

Supplementary Information for
**Organometallic Calcium and Strontium Borohydrides as Initiators for
the Polymerization of ϵ -Caprolactone and *L*-Lactide: Combined
Experimental and Computational Investigations**

Magdalena Kuzdrowska,^a Liana Annunziata,^b Sebastian Marks,^a Matthias Schmid,^{a,b} Cedric G.
Jaffredo,^b Peter W. Roesky,^{a*} Sophie M. Guillaume,^{b*} and Laurent Maron^{c*}

^a Institut für Anorganische Chemie and Helmholtz Research School: Energy-Related Catalysis, Karlsruher Institut für Technologie (KIT), Engesserstr. 15, 76131 Karlsruhe (Germany), Fax: (+49)721-608-44845, E-mail: roesky@kit.edu

^b Sciences Chimiques de Rennes (UMR 6226), CNRS - Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex (France), Fax: (+33) 2-2323-6939, E-mail: sophie.guillaume@univ-rennes1.fr

^c Université de Toulouse, INSA, UPS, CNRS-UMR5215, LPCNO, 135 Avenue de Ranguéil, 31077 Toulouse (France), E-mail: laurent.maron@irsamc.ups-tlse.fr

Computational details

Calculations were carried out at the DFT level using the hybrid functional B3PW91^[1] with the Gaussian 03^[2] suite of programs. Strontium, phosphorus and silicon have been represented by a relativistic effective-core potential (RECP)^[3] from the Stuttgart group and their corresponding optimized basis set. Polarized all-electron double- ζ 6-31G(d,p)^[4] basis sets were used for Ca, B, C, H, O and N. Geometry optimizations were carried out without any symmetry restriction. The nature of the extrema (minimum or transition state) was verified with analytical frequency calculations. The connectivity of the transition states were controlled by IRC calculations. For simplicity and in order to be in line with previous studies, the ligand of complex **2a** was simplified by replacing the phenyl backbone by a methyl group and the SiMe₃ substituents by simple SiH₃. Moreover, for this complex, the monomer was used as reference rather than the dimer. In all cases, the replacement of THF by ϵ -CL was done. It is noteworthy that for complex **2a** and **3a**, the replacement of one THF molecule was leading to the dissociation of the second one. Thus, we considered as reference the non-solvated complex unlike complex **1a** where one THF molecule remained coordinated after replacement.

References

- [1] a) J. P. Perdew, Y. Wang, *Phys. Rev. B* **1992**, *45*, 13244; b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.
- [2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, R. E. Stratman, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. Martin, D. J. Fox, T. Keith, M. A. AlLaham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. J. Wong, L. Andres, M. Head-Gordon, E. S. Replogle, J. A. Pople, *Gaussian 03; E.01 ed. Pittsburgh PA* **2006**.

- [3] a) P. Fuentealba, L. v. Szentpaly, H. Preuss, H. Stoll, *J. Phys. B: At., Mol. Opt. Phys.* **1985**, *18*, 1287; b) A. Bergner, M. Dolg, W. Küchle, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *80*, 1431.
- [4] J.-P. Blaudeau, M. P. McGrath, L. A. Curtiss, L. Radom, *J. Chem. Phys.* **1997**, *107*, 5016.

1b

37

scf done: -550.088318

C	-0.562508	0.989559	0.341821
C	-0.053372	-0.453293	0.439704
O	1.371975	-0.360574	0.706513
C	1.729123	1.021383	0.925774
C	0.716584	1.800402	0.104715
Sr	3.034789	-2.167254	0.123379
O	3.538723	-3.631723	2.114995
C	2.957407	-4.946640	2.324382
C	3.933718	-5.704289	3.231351
C	5.237066	-4.910243	3.089304
C	4.717393	-3.491251	2.938102
B	5.261906	-0.695346	0.119244
B	1.411759	-3.802947	-1.213322
H	1.643213	1.251250	1.996670
H	2.769274	1.146049	0.616511
H	0.629214	2.842530	0.422611
H	-0.174667	-1.014646	-0.490851
H	-0.526659	-1.016598	1.250198
H	-1.034267	1.295612	1.281402
H	-1.299605	1.108818	-0.456000
H	4.470871	-0.328916	-0.768281
H	0.990008	-3.607814	-0.059724
H	5.508917	-1.899712	-0.070674
H	2.559034	-4.275521	-1.120099
H	4.674012	-0.598865	1.210920
H	6.268797	-0.037368	0.101953
H	0.687109	-4.539691	-1.829129
H	1.506333	-2.694914	-1.771493
H	1.000073	1.785880	-0.953106
H	1.966553	-4.825359	2.773144
H	2.838307	-5.411069	1.341500
H	3.589259	-5.682451	4.270572
H	4.035745	-6.751386	2.935978
H	5.904559	-5.024464	3.947272
H	5.782380	-5.208444	2.187491
H	4.431180	-3.060403	3.907378
H	5.396311	-2.804083	2.428163

ϵ -CL adduct to 1b

42

scf done: -702.698952

O	-0.002763	0.051571	2.168762
C	0.234698	-0.290553	3.557908
C	-0.567758	0.720662	4.393208
C	-1.467874	1.414864	3.361438
C	-0.611808	1.354519	2.107794

Sr	-0.017656	-1.635617	0.283680
O	1.433084	-2.538787	-1.943422
C	1.322554	-3.253075	-3.198305
C	0.742425	-2.371930	-4.296410
C	1.331930	-0.957052	-4.312538
C	2.856960	-0.884923	-4.177164
C	3.426687	-1.407390	-2.825760
C	2.384779	-1.606344	-1.759820
O	2.336380	-0.983133	-0.709884
B	-1.674426	-0.380359	-1.417797
B	0.053881	-3.854897	1.756735
H	4.156040	-0.711313	-2.409350
H	3.943169	-2.364292	-2.965948
H	0.677632	-4.101547	-2.966676
H	3.158811	0.160776	-4.287427
H	3.334333	-1.432382	-4.997632
H	2.311240	-3.642791	-3.460247
H	1.036161	-0.464215	-5.244455
H	0.864079	-0.370629	-3.511634
H	0.930480	-2.881680	-5.250030
H	-0.342448	-2.299968	-4.174364
H	1.310474	-0.234203	3.756246
H	-0.092325	-1.324573	3.692368
H	-1.137463	0.232808	5.187782
H	0.102641	1.447185	4.863400
H	-2.393023	0.850649	3.205235
H	-1.732398	2.437155	3.644131
H	0.172339	2.124887	2.114435
H	-1.168166	1.413739	1.169422
H	-0.900966	-3.125992	2.080789
H	-1.481307	-1.558834	-1.759547
H	-0.571743	0.191716	-1.371014
H	-2.141685	-0.397888	-0.267128
H	-2.422688	0.175116	-2.181232
H	1.098513	-3.195125	1.895724
H	-0.070017	-4.116565	0.547666
H	0.077191	-4.859323	2.419442

Nucleophilic Attack TS to 1b

42

scf done: -702.645251

O	-1.071757	-0.346940	1.727235
C	-0.025536	-0.690962	2.664370
C	0.000182	0.478660	3.632861
C	-1.493240	0.795702	3.779528
C	-2.062047	0.481740	2.390313
Sr	-0.551738	-0.344548	-0.733830
O	0.451875	-2.439724	-1.658731

C	0.402652	-3.475567	-2.629690
C	0.827858	-3.023902	-4.052395
C	1.196087	-1.539973	-4.133411
C	2.501650	-1.166784	-3.398840
C	2.848015	-2.061578	-2.207982
C	1.814413	-2.087550	-1.078035
O	1.654265	-0.946918	-0.414708
B	-2.190309	1.539982	-1.682761
B	3.413359	-2.941167	1.550557
H	3.782388	-1.720335	-1.748335
H	3.039275	-3.085735	-2.554039
H	-0.635883	-3.823840	-2.638402
H	2.455936	-0.121926	-3.071083
H	3.337531	-1.223068	-4.106933
H	1.015787	-4.319058	-2.283379
H	1.283411	-1.257720	-5.189006
H	0.356870	-0.946803	-3.749549
H	1.674001	-3.629621	-4.398888
H	0.007102	-3.223415	-4.750846
H	0.890211	-0.840182	2.085948
H	-0.290727	-1.628765	3.171201
H	0.479511	0.227795	4.582554
H	0.539213	1.323111	3.189819
H	-1.944861	0.144353	4.534918
H	-1.683798	1.830383	4.074792
H	-2.205003	1.374671	1.774633
H	-3.008135	-0.067198	2.433636
H	3.798909	-1.858147	1.869596
H	-1.533902	0.990994	-2.588101
H	-1.378596	2.002132	-0.857872
H	-2.853150	0.657692	-1.108304
H	-2.896301	2.406299	-2.127649
H	2.036808	-2.964388	-0.419322
H	2.399016	-3.378871	2.010943
H	4.078797	-3.626117	0.831436

