196005	1.128624

6d conformation 2 HF=-624.6969896

1	-2.655611	-1.888144	-.669593
6	.182659	.796689	-.099832
7	-1.129021	.543619	-.709536
6	-2.634098	.096743	.169962
6	-2.343093	-1.255867	.156310
1	-2.501429	.669136	1.082783
1	-1.006655	-.110198	-1.486157
1	-3.390007	.496003	-.499615
1	-1.708445	-1.703167	.911834
6	.109079	1.558316	1.222413
1	1.111060	1.921024	1.467862
1	-.547273	2.421595	1.088520
1	-.246070	.939806	2.052865
8	.447419	1.521572	-1.198334
6	1.078219	-.458153	.021684
9	2.359266	-.100180	.219154
9	1.024652	-1.220516	-1.089774
9	.717375	-1.251563	1.068586

6e HF=-922.4084317

1	2.561846	-2.476539	-.298824

6	-.182803	.079822	.612129
7	1.142593	-.369969	1.032467
6	2.720896	-.354164	.022408
6	2.320570	-1.480715	-.659350
1	2.626794	.625760	-.429972
1	1.030766	-1.323992	1.386021
1	3.443453	-.424310	.829355
1	1.692485	-1.406650	-1.539203
6	-.093485	1.413829	-.173326
8	-.484338	.203973	1.901719
6	-1.060751	-.973241	-.119772
9	-2.354534	-.644334	-.036148
9	-.894505	-2.182289	.459494
9	-.752318	-1.111020	-1.432047
9	-1.319239	1.908978	-.397655
9	.617996	2.316510	.511564
9	.513118	1.251104	-1.380867

6f HF=-347.589499

1	2.421304	.586632	-1.299213
6	-1.020211	-.029335	.372300
7	.060046	-.756150	-.257749
6	1.827485	-.561248	.414995
6	1.997226	.597343	-.298957
1	1.563794	-.526697	1.468196
1	.069442	-.474357	-1.243395
1	2.274912	-1.491524	.080785
1	1.627972	1.546607	.073322
8	-1.864739	-.792709	-.262608
9	-1.035280	1.336266	.046974
1	-.969316	-.072895	1.472622

6g HF=-347.5886038

1	-2.739125	-.935733	.791679
6	1.011125	-.001028	.413561
7	-.047431	-.700904	-.293723
6	-1.649152	.207180	-.670489
6	-2.148549	-.047861	.584199
1	-1.194279	1.164859	-.897800
1	-.295251	-1.543563	.234973
1	-1.990815	-.363925	-1.527814
1	-1.927743	.607603	1.420842
8	1.836114	-.858927	-.118978
1	.940080	.077460	1.511101
9	1.063299	1.313478	-.054302

7a HF=-441.5005732

1	1.249411	2.467320	-0.778453
6	-1.478806	-0.290351	-0.056857
7	-0.097721	0.036154	-0.481341
6	1.298874	0.685217	0.423826
6	0.890385	1.977457	0.119360
1	1.080205	0.272545	1.410030
1	-0.101863	0.452759	-1.414494
8	2.401966	0.186293	-0.190934
1	0.194152	2.496966	0.764121
6	-1.524831	-0.708235	1.417850
1	-2.494099	-1.177245	1.615647
1	-0.746201	-1.450221	1.617497
1	-1.412214	0.139685	2.105143
8	-1.379038	-1.311343	-0.938056
6	-2.530302	0.769865	-0.402355
1	-3.529487	0.342308	-0.261624
1	-2.435816	1.058786	-1.454364
1	-2.449355	1.664598	0.225557
6	2.561194	-1.229586	-0.058324
1	1.705656	-1.751767	-0.499285
1	2.660792	-1.511420	0.999120
1	3.480353	-1.483196	-0.588585

7a conformation 2 HF=-441.5020157

8	-2.603374	-0.307613	0.288822
6	1.686090	0.262156	0.079757
7	0.580507	-0.454128	0.754000
6	-0.605145	-1.518411	-0.104765
6	-1.548791	-0.583688	-0.495071
1	0.035998	-1.927728	-0.876846
1	0.008966	0.247640	1.229263
1	-3.629257	0.912249	-1.061696
1	-1.428534	0.025207	-1.389502
6	2.519397	-0.708981	-0.769745
1	3.481334	-0.237429	-0.995820
1	2.711539	-1.619511	-0.195224
1	2.041501	-0.970397	-1.723264
8	2.180897	0.487812	1.316458
6	1.302047	1.531880	-0.697347
1	2.211930	2.091067	-0.944181
1	0.676112	2.176721	-0.069947
1	0.775910	1.319340	-1.637080
1	-0.874811	-2.210114	0.686983
1	-4.200413	0.893480	0.631701
6	-3.318786	0.894076	-0.009949
1	-2.702872	1.774593	0.208086

7b HF=-419.2255747

6	-2.749512	0.191338	-0.187607
6	1.531481	0.209014	0.039914
7	0.277026	-0.155062	0.695013
6	-0.842903	-1.331098	0.199864
6	-1.640336	-0.542269	-0.658064
1	-0.209393	-2.085905	-0.256193
1	-0.237937	0.675203	0.993056
1	-1.274174	-1.655063	1.143765
1	-1.351288	-0.402634	-1.694996
6	2.166804	-0.922732	-0.758529
1	3.218731	-0.675168	-0.932551
1	2.130803	-1.855779	-0.190156
1	1.687097	-1.062716	-1.733841
8	1.858599	0.229745	1.381217
6	1.561681	1.561052	-0.661477
1	2.602926	1.864523	-0.815359
1	1.077501	2.321530	-0.040794
1	1.067340	1.525091	-1.637878
7	-3.668982	0.800937	0.200788