Borane complex of 1b

42

scf done: -702.717191

O	-0.613303	-0.251881	1.977170
C	-0.149291	-0.930176	3.168495
C	-0.870031	-0.245994	4.319939
C	-2.223236	0.085450	3.686060
C	-1.827816	0.491415	2.270759
Sr	0.613817	-0.047819	-0.235573
O	0.964777	-2.265064	-1.427340
C	0.306984	-3.314997	-2.135909
C	0.267458	-3.103980	-3.670805

C	0.848181	-1.756832	-4.110065
C	2.380792	-1.655590	-3.958383
C	2.971816	-2.520877	-2.842953
C	2.428581	-2.254412	-1.447959
O	2.772165	-1.003602	-0.987105
B	-1.153291	1.554357	-1.411167
B	3.112172	-0.873654	0.500930
H	4.054999	-2.369352	-2.781060
H	2.828088	-3.583340	-3.076617
H	-0.707725	-3.330336	-1.727621
H	2.667064	-0.610145	-3.801733
H	2.858825	-1.965130	-4.895677
H	0.774062	-4.273387	-1.872633
H	0.578325	-1.583825	-5.157842
H	0.357544	-0.957189	-3.544882
H	0.800821	-3.919205	-4.174656
H	-0.773590	-3.170645	-4.005594
H	0.939691	-0.848815	3.202456
H	-0.420524	-1.991495	3.098177
H	-0.948325	-0.887712	5.201233
H	-0.344236	0.670555	4.609095
H	-2.864051	-0.803055	3.668490
H	-2.762952	0.881353	4.205334
H	-1.598761	1.559877	2.197569
H	-2.573288	0.246028	1.510663
H	2.971675	0.334512	0.750297
H	-0.198150	1.308014	-2.166334
H	-0.692786	2.071476	-0.376720
H	-1.668655	0.466750	-1.089676
H	-1.953485	2.278842	-1.941466
H	2.762201	-3.038332	-0.748806
H	2.252199	-1.502417	1.150079
H	4.224784	-1.252582	0.777116

Ring Opening TS to 1b

42

scf done: -702.689098

C	-0.215587	-0.741662	0.217224
C	0.137497	-0.065099	1.550347
O	1.573726	0.137108	1.533348
C	2.140138	-0.571252	0.409828
C	1.041058	-0.531748	-0.637912
Sr	2.771093	2.194788	2.370387
O	4.502157	1.917628	1.004090
C	5.838081	1.984839	0.659983
C	6.519212	3.294164	1.109905
C	6.230794	3.740456	2.547033
C	6.954983	3.074792	3.727364

C	6.839824	1.559507	3.964377
C	5.469965	0.915965	3.800816
O	4.381656	1.638208	4.438235
B	4.201918	1.838241	5.790381
B	0.751298	3.772802	3.136730
H	7.231209	1.348587	4.968943
H	7.491868	1.014795	3.269011
H	5.987759	1.897467	-0.432549
H	6.607397	3.583375	4.635365
H	8.026705	3.303736	3.658023
H	6.408126	1.132303	1.091167
H	6.463656	4.810216	2.621972
H	5.147135	3.686169	2.712021
H	7.603706	3.217250	0.943415
H	6.161641	4.095613	0.449699
H	2.371819	-1.602470	0.712010
H	3.064953	-0.052276	0.141180
H	1.024205	0.448760	-1.125846
H	1.164864	-1.295740	-1.409883
H	-1.113359	-0.312138	-0.233891
H	-0.397009	-1.810948	0.366731
H	-0.121368	-0.683019	2.416561
H	-0.325884	0.918288	1.671054
H	3.546805	1.044784	6.412467
H	1.858547	4.315160	3.311075
H	0.731248	2.722162	3.801471
H	0.673210	3.459414	1.931974
H	-0.144834	4.513379	3.447563
H	5.197280	0.886237	2.742641
H	5.477379	-0.106974	4.197300
H	4.669076	2.812761	6.313166

Product from 1b

42

scf done: -702.713607

C	-0.142817	-0.744350	0.365392
C	0.190654	-0.049465	1.693796
O	1.625151	0.170361	1.687550
C	2.209261	-0.538273	0.572536
C	1.116706	-0.523954	-0.482589
Sr	2.745706	2.315939	2.411092
O	4.463019	2.006051	1.035219
C	5.786208	2.091596	0.651320
C	6.476015	3.386832	1.128495
C	6.209405	3.784305	2.583730
C	6.946015	3.073252	3.728748
C	6.867651	1.545408	3.892594
C	5.514190	0.865095	3.738467

O	4.419748	1.570096	4.400802
B	4.235561	1.486797	5.742510
B	0.601540	3.865957	2.811996
H	7.285105	1.299984	4.877687
H	7.518888	1.053632	3.158842
H	5.901686	2.045943	-0.447852
H	6.595373	3.532821	4.662256
H	8.013115	3.324891	3.669658
H	6.373542	1.227150	1.031962
H	6.444265	4.850491	2.694423
H	5.127264	3.724058	2.758597
H	7.557680	3.316519	0.942726
H	6.107577	4.209603	0.501476
H	2.454615	-1.563430	0.884674
H	3.126317	-0.004729	0.305012
H	1.089041	0.452047	-0.978852
H	1.256961	-1.292716	-1.247060
H	-1.043101	-0.331366	-0.096010
H	-0.310106	-1.814758	0.523614
H	-0.067373	-0.661978	2.564280
H	-0.284791	0.929755	1.798856
H	3.315462	2.104946	6.190834
H	1.664939	4.463227	3.065802
H	0.537310	2.871863	3.555482
H	0.670528	3.458173	1.636707
H	-0.345939	4.593190	2.960251
H	5.217456	0.835593	2.687603
H	5.552524	-0.152282	4.141616
H	4.966545	0.808183	6.407266

Dimer 2b

114

scf done: -1825.674721

C	7.445945	11.204163	9.255697
C	7.123280	11.119412	7.871669
C	6.220796	12.175244	7.563251
C	5.990205	12.918231	8.754711
C	6.744261	12.316507	9.803380
C	8.243951	10.185388	10.020141
H	7.653417	9.281498	10.228613
H	8.577619	10.567917	10.990427
H	9.136868	9.856892	9.474360
C	7.547542	10.015309	6.945492
H	8.554647	9.650909	7.175866
H	7.552070	10.338463	5.898314
H	6.872328	9.148981	7.005376
C	5.522357	12.389009	6.250835
H	6.118662	12.026848	5.406650

H	5.313415	13.447419	6.062139
H	4.559169	11.859549	6.211807
C	5.004542	14.042964	8.902681
H	4.977105	14.690362	8.018069
H	5.233303	14.679191	9.764964
H	3.979615	13.673479	9.052327
C	6.657994	12.676963	11.259913
H	6.521035	13.753076	11.416658
H	7.555050	12.380911	11.815005
H	5.810009	12.180611	11.753442
C	8.042936	16.346646	10.233883
H	8.621574	15.672705	10.867682
H	6.974618	16.208789	10.447684
C	8.440541	17.831090	10.351814
H	7.672774	18.396156	10.887646
H	9.378010	17.955253	10.900476
C	8.584076	18.295015	8.884711
H	9.637227	18.430760	8.622454
H	8.066464	19.236795	8.684019
C	7.993167	17.134739	8.087654
H	6.901550	17.227613	7.990562
H	8.424656	16.988720	7.097761
C	10.719525	12.915188	11.065179
H	10.818464	11.970287	10.519919
H	9.938626	12.811008	11.823740
C	12.060243	13.375214	11.627927
H	12.690311	12.534258	11.929113
H	11.914661	14.020983	12.501606
C	12.634409	14.175529	10.457416
H	13.412062	14.884856	10.753016
H	13.045118	13.503653	9.697284
C	11.390997	14.867128	9.918931
H	11.173394	15.794383	10.466579
H	11.448887	15.092631	8.850682
B	8.676398	14.673881	5.435002
O	8.301426	15.974771	8.873654
O	10.307970	13.938268	10.130355
Sr	8.685708	13.463878	8.049552
H	7.648909	15.016242	5.995040
H	9.653861	15.020216	6.108273
H	8.671078	13.440544	5.354332
H	8.765117	15.165878	4.326071
C	12.414387	15.707836	3.282811
C	12.737051	15.792588	4.666839
C	13.639535	14.736756	4.975257
C	13.870126	13.993768	3.783797
C	13.116071	14.595492	2.735128
C	11.616381	16.726612	2.518367

H	12.206915	17.630502	2.309895
H	11.282713	16.344083	1.548081
H	10.723463	17.055108	3.064148
C	12.312790	16.896690	5.593016
H	11.305684	17.261091	5.362642
H	12.308261	16.573536	6.640194
H	12.988003	17.763019	5.533133
C	14.337974	14.522990	6.287674
H	13.741668	14.885152	7.131858
H	14.546916	13.464581	6.476369
H	15.301162	15.052450	6.326701
C	14.855789	12.869035	3.635827
H	14.883225	12.221637	4.520439
H	14.627028	12.232809	2.773545
H	15.880716	13.238520	3.486181
C	13.202337	14.235037	1.278596
H	13.339297	13.158924	1.121850
H	12.305281	14.531089	0.723503
H	14.050323	14.731389	0.785066
C	11.817395	10.565354	2.304625
H	11.238757	11.239295	1.670825
H	12.885713	10.703211	2.090823
C	11.419790	9.080910	2.186694
H	12.187556	8.515844	1.650862
H	10.482320	8.956748	1.638032
C	11.276255	8.616985	3.653797
H	10.223104	8.481240	3.916054
H	11.793867	7.675205	3.854488
C	11.867165	9.777261	4.450853
H	12.958781	9.684387	4.547945
H	11.435675	9.923280	5.440747
C	9.140807	13.996813	1.473328
H	9.041868	14.941713	2.018589
H	9.921706	14.100992	0.714768
C	7.800089	13.536787	0.910580
H	7.170021	14.377743	0.609395
H	7.945670	12.891018	0.036902
C	7.225922	12.736471	2.081091
H	6.448269	12.027145	1.785491
H	6.815213	13.408348	2.841223
C	8.469334	12.044873	2.619576
H	8.686937	11.117617	2.071929
H	8.411443	11.819369	3.687826
B	11.183932	12.238119	7.103506
O	11.558905	10.937229	3.664854
O	9.552361	12.973732	2.408153
Sr	11.174623	13.448122	4.488956
H	12.211422	11.895757	6.543469

H	10.206470	11.891784	6.430235
H	11.189253	13.471456	7.184175
H	11.095213	11.746122	8.212437

Monomer 2b

31

scf done: -448.027046

C	-8.724148	5.869938	3.855477
C	-9.483979	6.611046	2.903491
C	-10.846474	6.205199	3.014988
C	-10.928404	5.213243	4.035980
C	-9.616764	5.005590	4.555199
C	-8.962656	7.717793	2.028086
C	-12.010310	6.812190	2.280130
C	-12.192918	4.590949	4.562039
C	-9.260418	4.128290	5.724173
C	-7.263141	6.059926	4.158928
Sr	-9.530688	4.013876	1.987187
B	-9.062480	2.109332	0.216343
H	-8.989280	1.672619	1.381907
H	-8.849990	1.244670	-0.588612
H	-10.200707	2.597051	0.068780
H	-11.733240	7.171321	1.282506
H	-12.837969	6.105279	2.152953
H	-12.419351	7.677063	2.819995
H	-9.014678	8.690611	2.535716
H	-7.913688	7.568964	1.748209
H	-9.535697	7.820502	1.099618
H	-6.794332	5.146019	4.540896
H	-6.691545	6.375554	3.278903
H	-7.108844	6.832653	4.924347
H	-9.916752	3.254496	5.805163
H	-8.230648	3.757700	5.669305
H	-9.346040	4.671574	6.675117
H	-12.969058	4.508902	3.792789
H	-12.026732	3.585703	4.965566
H	-12.624652	5.186402	5.377994
H	-8.238495	3.039344	0.111304

Adduct of ϵ -CL to monomer 2b

49

scf done: -833.042082

C	-8.652522	6.026097	3.879472
C	-9.425576	6.793802	2.960675
C	-10.733778	6.231795	2.907776
C	-10.767661	5.113623	3.790328
C	-9.481176	4.987187	4.390959
C	-8.983055	8.056724	2.275071

C	-11.904412	6.791089	2.148140
C	-11.982682	4.289790	4.117246
C	-9.096410	4.002235	5.459936
C	-7.248416	6.328568	4.322325
Sr	-9.111368	4.326317	1.707563
O	-6.697265	3.263381	1.917906
C	-6.075341	3.774273	0.999276
C	-4.726890	3.310693	0.518377
C	-4.724295	2.765769	-0.941129
C	-6.002295	3.044672	-1.739041
C	-6.290271	4.525385	-2.010299
C	-6.071025	5.412351	-0.793725
O	-6.651217	4.837020	0.403469
B	-9.972136	3.382923	-0.649037
H	-5.008741	5.598500	-0.605825
H	-6.568798	6.377540	-0.896557
H	-5.637497	4.908728	-2.805130
H	-7.322985	4.626820	-2.357029
H	-6.863531	2.609056	-1.217350
H	-5.945454	2.516968	-2.696674
H	-3.853056	3.169911	-1.468868
H	-4.581168	1.682349	-0.894306
H	-4.032165	4.153005	0.619981
H	-4.403314	2.545638	1.225401
H	-10.870706	3.337043	0.206185
H	-10.358427	2.964898	-1.710995
H	-9.596967	4.566165	-0.741904
H	-7.901401	8.073642	2.097165
H	-9.475620	8.199150	1.306069
H	-9.213078	8.948276	2.875475
H	-7.230670	6.977911	5.209068
H	-6.693117	5.421385	4.586600
H	-6.673967	6.847249	3.545948
H	-9.662080	3.066274	5.385047
H	-8.032282	3.742360	5.420243
H	-9.285154	4.399293	6.467276
H	-12.664948	4.204289	3.264341
H	-11.723034	3.271247	4.428306
H	-12.561661	4.729434	4.941445
H	-11.592184	7.327477	1.245483
H	-12.604275	6.010587	1.830925
H	-12.478519	7.504069	2.756653
H	-9.014051	2.712100	-0.224127

Nucleophilic Attack TS for 2b

49

scf done: -832.986780

Sr	-8.646219	6.325431	4.248707
----	-----------	----------	----------

O	-9.617350	7.314116	2.376710
C	-10.763390	6.686266	2.237820
H	-10.716652	5.805325	1.542866
O	-11.052264	5.918929	3.584169
C	-12.253380	6.179450	4.299802
H	-12.431971	7.261164	4.356318
H	-12.085615	5.837820	5.329107
C	-13.473384	5.472503	3.708484
H	-14.373725	5.949514	4.118969
H	-13.492998	4.427670	4.041334
C	-13.501884	5.498188	2.179343
H	-12.738919	4.803661	1.809709
H	-14.461691	5.093241	1.836011
C	-13.284406	6.869880	1.529228
H	-14.114343	7.537417	1.794635
H	-13.354180	6.730518	0.443723
C	-11.949481	7.572355	1.859002
H	-12.067172	8.322974	2.648676
H	-11.599338	8.133304	0.986520
B	-9.974432	3.744873	2.021313
H	-8.948349	4.249431	2.397974
H	-10.191891	3.727527	0.848307
H	-10.657029	3.144387	2.790771
C	-8.257470	6.222998	7.016169
C	-7.540070	5.094398	6.526686
C	-6.421740	5.571398	5.783545
C	-6.445545	6.995880	5.816758
C	-7.581863	7.399559	6.576447
C	-9.439112	6.180402	7.945437
C	-7.839355	3.654811	6.842314
C	-5.336622	4.721764	5.180782
C	-5.391445	7.909285	5.253570
C	-7.926321	8.811860	6.963151
H	-10.092093	7.053112	7.828825
H	-10.056773	5.288189	7.790207
H	-9.127831	6.163894	8.999402
H	-7.425180	9.111551	7.894237
H	-7.624601	9.537970	6.199561
H	-9.001003	8.947147	7.131513
H	-4.902260	7.484439	4.369286
H	-5.797530	8.884879	4.962185
H	-4.594537	8.109030	5.983462
H	-5.706170	3.740768	4.860144
H	-4.872558	5.195375	4.307605
H	-4.525189	4.529089	5.896467
H	-8.909814	3.476760	6.997157
H	-7.510123	2.976708	6.046432
H	-7.332936	3.325578	7.760493