7c HF=-554.863436

6	-1.849636	-0.335053	-0.025214
6	2.216704	0.379987	0.081156
7	1.157533	-0.484839	0.565530
6	0.232183	-1.626272	-0.305923
6	-0.723595	-0.743013	-0.842278
1	0.949786	-2.086384	-0.978758
1	0.504303	0.000295	1.183016
1	-0.087022	-2.277470	0.503545
1	-4.492570	1.427811	-0.680446
6	2.987358	-0.182252	-1.105734
1	3.943468	0.345033	-1.184522
1	3.198020	-1.243546	-0.951199
1	2.445099	-0.045999	-2.048054
8	2.660421	-0.046723	1.323880
6	1.896495	1.864919	-0.025286
1	2.830627	2.435912	-0.066455
1	1.337088	2.195601	0.855325
1	1.316045	2.089744	-0.926054
8	-1.995438	-0.600108	1.165016
8	-2.748892	0.407741	-0.727438
6	-3.885973	0.853028	0.021005
1	-0.585466	-0.285831	-1.815324
1	-4.454379	0.003077	0.409350

1	-3.577676	1.480287	0.862844

7d oxygen transfer HF=-366.2621678

1	-1.758813	-1.986914	0.182433
6	0.584835	0.537537	0.008377
8	-0.603875	-0.295554	-0.518809
6	-2.782344	-0.149441	-0.244719
6	-1.807969	-0.923406	0.404082
1	-2.995395	0.861651	0.084653
6	0.684865	0.518792	1.535274
1	-3.206771	-0.467262	-1.190100
1	-1.571024	-0.689480	1.438397
6	0.416714	1.950949	-0.538566
7	1.433515	-0.219155	-0.777052
1	0.311069	1.904988	-1.624272
1	1.299898	2.554761	-0.297471
1	-0.463618	2.440070	-0.108552
1	-0.143139	1.068669	1.994905
1	1.613476	1.020967	1.830385
1	0.704042	-0.491420	1.951225
6	1.985998	-1.435938	-0.229207
1	2.982060	-1.225375	0.200809
1	1.391610	-1.925837	0.555688
1	2.140416	-2.157248	-1.039704

7d HF=-366.2731196

1	2.757339	0.066995	1.208521
6	-0.969052	-0.110363	-0.041199
7	0.367594	0.376254	-0.456898
6	1.778952	-0.683418	-0.568570
6	2.127004	-0.702612	0.776594
1	1.344114	-1.570143	-1.016638
6	0.750500	1.749981	-0.045845
1	2.390042	-0.109368	-1.261476
1	1.674944	-1.412191	1.461724
8	-1.425251	0.675063	-1.051826
6	-1.444967	0.277741	1.365058
1	-2.507437	0.025514	1.452426
1	-0.902701	-0.259129	2.151552
1	-1.350059	1.353258	1.532769
6	-1.149709	-1.612279	-0.300020
1	-0.617548	-2.247112	0.418231
1	-0.834293	-1.856452	-1.317813
1	-2.218364	-1.837458	-0.221870
1	-0.013576	2.423646	-0.427220
1	1.706806	1.989051	-0.518551

1	0.843211	1.884806	1.035128

7e oxygen transfer HF=-735.651071

1	-2.777460	-2.420715	1.041873
6	-0.918214	0.967079	-0.070091
8	-1.313989	-0.505782	-0.144164
6	-2.799443	-1.090670	-0.666188
6	-3.121969	-1.475982	0.637185
1	-3.314697	-0.245359	-1.111281
6	-0.989958	1.426377	1.389292
1	-2.494356	-1.847152	-1.383444
1	-3.606730	-0.786079	1.319274
6	-1.778304	1.840370	-0.985473
7	0.282186	0.607316	-0.636650
14	1.719511	-0.186159	-0.048593
1	-1.759382	1.448409	-2.005363
1	-1.353014	2.849819	-1.003384
1	-2.813223	1.924611	-0.633740
1	-2.028846	1.530779	1.721923
1	-0.507119	2.405876	1.488457
1	-0.482961	0.716786	2.044419
6	1.734046	-0.817129	1.744031
6	3.124127	1.073422	-0.252459
6	2.044948	-1.658070	-1.190388
1	2.992839	1.937528	0.409627
1	3.172688	1.445446	-1.281782
1	4.092251	0.614936	-0.012755
1	1.260882	-2.416588	-1.083935
1	3.007856	-2.133581	-0.964311
1	2.060438	-1.340666	-2.238979
1	0.869020	-1.457490	1.951468
1	1.736076	-0.002110	2.477129
1	2.637799	-1.415569	1.919516

7e HF=-735.6664149

1	0.103074	2.661917	1.239803
6	1.472106	-0.712955	-0.035915
7	0.435196	0.281798	-0.326604
6	0.984494	2.199940	-0.656147
6	0.983079	2.333151	0.701043
1	1.898676	2.004825	-1.204527
14	-1.312783	-0.168116	-0.020741
1	0.140579	2.525877	-1.252942
1	1.866489	2.111982	1.290769
8	0.508689	-1.570405	-0.504022
6	1.878284	-0.925064	1.424539