Borate complex for 2b

49

scf done: -833.059155

Sr	-6.559552	7.142337	-0.371482
O	-8.123378	5.388031	-1.424720
C	-9.056207	5.265474	-2.497990
H	-8.515443	5.031839	-3.425177
H	-9.484975	6.264887	-2.619550
C	-10.164502	4.247128	-2.271955
H	-10.790944	4.280163	-3.173426
H	-10.800473	4.570517	-1.440085
C	-9.672697	2.806354	-2.037525
H	-9.576798	2.617120	-0.962616
H	-10.439927	2.106729	-2.387946
C	-8.345481	2.479166	-2.732946
H	-8.170504	1.401863	-2.644005
H	-8.449898	2.671635	-3.808105
C	-7.107507	3.238023	-2.184808
H	-6.375197	2.527519	-1.790004
H	-6.588473	3.787305	-2.979225
C	-7.351693	4.201244	-1.030210
H	-7.916002	3.719084	-0.220924
O	-6.160759	4.697661	-0.547406
B	-6.027231	4.832293	0.975676
H	-5.075771	5.607924	1.137426
H	-5.847962	3.779045	1.538130
H	-7.061043	5.390518	1.408450
C	-5.290421	9.608661	-0.523923
C	-6.410480	9.838512	0.326710
C	-7.591881	9.737332	-0.463632
C	-7.201732	9.447956	-1.803626
C	-5.779412	9.365914	-1.840461
C	-3.844331	9.723439	-0.126367
C	-4.939687	9.185509	-3.075321
C	-8.116675	9.387642	-2.995072
C	-8.993310	10.016947	0.005675
C	-6.348568	10.235162	1.776192
H	-5.482627	9.801590	2.289125
H	-6.269867	11.324681	1.895677
H	-7.241528	9.924800	2.330521
H	-3.193087	9.084166	-0.733493
H	-3.472213	10.750504	-0.245286
H	-3.679432	9.450422	0.921870
H	-5.440929	8.572376	-3.833600
H	-4.710341	10.147312	-3.555051
H	-3.976590	8.709648	-2.857772
H	-9.129832	9.070290	-2.722946

H	-8.218996	10.369807	-3.477751
H	-7.754206	8.699221	-3.767653
H	-9.130271	9.780125	1.066860
H	-9.258473	11.076671	-0.114079
H	-9.742763	9.444279	-0.553177

Ring Opening TS for 2b

49

scf done: -832.992849

Sr	-6.860665	7.276815	-1.005515
O	-8.315779	5.645161	-1.730795
C	-9.085894	5.195568	-2.796582
H	-8.451682	4.755368	-3.592968
H	-9.600704	6.040916	-3.288420
C	-10.148690	4.155805	-2.413526
H	-10.528385	3.698671	-3.338377
H	-11.002580	4.662912	-1.945689
C	-9.671259	3.067125	-1.446114
H	-9.564635	3.513440	-0.450755
H	-10.472421	2.325015	-1.339164
C	-8.384782	2.307830	-1.806444
H	-8.246369	1.510237	-1.065310
H	-8.510970	1.801599	-2.771450
C	-7.092958	3.137811	-1.873766
H	-6.213223	2.485149	-1.864785
H	-7.028463	3.705686	-2.807001
C	-6.950295	4.138443	-0.771188
H	-7.722513	4.247246	-0.015503
O	-5.906128	4.959245	-0.732135
B	-5.278129	4.043590	0.378389
H	-4.262685	3.553006	-0.039892
H	-6.127785	3.111899	0.415688
H	-5.301084	4.612721	1.443745
C	-5.459346	9.639001	-0.483347
C	-6.649410	9.736017	0.293425
C	-7.750868	9.878649	-0.601671
C	-7.241506	9.864775	-1.931442
C	-5.825006	9.711486	-1.858845
C	-4.057082	9.580384	0.056685
C	-4.873266	9.757256	-3.023067
C	-8.040334	10.097214	-3.184012
C	-9.181747	10.124379	-0.208803
C	-6.716916	9.801716	1.794791
H	-5.921569	9.218076	2.273131
H	-6.610580	10.831839	2.162252
H	-7.671785	9.430917	2.185403
H	-3.368529	9.072085	-0.627969
H	-3.644088	10.584741	0.224644

H	-4.002216	9.057251	1.018444
H	-5.314804	9.348372	-3.939553
H	-4.568188	10.786398	-3.258361
H	-3.951411	9.197064	-2.828278
H	-9.068943	9.730086	-3.094072
H	-8.109447	11.166332	-3.428916
H	-7.596039	9.606735	-4.057825
H	-9.432150	9.667681	0.755626
H	-9.397262	11.197457	-0.110368
H	-9.889404	9.729933	-0.946876

Product for 2b

49

scf done: -833.061119

Sr	-7.197503	7.215212	-1.738353
O	-8.794991	5.868982	-2.413254
C	-9.705167	4.932290	-2.859578
H	-9.219282	4.179747	-3.516896
H	-10.490272	5.391302	-3.489730
C	-10.420142	4.169915	-1.731644
H	-11.024755	3.370765	-2.185952
H	-11.126340	4.851722	-1.238678
C	-9.521015	3.571234	-0.641599
H	-9.074150	4.397007	-0.072601
H	-10.164681	3.043498	0.073514
C	-8.419772	2.603577	-1.106903
H	-8.140873	1.942846	-0.273617
H	-8.821642	1.942262	-1.884732
C	-7.153678	3.283547	-1.653563
H	-6.514540	2.552563	-2.163784
H	-7.446911	4.046382	-2.380094
C	-6.348124	3.979650	-0.565559
H	-7.003615	4.408277	0.198487
O	-5.606627	5.101580	-1.119252
B	-4.266905	5.047351	-1.313249
H	-3.647971	4.075712	-0.985220
H	-5.637978	3.308947	-0.070644
H	-3.767103	6.008289	-1.822414
C	-5.722468	9.146814	-0.286055
C	-7.073316	9.271889	0.151452
C	-7.840792	9.793251	-0.930482
C	-6.965725	9.981039	-2.038981
C	-5.656215	9.581941	-1.639580
C	-4.553667	8.749401	0.572012
C	-4.404990	9.715058	-2.463263
C	-7.334458	10.613455	-3.353065
C	-9.292378	10.181886	-0.877853
C	-7.571838	9.031662	1.550080

H	-7.014802	8.236739	2.060685
H	-7.475302	9.928903	2.177686
H	-8.631115	8.750668	1.570516
H	-3.752697	8.277471	-0.008760
H	-4.103266	9.616144	1.076182
H	-4.839634	8.046067	1.363267
H	-4.598807	9.599478	-3.536420
H	-3.935306	10.700867	-2.338271
H	-3.646594	8.972464	-2.189033
H	-8.370325	10.399690	-3.640876
H	-7.239400	11.707902	-3.319339
H	-6.692620	10.272240	-4.173946
H	-9.858864	9.570808	-0.166196
H	-9.423436	11.228233	-0.567522
H	-9.784727	10.079382	-1.851547

3b

36

scf done: -390.400941

Sr	-10.127316	2.532580	-0.534100
B	-8.935812	3.871243	1.429297
H	-8.512048	4.234546	0.316776
H	-10.164660	4.062231	1.447331
H	-8.744029	2.642368	1.520572
H	-8.387093	4.464171	2.320272
Si	-8.596490	2.476794	-4.138822
H	-8.568375	3.944691	-3.841501
H	-7.185689	2.039309	-4.428914
H	-9.371355	2.281063	-5.414144
N	-9.310895	1.679587	-2.760166
P	-9.581745	0.065693	-2.602876
C	-10.301554	-0.643459	-4.155766
H	-9.581339	-0.548368	-4.973585
H	-11.202031	-0.086689	-4.421776
H	-10.547784	-1.698226	-4.010234
C	-8.031981	-0.908137	-2.380333
H	-7.548114	-0.588411	-1.454903
H	-8.251065	-1.978041	-2.331348
H	-7.362406	-0.709868	-3.220634
C	-10.508768	-0.225270	-1.120792
H	-10.179818	-1.122767	-0.598771
P	-12.242097	0.076212	-0.918324
N	-12.491287	1.697088	-0.803823
C	-13.353024	-0.684200	-2.191109
H	-13.225916	-0.160450	-3.140133
H	-13.111495	-1.742548	-2.317269
H	-14.396105	-0.585092	-1.876759
Si	-14.040363	2.501993	-0.811292

H	-13.782057	3.971739	-0.681799
H	-14.821543	2.282200	-2.078685
H	-14.944076	2.091587	0.320577
C	-12.694219	-0.837661	0.618538
H	-12.053097	-0.493921	1.433083
H	-12.566834	-1.914516	0.479520
H	-13.735916	-0.622185	0.868118

Adduct of ϵ -CL to 3b

54

scf done: -775.408779

B	-8.657116	4.428191	4.860152
H	-9.550568	5.284151	4.743744
H	-8.261130	4.131071	3.724592
H	-7.752292	4.837239	5.547610
Sr	-10.707691	3.510384	3.342416
O	-12.061594	1.981807	5.045732
C	-12.322992	2.661559	6.026984
C	-12.831858	2.102629	7.331513
C	-11.880269	2.328923	8.543388
C	-10.708379	3.279043	8.276085
C	-11.103729	4.731902	7.991142
C	-12.294522	4.853934	7.052136
O	-12.162011	3.987201	5.903835
N	-12.533767	4.804392	2.096013
Si	-14.188068	5.179339	2.476763
P	-11.734939	5.282505	0.739487
C	-10.173875	4.479588	0.640085
P	-9.859367	2.795236	0.235861
C	-10.565565	2.216988	-1.379289
C	-12.819020	5.108519	-0.755008
C	-11.326610	7.081893	0.753711
C	-8.039631	2.726789	-0.056551
N	-10.346211	1.823447	1.468203
Si	-10.415698	0.084044	1.414148
H	-9.166151	3.408822	5.357745
H	-11.490406	-0.452350	0.504113
H	-14.483541	6.657279	2.558179
H	-15.191719	4.616763	1.504178
H	-14.502069	4.596448	3.821763
H	-9.133045	-0.565519	0.957124
H	-10.705776	-0.415180	2.795458
H	-9.364213	5.148757	0.358599
H	-7.761482	3.334849	-0.921453
H	-7.535567	3.101428	0.837136
H	-7.745467	1.688547	-0.227421
H	-10.281346	2.902358	-2.181784
H	-10.194603	1.213649	-1.609553

H	-11.653714	2.174882	-1.299797
H	-13.694880	5.757376	-0.661221
H	-12.261461	5.376597	-1.655785
H	-13.160150	4.073779	-0.827619
H	-10.858580	7.382385	-0.187377
H	-12.243306	7.656073	0.907517
H	-10.640764	7.270735	1.582571
H	-13.239442	4.624137	7.556197
H	-11.375063	5.249414	8.920589
H	-12.374819	5.854584	6.625488
H	-10.244201	5.254312	7.560718
H	-10.030636	3.259817	9.136073
H	-10.118498	2.905256	7.430096
H	-12.468203	2.686451	9.396691
H	-11.472748	1.356965	8.836805
H	-13.813849	2.553417	7.519860
H	-12.999833	1.039386	7.155037

Nucleophilic Attack TS for 3b

54

scf done: -775.348373

B	-8.770626	4.846781	4.782500
H	-9.652461	5.457800	4.245012
H	-8.375457	3.816936	4.315790
H	-8.161215	5.385118	5.653795
Sr	-11.179417	3.423048	3.020356
O	-10.987656	3.083225	5.214537
C	-10.602760	3.438571	6.460563
C	-10.777888	2.288916	7.459869
C	-10.519246	2.618625	8.932554
C	-11.325603	3.812897	9.479973
C	-12.698116	3.974675	8.822339
C	-12.586093	4.471749	7.353821
O	-11.248855	4.642507	6.920844
N	-12.600690	4.994618	1.608202
Si	-14.183133	5.687438	1.844099
P	-11.599175	5.301957	0.342507
C	-10.203215	4.218360	0.406117
P	-10.207949	2.494226	0.008894
C	-10.982328	2.045672	-1.614166
C	-12.534682	5.314348	-1.258491
C	-10.869886	6.996509	0.397017
C	-8.429378	2.079341	-0.258952
N	-10.887605	1.640805	1.237209
Si	-11.233857	-0.068147	1.229203
H	-9.525107	3.757992	6.487418
H	-12.217622	-0.482432	0.166857
H	-14.186594	7.192860	1.910186

H	-15.172841	5.316104	0.771480
H	-14.713261	5.173852	3.147447
H	-10.016740	-0.933811	1.029043
H	-11.826436	-0.417597	2.559316
H	-9.285869	4.710252	0.085744
H	-8.032519	2.614989	-1.125371
H	-7.866969	2.357247	0.634967
H	-8.334603	1.002846	-0.419945
H	-10.571605	2.665289	-2.415179
H	-10.791455	0.991429	-1.834998
H	-12.061726	2.194534	-1.548094
H	-13.265766	6.128221	-1.254336
H	-11.845870	5.449933	-2.096144
H	-13.069507	4.369413	-1.370500
H	-10.258379	7.185761	-0.489243
H	-11.678213	7.729984	0.446592
H	-10.254377	7.083189	1.294900
H	-13.121833	3.800997	6.667501
H	-13.243253	3.022508	8.862638
H	-13.046883	5.460792	7.260034
H	-13.293438	4.688917	9.404194
H	-11.451715	3.696936	10.563548
H	-10.762865	4.738288	9.325117
H	-10.757503	1.721414	9.519292
H	-9.448704	2.802924	9.091706
H	-11.800448	1.911658	7.324994
H	-10.121042	1.473330	7.135957

Borate complex of 3b

54

scf done: -775.415578

B	-8.825805	4.729269	4.924481
H	-9.216173	5.709560	4.265874
H	-8.233177	3.963953	4.130752
H	-8.097706	5.070660	5.819343
Sr	-10.555535	3.879982	3.036091
O	-10.085850	3.991792	5.403186
C	-10.145299	3.561555	6.734121
C	-11.187965	2.448512	6.827639
C	-11.521800	1.982813	8.248395
C	-11.945913	3.107014	9.213688
C	-12.682820	4.259237	8.526382
C	-11.735361	5.111522	7.638117
O	-10.402207	4.627824	7.620406
N	-12.407634	5.051418	1.783400
Si	-13.983986	5.606977	2.278703
P	-11.730863	5.254225	0.298166
C	-10.219010	4.341904	0.209221

P	-10.076058	2.586996	0.059573
C	-10.981493	1.818191	-1.363591
C	-12.963901	4.903639	-1.039855
C	-11.238822	6.999838	-0.034944
C	-8.307170	2.301735	-0.376572
N	-10.506411	1.884510	1.483097
Si	-10.749692	0.180096	1.755724
H	-9.157038	3.199590	7.047025
H	-11.869942	-0.409722	0.941542
H	-14.166058	7.098828	2.180607
H	-15.116555	4.992738	1.500039
H	-14.164100	5.222905	3.716429
H	-9.535494	-0.666211	1.476523
H	-11.100356	0.003043	3.202414
H	-9.438140	4.876112	-0.329405
H	-8.071848	2.736032	-1.351875
H	-7.681195	2.760832	0.391640
H	-8.115363	1.226361	-0.399419
H	-10.741735	2.347616	-2.289137
H	-10.694296	0.767136	-1.462209
H	-12.056031	1.868803	-1.178096
H	-13.790122	5.617950	-0.978132
H	-12.489636	4.981327	-2.021320
H	-13.364352	3.897487	-0.901298
H	-10.842454	7.103328	-1.048461
H	-12.111694	7.646029	0.084645
H	-10.476203	7.290952	0.690629
H	-12.121051	5.200653	6.613547
H	-13.516066	3.864985	7.929689
H	-11.656808	6.127120	8.036658
H	-13.136898	4.900594	9.290793
H	-12.584014	2.683055	9.998199
H	-11.062330	3.515055	9.713023
H	-12.330906	1.245543	8.168663
H	-10.665435	1.444324	8.673004
H	-12.102644	2.804333	6.332917
H	-10.829946	1.598364	6.234150