1	2.394557	-1.888195	1.512697
1	2.564611	-0.145648	1.774034
1	1.001692	-0.944081	2.074174
6	2.683944	-0.604706	-0.965016
1	3.356724	0.211690	-0.676042
1	2.346974	-0.455010	-1.993827
1	3.255137	-1.538059	-0.917073
6	-2.104476	-0.938555	-1.552550
6	-1.696087	-1.146091	1.551998
6	-2.223722	1.495078	0.200921
1	-3.198979	-0.881046	-1.497453
1	-1.811333	-1.985294	-1.668612
1	-1.790541	-0.405336	-2.458028
1	-1.319857	-0.644698	2.451810
1	-1.279062	-2.155524	1.517420
1	-2.785732	-1.226680	1.662547
1	-1.997029	1.995804	1.148911
1	-3.301999	1.287773	0.204007
1	-2.046621	2.209198	-0.612130

7f HF=-777.3122769

1	-0.164941	2.388953	1.426388
6	1.458337	-0.857728	-0.154791
7	0.785509	0.445314	-0.433905
6	1.471289	2.176577	0.048215
6	0.856746	2.059070	1.272857
1	2.531194	1.974853	-0.059481
6	-0.627071	0.556010	-0.657966
1	1.016468	2.751941	-0.749105
1	1.355094	1.588891	2.114254
8	0.726878	-1.281600	-1.219811
6	1.225310	-1.553239	1.189576
1	1.643834	-2.563529	1.122737
1	1.746647	-1.030720	1.999098
1	0.172407	-1.641760	1.443715
6	2.955944	-0.720336	-0.457929
1	3.501986	-0.208944	0.343228
1	3.095999	-0.189562	-1.402569
1	3.376950	-1.725818	-0.560359
8	-1.044915	1.487797	-1.303174
6	-1.697770	-0.308480	0.090078
9	-2.914595	0.090025	-0.290956
9	-1.572105	-0.038879	1.419320
9	-1.634035	-1.631404	-0.065801

7f conformation 2 HF=-777.3157677

1	0.398599	2.655021	1.096858
6	1.668626	-0.721502	-0.043798
7	0.581441	0.244241	-0.306072
6	0.723272	2.006520	-0.929542
6	1.118214	2.381449	0.334112
1	1.451703	1.866149	-1.721628
6	-0.527631	0.005372	0.613932
1	-0.297568	2.164441	-1.260906
1	2.161750	2.351148	0.628114
8	0.631469	-1.634655	-0.069963
6	2.421022	-0.636066	1.284043
1	2.932608	-1.591843	1.444255
1	3.181736	0.152920	1.272536
1	1.732050	-0.465787	2.111626
6	2.596889	-0.822945	-1.252541
1	3.275199	0.036091	-1.321468
1	2.006083	-0.901444	-2.168542
1	3.209551	-1.724747	-1.153570
8	-0.550385	0.244460	1.796187
6	-1.859278	-0.237203	-0.140432
9	-2.755453	-0.817216	0.660812
9	-1.749349	-0.952673	-1.259421
9	-2.341548	0.993907	-0.489078

7f oxygen transfer HF=-777.3242641

1	-2.360119	-2.466090	-0.193503
6	-1.211141	0.834482	0.180004
8	-1.596303	-0.367197	-0.542546
6	-3.684287	-0.900845	-0.836525
6	-2.877432	-1.551712	0.072387
1	-4.292722	-0.051389	-0.544725
6	-1.424257	0.777055	1.689917
1	-3.697857	-1.187475	-1.881912
1	-2.949901	-1.344965	1.133760
6	-1.819264	2.079268	-0.454847
7	0.097563	0.594604	-0.346808
6	0.912915	-0.335499	0.250220
1	-1.664190	2.053837	-1.535483
1	-1.335451	2.975029	-0.051708
1	-2.891560	2.142828	-0.239565
1	-2.490215	0.861325	1.930901
1	-0.919251	1.632993	2.150303
1	-1.019667	-0.140802	2.115674
8	0.655160	-1.288320	0.971367
6	2.388008	-0.088031	-0.172402
9	2.556335	-0.347910	-1.484038

9	3.220388	-0.876679	0.519576
9	2.752155	1.193290	0.046776

10a HF=-782.7528036

6	-1.338285	-1.209494	-0.284595
6	2.670352	-0.133819	0.422440
7	1.747818	-0.896085	-0.376073
6	0.501964	-0.315369	-1.583461
6	-0.632697	-0.035181	-0.789494
1	1.000087	0.530790	-2.043600
1	1.231331	-1.639317	0.113111
1	0.507231	-1.231631	-2.164930
6	-0.848598	1.360187	-0.421230
6	3.010223	1.249978	-0.078732
1	3.901458	1.620099	0.438063
1	3.215173	1.219744	-1.151200
1	2.174744	1.935220	0.095536
8	3.200478	-1.224010	-0.335998
6	2.641973	-0.339407	1.919642
1	3.629400	-0.122603	2.340697
1	2.378668	-1.371752	2.167677
1	1.918400	0.338679	2.384219
8	-0.798043	-2.319818	-0.210567
8	-2.618182	-1.023317	0.095015
6	-3.272665	-2.177735	0.635407
8	-0.078478	2.275517	-0.710145
8	-1.979742	1.587804	0.292586
6	-2.204748	2.953862	0.653207
1	-1.392512	3.334945	1.279801
1	-3.145261	2.956640	1.206645
1	-2.283720	3.586251	-0.235733
1	-2.726669	-2.568969	1.498678
1	-3.351939	-2.968292	-0.116146
1	-4.264481	-1.834742	0.933466

10b HF=-511.4749837

6	-2.601468	-0.584864	0.216827
6	1.766935	-0.193422	0.159206
7	0.580782	-0.957620	-0.201184
6	-0.605331	-0.510673	-1.243694
6	-1.566849	0.160068	-0.401511
1	-0.084570	0.100569	-1.976770
1	0.159569	-1.455566	0.589212
1	-0.929287	-1.460642	-1.666642
6	-1.323511	1.507532	-0.041345
6	2.136447	0.980662	-0.716093

1	3.183981	1.236323	-0.528346
1	2.032363	0.735080	-1.774888
1	1.515963	1.848789	-0.471627
8	2.002909	-1.486936	-0.386825
6	2.031221	-0.035056	1.638689
1	3.098614	0.144044	1.801367
1	1.746824	-0.937010	2.189139
1	1.473671	0.822827	2.028414
7	-3.435796	-1.234176	0.715436
7	-1.037137	2.608310	0.233213

11a HF=-228.8593725

1	-1.110793	1.632223	0.173188
1	2.360304	0.619598	-1.328884
6	-1.132333	0.586145	0.478214
7	-2.144282	-0.194415	-0.185110
1	-2.615881	0.147741	-1.017560
1	-1.100030	0.450482	1.557572
7	-0.349975	-0.392322	-0.255281
6	1.861708	-0.631368	0.326568
6	2.090804	0.558262	-0.276844
1	2.065823	1.494400	0.275605
1	1.968457	-1.570887	-0.207173
1	1.687510	-0.703016	1.396634
1	-0.177308	-0.029115	-1.202399
1	-2.539363	-1.012497	0.268123

11a rb3lyp/6-31+g(d) HF=-228.8649937

1	-1.101689	1.631399	0.160068
1	2.373535	0.624595	-1.322612
6	-1.126311	0.587667	0.472777
7	-2.149225	-0.191891	-0.175898
1	-2.629303	0.150649	-1.004096
1	-1.080859	0.455406	1.552268
7	-0.355718	-0.396510	-0.264407
6	1.865318	-0.632584	0.327173
6	2.093260	0.560346	-0.273223
1	2.055282	1.495749	0.280644
1	1.982203	-1.571300	-0.206671
1	1.678842	-0.705971	1.395412
1	-0.190317	-0.049618	-1.219256
1	-2.546698	-1.004672	0.286020

11a rb3lyp/6-311g(d) HF=-228.9116255

1	-1.096046	1.625904	0.158545
1	2.368475	0.621966	-1.319784

6	-1.123805	0.585066	0.471121
7	-2.148084	-0.189758	-0.176481
1	-2.620278	0.150038	-1.004583
1	-1.082123	0.456644	1.548413
7	-0.351091	-0.398169	-0.261517
6	1.859870	-0.629175	0.325961
6	2.088088	0.558225	-0.272822
1	2.051772	1.492719	0.278139
1	1.977789	-1.566649	-0.204429
1	1.676577	-0.702513	1.392224
1	-0.182854	-0.048301	-1.210340
1	-2.544011	-0.999016	0.282244

11a MP2=-228.0736036

1	-1.032025	1.632293	0.151535
1	2.306072	0.629161	-1.298841
6	-1.051295	0.588798	0.463708
7	-2.080863	-0.183645	-0.171155
1	-2.546304	0.141703	-1.016282
1	-1.002292	0.459022	1.543003
7	-0.279328	-0.394859	-0.268694
6	1.727564	-0.642990	0.323010
6	1.993482	0.561453	-0.260411
1	1.931398	1.490156	0.299690
1	1.895899	-1.574665	-0.206176
1	1.539116	-0.722022	1.389088
1	-0.130138	-0.039334	-1.226385
1	-2.458898	-1.010356	0.285478

11b HF=-268.1856996

1	0.918215	0.003765	1.547690
1	-2.724775	-0.952215	0.996828
6	0.970252	0.074172	0.459466
7	1.815445	-0.957952	-0.092289
1	2.106648	-1.763996	0.451399
6	1.218894	1.472819	-0.048677
7	-0.012509	-0.709390	-0.291794
6	-2.016701	0.147590	-0.693285
6	-2.278397	-0.032518	0.625809
1	-2.091163	0.748866	1.358069
1	-2.285288	-0.599685	-1.433635
1	-1.669616	1.101088	-1.079191
1	-0.324021	-1.494369	0.295136
1	2.245712	-0.827668	-1.002159
1	0.418621	2.140228	0.283621
1	1.257471	1.492003	-1.142565