Ring Opening TS for 3b

54

scf done: -775.364738

C	-7.368235	7.669929	-1.197769
Sr	-8.893971	5.185598	-1.530857
N	-8.967644	6.929726	-3.366484
Si	-9.873118	7.005385	-4.852866
P	-7.870772	8.041071	-2.846122
C	-8.500751	9.762088	-3.123890
P	-8.315810	7.897914	0.272304

N	-9.507450	6.766852	0.355679
Si	-10.796615	6.724221	1.527564
C	-6.305963	8.008757	-3.823467
C	-7.088109	7.745849	1.640432
C	-9.007557	9.600152	0.520385
O	-9.731090	3.015347	-1.683521
C	-10.512435	2.186893	-2.474472
C	-10.935357	0.877248	-1.790774
C	-9.829249	0.176192	-0.994365
C	-8.492021	-0.079584	-1.705611
C	-7.705974	1.161766	-2.154061
C	-7.679473	2.271882	-1.148430
O	-7.079832	3.425433	-1.436969
B	-5.866784	2.946898	-0.583420
H	-6.349550	8.550414	1.591378
H	-9.997483	1.921753	-3.421866
H	-8.210707	2.188678	-0.205536
H	-9.014150	7.060450	-6.090303
H	-10.806080	8.184093	-4.942007
H	-10.706204	5.762450	-4.939154
H	-6.542502	8.137483	-4.882341
H	-5.826622	7.038091	-3.678851
H	-5.629828	8.804479	-3.499911
H	-8.648535	9.938529	-4.193399
H	-9.461167	9.875632	-2.617469
H	-7.788178	10.490856	-2.729651
H	-6.301327	7.813532	-1.039071
H	-9.798941	9.775343	-0.211074
H	-9.436743	9.686971	1.523001
H	-8.219159	10.346721	0.396217
H	-7.613780	7.789566	2.597247
H	-6.585688	6.780242	1.551067
H	-10.321846	6.641672	2.955973
H	-11.618516	5.501911	1.253968
H	-11.716748	7.915085	1.465554
H	-6.673519	0.893913	-2.403567
H	-8.127365	1.593373	-3.066648
H	-7.857935	-0.666646	-1.028361
H	-8.654749	-0.712489	-2.587083
H	-9.647903	0.749409	-0.078404
H	-10.211934	-0.793789	-0.651759
H	-11.333498	0.200204	-2.560415
H	-11.762529	1.079639	-1.097814
H	-11.433259	2.706455	-2.800923
H	-6.264768	1.786245	-0.267852
H	-4.905890	2.780855	-1.290241
H	-5.780519	3.589090	0.435917

Product for 3b

54

scf done: -775.429240

C	-7.352145	7.488692	-1.180145
Sr	-8.910152	5.004232	-1.871539
N	-8.802058	6.949006	-3.515210
Si	-9.610454	7.188492	-5.041626
P	-7.769832	8.015104	-2.809824
C	-8.419449	9.747654	-2.948635
P	-8.388155	7.554898	0.243465
N	-9.541900	6.386803	0.176433
Si	-10.878040	6.231958	1.286425
C	-6.148632	8.127355	-3.686750
C	-7.230066	7.334784	1.665861
C	-9.150133	9.208412	0.601705
O	-10.123915	3.212602	-2.317043
C	-10.775492	2.059975	-2.697201
C	-11.136803	1.129228	-1.526331
C	-10.003783	0.816521	-0.540223
C	-8.725516	0.198023	-1.131102
C	-7.770363	1.200794	-1.797921
C	-7.101452	2.128139	-0.795166
O	-6.719246	3.374918	-1.435500
B	-5.436574	3.635818	-1.773013
H	-6.523511	8.166900	1.725154
H	-10.169244	1.467034	-3.417178
H	-7.793414	2.408073	0.004126
H	-8.667753	7.455273	-6.189318
H	-10.587108	8.335506	-5.040970
H	-10.371668	5.940866	-5.362350
H	-6.329296	8.379168	-4.734495
H	-5.654479	7.155134	-3.631588
H	-5.512178	8.890476	-3.230904
H	-8.488381	10.035482	-4.001952
H	-9.418901	9.791657	-2.511619
H	-7.757436	10.441642	-2.424618
H	-6.304240	7.662547	-0.942276
H	-9.908499	9.424245	-0.153457
H	-9.634378	9.191514	1.582662
H	-8.383861	9.987508	0.587871
H	-7.809417	7.279917	2.590540
H	-6.684328	6.398718	1.529712
H	-10.450684	6.120000	2.729766
H	-11.628648	4.986097	0.938172
H	-11.848370	7.383192	1.237982
H	-6.997916	0.672255	-2.370803
H	-8.338550	1.831677	-2.486691
H	-8.184655	-0.341871	-0.340221

H	-8.999999	-0.562986	-1.872511
H	-9.756583	1.739599	-0.001295
H	-10.397309	0.130840	0.221313
H	-11.532454	0.189326	-1.940579
H	-11.955083	1.585620	-0.953070
H	-11.716692	2.276663	-3.238732
H	-6.208475	1.685309	-0.340445
H	-4.569125	2.853500	-1.500873
H	-5.233569	4.670056	-2.339513

1a

37

scf done: -1196.902153

C	-0.501979	0.851199	0.455763
C	0.033637	-0.581871	0.509395
O	1.457702	-0.467949	0.776663
C	1.805669	0.922337	0.962796
C	0.754389	1.680875	0.171898
Ca	3.027554	-2.144502	0.178475
O	3.460577	-3.507623	2.071343
C	2.880083	-4.828303	2.247948
C	3.803498	-5.567548	3.217911
C	5.128277	-4.811668	3.076736
C	4.646996	-3.383407	2.888320
B	5.131448	-0.829714	0.003449
B	1.616225	-3.660296	-1.190176
H	1.757551	1.163549	2.033451
H	2.831234	1.054378	0.612285
H	0.662231	2.723217	0.487874
H	-0.078786	-1.115356	-0.438429
H	-0.424021	-1.180376	1.303199
H	-0.933515	1.138204	1.420593
H	-1.276485	0.968516	-0.306219
H	4.296807	-0.482608	-0.848958
H	1.139700	-3.502278	-0.052529
H	5.331475	-2.045811	-0.153041
H	2.768131	-4.104661	-1.049631
H	4.602669	-0.682738	1.119301
H	6.149354	-0.197289	-0.090002
H	0.935933	-4.394080	-1.856332
H	1.718946	-2.534876	-1.706796
H	1.001503	1.664163	-0.894932
H	1.860347	-4.712926	2.627288
H	2.832783	-5.300680	1.262723
H	3.429581	-5.486992	4.244287
H	3.885258	-6.629494	2.973178
H	5.782005	-4.922545	3.945710
H	5.675826	-5.145106	2.188735