1	2.163360	1.850989	0.353510

11c HF=-268.1783519

1	-0.556034	0.446814	1.536459
1	2.597262	1.688743	-0.256245
6	-0.483957	-0.385214	0.834379
7	-1.597487	-0.468315	-0.065275
6	-2.613892	0.572608	-0.223012
1	-0.224686	-1.322523	1.326633
7	0.224238	-0.190113	-0.421940
6	2.387600	-0.433138	-0.415568
6	2.488482	0.739433	0.262832
1	2.495634	0.772044	1.349316
1	2.478471	-0.473024	-1.496508
1	2.390638	-1.388693	0.101011
1	-2.930336	0.626377	-1.266528
1	-2.201856	1.536481	0.084386
1	-3.478865	0.339566	0.410107
1	0.167183	0.805556	-0.673704
1	-1.794069	-1.384481	-0.456206

11d HF=-307.4950714

1	0.047919	-1.114955	1.369500
1	-3.165194	-1.339872	-0.631295
6	0.156783	-0.140690	0.889129
7	1.330322	-0.022168	0.074970
7	-0.536742	0.096567	-0.370624
6	-2.544855	0.683362	-0.301460
6	-2.905424	-0.570659	0.091753
1	-2.961321	-0.845003	1.141834
1	-2.601482	0.986522	-1.342060
1	-2.411850	1.483043	0.421296
1	-0.617933	-0.798790	-0.869236
1	0.020713	0.676399	1.598780
6	2.001333	1.273775	-0.052258
1	1.283052	2.076869	0.113009
1	2.810516	1.341864	0.686416
1	2.420575	1.370198	-1.056174
6	2.086663	-1.214453	-0.315944
1	2.952571	-1.331159	0.349310
1	1.459074	-2.104319	-0.234866
1	2.441292	-1.109598	-1.344259

11e HF=-346.8158577

1	-0.079471	-0.188169	-1.641921
1	3.095793	-1.730317	-0.323330

6	-0.162880	0.275554	-0.655556
7	-1.341933	-0.211104	0.023076
6	-2.073362	-1.357885	-0.519421
7	0.554733	-0.421205	0.423411
6	2.502960	-0.012839	0.816576
6	2.873428	-0.666279	-0.325172
1	2.422840	1.068789	0.842844
1	-2.385421	-2.022926	0.290435
1	-1.446357	-1.910970	-1.221892
1	-2.968182	-1.005964	-1.050620
1	0.610794	-1.419005	0.188285
6	-2.035397	0.579236	1.042028
1	-2.820915	1.188221	0.576214
1	-2.493251	-0.099676	1.764904
1	-1.333734	1.224383	1.567238
1	2.536663	-0.507536	1.781984
1	2.963662	-0.147794	-1.275801
6	0.065759	1.770634	-0.739488
1	-0.721692	2.232266	-1.342914
1	0.086770	2.247299	0.243097
1	1.019845	1.967037	-1.237725

11f HF=-346.8963602

1	-0.081012	-0.260333	-1.650525
1	3.071286	-1.700793	-0.326636
6	-0.137341	0.225554	-0.647704
7	-1.327645	-0.208709	0.044713
6	-2.085617	-1.331194	-0.496368
7	0.555154	-0.459252	0.448722
6	2.441316	-0.006872	0.823014
6	2.832668	-0.639918	-0.322533
1	2.336056	1.073113	0.858734
1	-2.521746	-1.912402	0.322313
1	-1.429679	-1.972387	-1.090412
1	-2.897361	-0.956037	-1.137845
1	0.593325	-1.481501	0.238226
6	-2.021055	0.651790	0.995239
1	-2.762617	1.271562	0.470310
1	-2.537223	0.026892	1.729908
1	-1.311314	1.296860	1.514875
1	2.513005	-0.504707	1.785874
1	2.879131	-0.118568	-1.275252
6	0.129324	1.710331	-0.761236
1	-0.653158	2.174211	-1.371783
1	0.168647	2.212562	0.209531
1	1.084330	1.869106	-1.273831

11g HF=-644.5237785

1	0.422375	-0.087576	-1.517032
1	3.144970	-2.286714	-0.104363
6	0.570177	0.529764	-0.630551
7	-0.603787	0.468210	0.245471
6	-1.643121	-0.503484	-0.091127
7	1.110270	-0.157005	0.543118
6	3.316019	-0.335292	0.749910
6	3.273689	-1.220728	-0.277099
1	3.545390	0.713352	0.587372
9	-2.336993	-0.819822	0.992722
9	-1.071826	-1.608812	-0.592727
9	-2.461168	0.013058	-1.008876
1	0.916934	-1.161343	0.440341
6	-1.005876	1.598522	1.106788
1	-1.567521	2.330182	0.517543
1	-1.622902	1.214843	1.917704
1	-0.112763	2.055220	1.527750
1	3.274082	-0.662370	1.784260
1	3.404493	-0.906952	-1.309679
6	1.150381	1.882072	-0.967964
1	0.451832	2.442130	-1.597122
1	1.392323	2.469461	-0.080398
1	2.067674	1.736390	-1.546312

11g conformation 2 HF=-644.5194148

1	-0.159529	-0.292583	-1.598643
1	2.960183	-2.273112	-0.882629
6	-0.236496	-0.196708	-0.513426
7	-1.451434	-0.765364	-0.007821
6	-2.267873	-1.600165	-0.898712
7	0.390631	-1.220088	0.306186
6	2.471925	-1.065029	0.817140
6	2.781162	-1.273985	-0.492660
1	2.407305	-0.064481	1.230893
1	0.429362	-2.084290	-0.247617
6	-2.106013	-0.273663	1.214250
1	-2.814826	0.520497	0.950805
1	-2.641749	-1.103954	1.677437
1	-1.363572	0.110279	1.909216
1	2.461679	-1.881642	1.532670
1	2.881929	-0.445497	-1.187982
6	0.114358	1.255694	-0.157583
9	0.349585	1.432365	1.151263
9	1.226134	1.597805	-0.830833

9	-0.891167	2.053157	-0.533736
1	-3.089582	-0.996672	-1.305855
1	-2.684750	-2.438057	-0.335352
1	-1.664175	-1.979119	-1.725798

12a HF=-461.3532016

1	1.547487	1.161195	1.334516
1	-1.946908	-0.490270	1.815556
6	1.233475	0.776582	0.359934
7	2.061732	-0.352505	-0.023377
6	2.977288	-0.943553	0.956105
7	0.222415	-0.277950	0.381737
6	-2.303253	0.784627	0.125230
6	-1.730066	0.451723	1.324476
1	-2.212906	1.790008	-0.280030
1	2.981156	-2.032090	0.855636
1	2.673105	-0.672332	1.969211
1	3.994293	-0.567635	0.782447
1	0.291006	-0.749269	1.290994
6	2.301456	-0.694240	-1.427213
1	3.184817	-0.159056	-1.798016
1	2.476094	-1.769703	-1.503499
1	1.433665	-0.437346	-2.031570
8	-2.970263	0.012192	-0.704054
1	-1.352674	1.256343	1.945836
6	1.017355	1.899682	-0.630457
1	1.965745	2.401560	-0.846118
1	0.573676	1.548340	-1.564620
1	0.345513	2.641517	-0.189070
6	-3.217065	-1.361818	-0.346117
1	-2.267170	-1.892973	-0.237976
1	-3.792298	-1.777690	-1.171604
1	-3.796672	-1.412968	0.580474

12b HF=-439.0480789

1	0.583818	0.087571	-1.632783
6	-3.120394	0.440349	-0.110110
6	0.882972	-0.357277	-0.680104
7	1.794156	0.526467	0.016737
6	1.957976	1.908672	-0.440117
7	0.001734	-0.055569	0.454756
6	-1.553399	-1.158026	0.897443
6	-2.322797	-0.731362	-0.167391
1	-1.085928	-2.135307	0.856818
1	1.996175	2.586378	0.416876
1	1.133054	2.193461	-1.096378

1	2.898734	1.995521	-1.000799
1	-0.452544	0.850510	0.292850
6	2.785561	0.033609	0.975418
1	3.736416	-0.153912	0.460221
1	2.940523	0.792103	1.745712
1	2.438177	-0.882179	1.449498
1	-1.706872	-0.743336	1.888025
1	-2.305549	-1.263269	-1.116121
6	1.267793	-1.811521	-0.854281
1	2.153189	-1.886688	-1.492758
1	1.470817	-2.309925	0.096142
1	0.455656	-2.344874	-1.357549
7	-3.744738	1.424428	-0.076479

12c HF=-574.6981099

1	-1.020799	0.178522	1.544764
6	2.191130	-0.064632	-0.180702
6	-1.547443	-0.292324	0.709574
7	-2.395351	0.680541	0.050653
6	-2.221744	2.102730	0.348100
7	-0.829005	-0.286937	-0.563394
6	0.471614	-1.603562	-1.116291
6	1.334408	-1.279542	-0.093603
1	-0.088363	-2.531874	-1.084883
1	-2.347459	2.693144	-0.563176
1	-1.226710	2.284905	0.759665
1	-2.972500	2.422123	1.084114
1	-0.199332	0.526944	-0.620042
6	-3.620038	0.299287	-0.652793
1	-4.474903	0.327660	0.035471
1	-3.794863	1.006725	-1.466339
1	-3.523047	-0.699399	-1.074950
1	0.599772	-1.158488	-2.097697
1	3.784100	1.787776	0.880213
6	-2.147240	-1.619800	1.125814
1	-2.907483	-1.462341	1.896813
1	-2.594634	-2.156748	0.286565
1	-1.365073	-2.250769	1.558340
8	1.844313	0.941573	-0.783827
8	3.327033	-0.215535	0.486883
6	4.254459	0.900952	0.450582
1	1.382558	-1.873492	0.815251
1	4.551134	1.102694	-0.580406
1	5.106446	0.580436	1.046953

12d HF=-386.120219

1	-0.215277	-0.029432	-1.661690
1	3.284817	-1.024904	-0.606980
6	-0.237188	0.403678	-0.655170
7	-1.476523	0.041318	-0.013634
6	-2.350585	-0.979100	-0.572600
7	0.499184	-0.399033	0.333807
6	2.381254	0.252993	0.860620
6	2.899256	-0.038075	-0.369311
1	2.118865	1.269948	1.128820
1	-2.519167	-1.792623	0.145163
1	-1.929126	-1.388069	-1.491746
1	-3.325826	-0.530249	-0.804743
6	-1.995242	0.775077	1.139594
1	-2.736046	1.518127	0.815601
1	-2.479312	0.073865	1.824815
1	-1.187727	1.273946	1.672527
1	2.477325	-0.440038	1.689985
1	2.940438	0.703315	-1.161475
6	0.085612	1.887903	-0.712735
1	-0.698588	2.395455	-1.282865
1	0.145285	2.346149	0.276788
1	1.030915	2.058066	-1.232829
6	0.577755	-1.844177	0.046554
1	1.407937	-2.267014	0.613699
1	-0.328937	-2.325443	0.428208
1	0.690633	-2.086885	-1.016203