H	4.373812	-2.919829	3.845952
H	5.344101	-2.729694	2.360140

ϵ -CL adduct to 1a

42

scf done: -1349.511042

O	-0.062171	-0.019215	1.998827
C	0.266346	-0.315820	3.380329
C	-0.344873	0.815414	4.212368
C	-1.411761	1.397452	3.278540
C	-0.743489	1.248944	1.922218
Ca	-0.035855	-1.637319	0.259506
O	1.447316	-2.495326	-1.814442
C	1.453098	-3.262736	-3.041312
C	0.837650	-2.484071	-4.198198
C	1.236317	-1.004627	-4.217765
C	2.731686	-0.717366	-4.033866
C	3.334532	-1.189756	-2.678263
C	2.291985	-1.469003	-1.633164
O	2.139695	-0.822685	-0.605979
B	-1.728589	-0.669191	-1.314475
B	0.100820	-3.715878	1.614332
H	4.000730	-0.434862	-2.258353
H	3.926884	-2.101848	-2.814339
H	0.880760	-4.158044	-2.796145
H	2.879005	0.364085	-4.109832
H	3.308816	-1.167176	-4.849531
H	2.482973	-3.567338	-3.250989
H	0.909109	-0.566842	-5.166639
H	0.665840	-0.478704	-3.441761
H	1.147887	-2.982814	-5.125220
H	-0.253167	-2.549352	-4.143829
H	1.355010	-0.375968	3.476862
H	-0.159524	-1.295839	3.612091
H	-0.754211	0.451301	5.158043
H	0.409302	1.575287	4.443543
H	-2.328459	0.799199	3.312001
H	-1.667619	2.434600	3.510811
H	-0.006802	2.045087	1.745755
H	-1.430069	1.201437	1.074308
H	-0.861381	-3.009212	1.957677
H	-1.383771	-1.807357	-1.663733
H	-0.706545	0.036300	-1.259781
H	-2.177930	-0.761618	-0.162108
H	-2.542917	-0.203663	-2.069381
H	1.128298	-3.024691	1.729459
H	-0.045187	-3.967439	0.408032
H	0.168942	-4.721082	2.271760

Nucleophilic Attack TS to 1a

42

scf done: -1349.461498

O	-1.002386	-0.393526	1.560204
C	0.008820	-0.733819	2.535504
C	-0.063743	0.399586	3.543574
C	-1.575974	0.645236	3.631215
C	-2.075667	0.330453	2.213809
Ca	-0.369226	-0.228696	-0.701502
O	0.387485	-2.274119	-1.524598
C	0.228347	-3.336333	-2.455273
C	0.643576	-2.970803	-3.904989
C	1.090620	-1.514563	-4.059723
C	2.435983	-1.184333	-3.376551
C	2.776739	-2.060055	-2.170686
C	1.785021	-1.978259	-1.008260
O	1.704542	-0.795275	-0.400575
B	-1.899813	1.469501	-1.665500
B	3.604915	-2.803635	1.538252
H	3.746823	-1.760759	-1.757943
H	2.891069	-3.106325	-2.483090
H	-0.834287	-3.598340	-2.419626
H	2.446692	-0.131922	-3.071484
H	3.246358	-1.296806	-4.107037
H	0.784469	-4.211554	-2.093000
H	1.163667	-1.283193	-5.128600
H	0.297542	-0.859798	-3.679630
H	1.445339	-3.638566	-4.242806
H	-0.204964	-3.153897	-4.574000
H	0.953707	-0.824967	1.993675
H	-0.244240	-1.699336	2.994498
H	0.382710	0.136669	4.505978
H	0.455316	1.282205	3.154678
H	-2.028327	-0.037982	4.357244
H	-1.824262	1.665233	3.934716
H	-2.272495	1.224814	1.616341
H	-2.973902	-0.295747	2.212878
H	4.069621	-1.722234	1.732499
H	-1.080863	1.043789	-2.500230
H	-1.240359	1.928457	-0.714079
H	-2.539448	0.491413	-1.239941
H	-2.621394	2.302110	-2.144667
H	1.983788	-2.829424	-0.310403
H	2.629263	-3.155498	2.135055
H	4.149078	-3.566989	0.796321

Borane complex of 1a

42

scf done: -1349.530455

O	-0.522489	-0.262737	1.771139
C	-0.199608	-1.044750	2.946635
C	-1.051195	-0.462846	4.066907
C	-2.295683	0.005903	3.309358
C	-1.694325	0.556485	2.024411
Ca	0.782018	-0.053564	-0.213543
O	0.960115	-2.199414	-1.229692
C	0.231824	-3.255129	-1.856008
C	0.106118	-3.102641	-3.392546
C	0.659655	-1.772631	-3.911051
C	2.199956	-1.671623	-3.858848
C	2.862327	-2.518743	-2.769166
C	2.418781	-2.213526	-1.348135
O	2.802625	-0.952560	-0.947286
B	-0.640932	1.593696	-1.394350
B	3.124685	-0.756228	0.540699
H	3.948276	-2.375269	-2.787563
H	2.694443	-3.585163	-2.966286
H	-0.755744	-3.222333	-1.387125
H	2.495072	-0.624241	-3.736570
H	2.617802	-1.997098	-4.819183
H	0.688071	-4.215502	-1.581678
H	0.326559	-1.633787	-4.945601
H	0.207276	-0.952729	-3.343638
H	0.610618	-3.936835	-3.894946
H	-0.952457	-3.181248	-3.664248
H	0.877240	-0.975717	3.117280
H	-0.456874	-2.092477	2.746478
H	-1.266920	-1.198370	4.846107
H	-0.542831	0.388262	4.533017
H	-2.956240	-0.841480	3.094239
H	-2.874222	0.759814	3.849224
H	-1.370683	1.597180	2.137942
H	-2.347819	0.491437	1.152051
H	2.922095	0.452491	0.737912
H	0.377766	1.327256	-2.049089
H	-0.264523	2.018069	-0.287789
H	-1.242108	0.521654	-1.193341
H	-1.339693	2.391834	-1.959005
H	2.788122	-2.982202	-0.649889
H	2.280328	-1.397113	1.191483
H	4.247924	-1.072816	0.845329

Ring Opening TS to 1a

42

scf done: -1349.504742

C	-0.115775	-0.728250	0.352318
C	0.276243	-0.029566	1.663775
O	1.703914	0.206716	1.583802
C	2.243233	-0.519302	0.456964
C	1.107177	-0.516354	-0.550709
Ca	2.845328	2.162033	2.279837
O	4.433304	1.923995	0.951076
C	5.769642	2.005501	0.618115
C	6.436200	3.313444	1.091340
C	6.114356	3.743462	2.525583
C	6.804803	3.063374	3.718039
C	6.699322	1.544046	3.941744
C	5.350011	0.871265	3.721986
O	4.211439	1.605594	4.241996
B	3.892974	1.865229	5.560983
B	1.118818	3.703015	3.195208
H	7.051453	1.338379	4.961553
H	7.391396	1.012715	3.275236
H	5.926713	1.933354	-0.474648
H	6.424937	3.559913	4.619690
H	7.876640	3.300331	3.685998
H	6.343848	1.150968	1.041023
H	6.352503	4.810684	2.618253
H	5.027073	3.697816	2.662719
H	7.523827	3.241831	0.944903
H	6.088215	4.119959	0.432294
H	2.496573	-1.540859	0.774344
H	3.150701	0.010442	0.153585
H	1.057949	0.454221	-1.055854
H	1.214867	-1.293442	-1.312014
H	-1.033843	-0.314813	-0.072436
H	-0.279808	-1.797189	0.522650
H	0.069360	-0.645429	2.545414
H	-0.204423	0.943690	1.795893
H	3.180571	1.094645	6.145765
H	2.237976	4.239875	3.131515
H	1.226113	2.689765	3.909948
H	0.836040	3.314939	2.045035
H	0.289855	4.462824	3.619554
H	5.142915	0.780446	2.653685
H	5.344100	-0.129491	4.170981
H	4.317409	2.855849	6.087635

Product from 1a

42

scf done: -1349.528678

C	-0.123710	-0.669522	0.447176
C	0.251552	0.058952	1.744655

O	1.692757	0.226276	1.711366
C	2.234851	-0.503536	0.586241
C	1.114405	-0.481716	-0.438434
Ca	2.830398	2.211136	2.343491
O	4.416978	1.929862	1.023027
C	5.739111	2.042111	0.647876
C	6.397994	3.351144	1.129190
C	6.097899	3.747027	2.577479
C	6.807747	3.034890	3.738703
C	6.748538	1.504619	3.897062
C	5.412419	0.795555	3.709023
O	4.275042	1.516209	4.275971
B	4.036274	1.520252	5.613403
B	1.010360	3.837104	2.814177
H	7.142878	1.268922	4.893772
H	7.430674	1.025508	3.183468
H	5.861131	1.997103	-0.450745
H	6.424656	3.485840	4.663731
H	7.873247	3.298907	3.713167
H	6.341163	1.189214	1.032198
H	6.333072	4.812493	2.694029
H	5.012148	3.694022	2.727234
H	7.483441	3.297745	0.961296
H	6.026039	4.165700	0.493825
H	2.469399	-1.529473	0.903611
H	3.152732	0.014945	0.294264
H	1.089162	0.488534	-0.945906
H	1.220268	-1.262517	-1.196266
H	-1.033946	-0.262481	-0.000053
H	-0.292947	-1.734164	0.639552
H	-0.015045	-0.510677	2.641114
H	-0.187702	1.057630	1.818610
H	4.755927	0.904462	6.347853
H	2.138606	4.323496	3.011831
H	0.901169	2.839723	3.547982
H	0.988148	3.440044	1.634322
H	0.143462	4.643280	3.023660
H	5.166723	0.705159	2.649381
H	5.442118	-0.198339	4.167104
H	3.086989	2.144375	5.981279