12e HF=-755.5013231

1	1.093032	0.430179	1.629624
1	-2.107086	2.224591	0.785390
6	1.286319	0.617060	0.567297
7	1.727884	-0.613644	-0.051453
6	1.970909	-1.777173	0.805996
7	0.115771	0.482256	-0.294611
6	-0.687837	2.459708	-0.798223
6	-1.111024	2.536147	0.491336
1	0.256209	2.889503	-1.109557
1	1.952777	-2.689340	0.207809
1	1.214950	-1.843015	1.589258
1	2.959768	-1.681370	1.277333
14	-1.332465	-0.668384	0.003999
6	2.500821	-0.581677	-1.296086
1	3.572600	-0.478555	-1.078890
1	2.338599	-1.518013	-1.834820
1	2.168668	0.243377	-1.923007
1	-1.350957	2.142638	-1.593972

1	-0.485927	2.951707	1.275816
6	2.185964	1.835228	0.414156
1	3.142011	1.627261	0.906468
1	2.380924	2.086265	-0.630481
1	1.754609	2.708541	0.909274
6	-0.923722	-2.324915	-0.795657
6	-1.700879	-0.837726	1.843884
6	-2.807152	0.002640	-0.954284
1	-1.861614	-2.880043	-0.920876
1	-0.255192	-2.957982	-0.207571
1	-0.492003	-2.193790	-1.793933
1	-1.984523	0.114543	2.305361
1	-0.870528	-1.254163	2.425241
1	-2.547280	-1.524122	1.972679
1	-3.237819	0.937407	-0.585926
1	-3.597738	-0.755958	-0.890574
1	-2.574954	0.121684	-2.018704

12f conformation 1 HF=-797.1393618

1	-0.657113	-0.230498	-1.552266
1	2.021429	2.292492	0.040549
6	-1.256133	0.219784	-0.760811
7	-1.825818	-0.827710	0.055769
6	-1.520983	-2.239649	-0.181467
7	-0.487600	0.636570	0.431793
6	0.023857	2.634796	0.750713
6	1.001236	2.571587	-0.208497
1	-0.952095	3.051383	0.527766
1	-1.240035	-2.732261	0.754637
1	-0.719038	-2.348174	-0.908351
1	-2.425600	-2.726957	-0.570685
6	0.730608	-0.074339	0.802070
6	-2.950358	-0.567391	0.955853
1	-3.891217	-0.828990	0.453235
1	-2.843223	-1.186820	1.849694
1	-2.968690	0.478392	1.254610
1	0.258382	2.498337	1.801323
1	0.798947	2.806154	-1.249089
6	-2.190545	1.269110	-1.333602
1	-2.874742	0.789633	-2.040468
1	-2.779658	1.776830	-0.566569
1	-1.618163	2.017226	-1.889091
6	1.723526	-0.644434	-0.262368
8	1.018243	-0.170666	1.962374
9	2.966157	-0.424600	0.150657
9	1.564849	-0.052606	-1.467385

9	1.532500	-1.963929	-0.415336

12f conformation 2 HF=-797.1509029

1	-1.616749	0.341838	-1.595887
1	1.779810	2.260651	-1.102910
6	-1.687398	0.484815	-0.515339
7	-1.963742	-0.788091	0.110235
6	-2.088012	-1.997104	-0.700616
7	-0.364981	0.444401	0.147976
6	0.539887	2.311564	0.647289
6	0.830469	2.556986	-0.668773
1	-0.350552	2.722345	1.109059
1	-1.799006	-2.869777	-0.110722
1	-1.464661	-1.924677	-1.592120
1	-3.138162	-2.107770	-1.010709
6	0.625583	-0.327565	-0.562329
6	-2.471292	-0.856494	1.481059
1	-3.569685	-0.838342	1.470639
1	-2.138575	-1.790854	1.937941
1	-2.096728	-0.020528	2.069221
1	1.286092	1.911667	1.324010
1	0.124714	3.060742	-1.323234
6	-2.581930	1.659604	-0.166859
1	-3.595909	1.450009	-0.522023
1	-2.623063	1.862308	0.905507
1	-2.240108	2.561363	-0.681741
6	1.948586	-0.567995	0.222947
8	0.467275	-0.835741	-1.644514
9	2.404824	-1.781221	-0.061739
9	1.761487	-0.464974	1.547680
9	2.868143	0.345075	-0.147349

13a HF=-802.5749479

1	1.553823	0.733444	1.275253
6	-1.560207	-1.232203	-0.250859
6	2.042487	0.562014	0.311715
7	3.049668	-0.476145	0.442340
6	3.058525	-1.323748	1.635059
7	1.399537	-0.434951	-0.543073
6	0.003394	-0.032895	-1.777014
6	-0.982668	0.039747	-0.808324
1	0.348102	0.891145	-2.229018
1	3.288075	-2.356319	1.359381
1	2.086049	-1.290099	2.130254
1	3.825635	-0.964042	2.334570
1	0.906446	-1.145302	0.021030

6	4.233237	-0.537297	-0.414976
1	5.067506	-0.008943	0.064338
1	4.510685	-1.583478	-0.562365
1	4.027387	-0.088394	-1.384497
1	0.125549	-0.935100	-2.365439
6	-1.345153	1.373479	-0.236562
6	2.425726	1.868760	-0.346863
1	3.148025	2.401719	0.279178
1	2.851910	1.724893	-1.342359
1	1.527952	2.485994	-0.442340
8	-0.839969	-2.072327	0.271995
8	-2.865127	-1.329366	-0.412190
6	-3.498589	-2.529274	0.108909
8	-0.801528	2.408224	-0.576525
8	-2.304125	1.273970	0.685125
6	-2.762099	2.520428	1.264678
1	-3.348805	-2.585363	1.188721
1	-3.074409	-3.412109	-0.372759
1	-4.553170	-2.418145	-0.135313
1	-1.937323	3.020700	1.776901
1	-3.544579	2.237564	1.966507
1	-3.155226	3.171428	0.481274

13b HF=-531.2741304

1	-0.762596	0.496311	-1.452700
6	2.683350	-1.232658	0.060520
6	-1.099277	0.535179	-0.413876
7	-2.210736	-0.377887	-0.206538
6	-2.537199	-1.370104	-1.235351
7	-0.445137	-0.419521	0.490408
6	1.136372	0.038742	1.483594
6	2.047451	-0.009639	0.429083
1	0.822937	1.004331	1.863150
1	-2.775951	-2.329791	-0.769776
1	-1.701961	-1.489846	-1.928022
1	-3.413673	-1.021749	-1.798610
1	-0.116468	-1.227145	-0.051026
6	-3.213616	-0.169584	0.841724
1	-4.066737	0.377581	0.420998
1	-3.553884	-1.141418	1.205155
1	-2.789979	0.393317	1.670584
1	1.101085	-0.787104	2.185617
6	2.286219	1.142000	-0.379184
6	-1.222135	1.963585	0.068363
1	-2.009976	2.473668	-0.494468
1	-1.443960	2.036121	1.135605

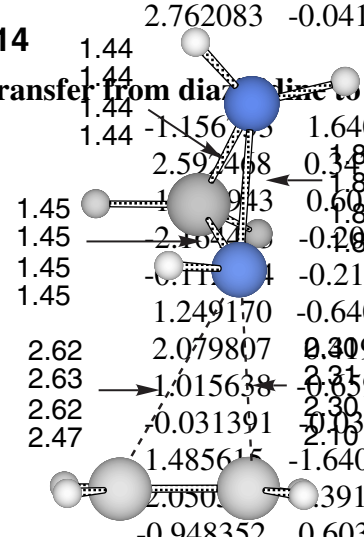
1	-0.284046	2.489037	-0.134250
7	3.165647	-2.247873	-0.244578
7	2.419973	2.094076	-1.036649

Nitrogen transfer from trimethyldiaziridinium to ethylene aziridine HF=-402.1693048

1	-0.456082	0.146523	-1.579585
1	0.258870	-1.246375	0.101966
6	-0.651487	0.443655	-0.545128
7	-1.769132	-0.311461	-0.005842
6	-2.325396	-1.420610	-0.785601
6	-0.620715	1.948008	-0.391750
7	0.043822	-0.319371	0.482012
7	2.056053	0.081775	0.440987
6	-2.625480	0.233904	1.050773
1	2.147310	0.762123	1.191849
6	3.156191	-0.898435	0.406339
6	3.096441	0.190285	-0.603825
1	-3.193283	-1.075394	-1.362819
1	-2.642282	-2.223458	-0.114928
1	-1.576132	-1.807016	-1.480477
1	-3.433784	0.835141	0.616166
1	-2.036500	0.843242	1.733860
1	-3.058747	-0.596590	1.612436
1	-1.416034	2.406537	-0.987474
1	-0.335902	2.323476	-0.767756
1	-0.172213	2.260490	0.649541
1	3.389238	-0.846660	1.206183
1	3.784928	1.027352	-0.528458
1	2.867203	-1.905223	0.115752
1	2.762083	-0.041612	-1.611203

Distances where calculated at: B3LYP/6-31G* and B3LYP/6-311G* and MP2/6-31G* respectively. Energies are activation energies in kcal/mol.

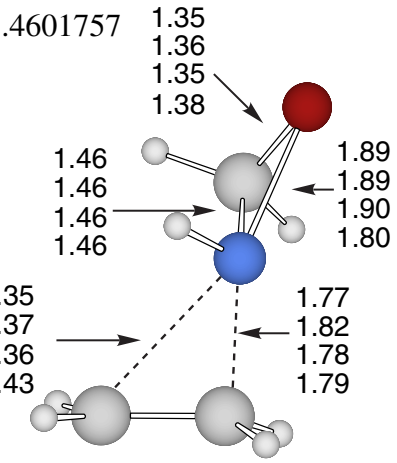
14



(B3LYP/6-31G*) = -0.3
(B3LYP/6-31+G*) = -1.5
(B3LYP/6-311G*) = -1.3
(MP2/6-31G*) = 4.9

14) Activation energies and transition state geometries for aziridination of ethylene by diaziridinium.

15



(B3LYP/6-31G*) = 22.0
(B3LYP/6-31+G*) = 20.9
(B3LYP/6-311G*) = 21.8
(MP2/6-31G*) = 20.8

15) Activation energies and transition state geometries for aziridination of ethylene by oxaziridine