2a

31

scf done: -1094.795063

C	-8.719334	5.815646	3.816646
C	-9.479186	6.561126	2.863948
C	-10.843816	6.153542	2.971502
C	-10.927460	5.155291	3.990207

C	-9.614578	4.948007	4.513607
C	-8.958764	7.681802	2.005629
C	-12.008924	6.775622	2.251009
C	-12.195131	4.547206	4.526060
C	-9.263194	4.080193	5.691280
C	-7.262813	6.017816	4.134597
Ca	-9.547844	4.076374	2.046524
B	-9.060200	2.310065	0.354938
H	-8.993157	1.848579	1.510395
H	-8.828047	1.462410	-0.456849
H	-10.204142	2.777702	0.191997
H	-11.734795	7.148724	1.257896
H	-12.839470	6.073602	2.116477
H	-12.409828	7.632467	2.808399
H	-9.013001	8.644665	2.530560
H	-7.909830	7.537742	1.723566
H	-9.531469	7.797562	1.078688
H	-6.790806	5.107983	4.521889
H	-6.685099	6.336330	3.259751
H	-7.125791	6.792861	4.900198
H	-9.920105	3.207382	5.776505
H	-8.233541	3.708626	5.643450
H	-9.353518	4.634046	6.635047
H	-12.975328	4.467083	3.760868
H	-12.035774	3.542971	4.934467
H	-12.614970	5.153322	5.339682
H	-8.244164	3.247051	0.265545

Adduct of ϵ -CL to monomer 2a

49

scf done: -1479.812653

C	-8.576583	5.815443	4.058147
C	-9.029364	6.685834	3.022560
C	-10.375576	6.335297	2.708660
C	-10.755742	5.248893	3.552265
C	-9.642249	4.924079	4.382202
C	-8.264118	7.852722	2.462648
C	-11.284107	7.061172	1.755199
C	-12.127310	4.638240	3.629829
C	-9.637238	3.916002	5.498582
C	-7.258886	5.913077	4.775107
Ca	-8.911043	4.268002	1.913924
O	-6.510251	3.710841	1.922565
C	-6.105947	4.185844	0.870938
C	-4.745620	3.943680	0.283541
C	-4.775089	3.165651	-1.066004
C	-6.158525	3.044541	-1.715461
C	-6.794346	4.369025	-2.152872

C	-6.665751	5.472732	-1.113307
O	-6.967871	4.991458	0.221974
B	-9.790005	2.697222	0.101421
H	-5.663533	5.911890	-1.098297
H	-7.383850	6.277155	-1.277033
H	-6.323103	4.742457	-3.071196
H	-7.851616	4.195769	-2.374320
H	-6.845028	2.536235	-1.026678
H	-6.082901	2.387828	-2.588154
H	-4.069733	3.636135	-1.760197
H	-4.397989	2.156156	-0.878981
H	-4.258581	4.918235	0.160072
H	-4.181399	3.398591	1.041361
H	-10.571249	2.713864	1.060794
H	-10.208896	1.986675	-0.773347
H	-9.651071	3.858858	-0.319661
H	-7.185957	7.657231	2.411706
H	-8.595331	8.116915	1.451605
H	-8.389085	8.754453	3.077816
H	-7.314529	6.598810	5.631895
H	-6.926594	4.945270	5.166809
H	-6.460358	6.287977	4.124338
H	-10.311486	3.075053	5.300562
H	-8.639566	3.497362	5.675652
H	-9.962963	4.361855	6.448418
H	-12.629990	4.626556	2.656692
H	-12.098591	3.603573	3.987982
H	-12.777173	5.195094	4.318936
H	-10.728900	7.559395	0.952179
H	-12.006094	6.388420	1.279121
H	-11.866112	7.841126	2.265237
H	-8.689346	2.286366	0.502907

Nucleophilic Attack TS to 2a

49

scf done: -1479.759714

Ca	-8.699762	6.267739	4.287857
O	-9.515873	7.375151	2.548235
C	-10.639678	6.740149	2.356346
H	-10.570525	5.857834	1.657906
O	-10.942294	5.918334	3.702673
C	-12.149101	6.159704	4.415033
H	-12.330584	7.240009	4.489740
H	-11.990252	5.801191	5.439671
C	-13.360011	5.460647	3.796353
H	-14.267171	5.937044	4.192151
H	-13.388811	4.413769	4.122097
C	-13.359887	5.492532	2.267026

H	-12.580135	4.809668	1.910896
H	-14.307030	5.074495	1.904787
C	-13.151565	6.867708	1.620727
H	-14.001299	7.519345	1.861624
H	-13.188130	6.725141	0.533950
C	-11.843157	7.599958	1.984784
H	-11.991245	8.325128	2.792503
H	-11.499045	8.193397	1.131373
B	-9.787107	3.855023	2.139404
H	-8.781319	4.463851	2.407244
H	-10.067800	3.741299	0.986045
H	-10.361386	3.248271	2.987303
C	-8.377769	6.215294	6.915566
C	-7.673092	5.075675	6.424766
C	-6.552325	5.541052	5.672929
C	-6.566674	6.967920	5.698006
C	-7.695629	7.384100	6.465022
C	-9.555000	6.188075	7.851000
C	-7.968005	3.640902	6.766904
C	-5.466064	4.679510	5.089117
C	-5.504958	7.871863	5.133860
C	-8.032537	8.802031	6.836620
H	-10.215542	7.052294	7.714442
H	-10.165754	5.287164	7.721264
H	-9.236676	6.200964	8.902332
H	-7.521521	9.110314	7.758878
H	-7.736799	9.516087	6.059694
H	-9.105529	8.941450	7.011921
H	-5.002761	7.430193	4.265760
H	-5.908072	8.840186	4.816100
H	-4.722188	8.084525	5.874620
H	-5.839034	3.700171	4.767492
H	-4.986169	5.145422	4.220781
H	-4.669092	4.485343	5.819800
H	-9.035836	3.465780	6.941246
H	-7.652152	2.950776	5.975977
H	-7.445860	3.328314	7.681506

Borane complex of 2a

49

scf done: -1479.832151

Ca	-6.709603	7.159956	-0.402304
O	-8.148197	5.479955	-1.350846
C	-9.048225	5.360802	-2.453450
H	-8.476691	5.184699	-3.374601
H	-9.516839	6.344829	-2.549639
C	-10.111930	4.286788	-2.285268
H	-10.703362	4.297240	-3.210683

H	-10.794936	4.565311	-1.474908
C	-9.551831	2.874163	-2.043842
H	-9.447311	2.697255	-0.967492
H	-10.285285	2.136860	-2.389151
C	-8.210599	2.605068	-2.737975
H	-7.986363	1.537694	-2.641248
H	-8.323563	2.785630	-3.814348
C	-7.006693	3.423055	-2.198489
H	-6.221954	2.749089	-1.842229
H	-6.541222	4.024128	-2.988467
C	-7.281626	4.335354	-1.012714
H	-7.786796	3.797671	-0.200138
O	-6.118145	4.913541	-0.551522
B	-6.001623	5.090330	0.979164
H	-5.742427	4.073128	1.569212
H	-7.088586	5.561794	1.379072
H	-5.120669	5.943050	1.114169
C	-5.347303	9.421799	-0.542325
C	-6.446091	9.688319	0.328918
C	-7.644301	9.640356	-0.444145
C	-7.285344	9.345706	-1.794119
C	-5.865878	9.206549	-1.853194
C	-3.892241	9.484656	-0.167298
C	-5.050759	9.010785	-3.102174
C	-8.217613	9.347457	-2.973984
C	-9.022212	9.992084	0.046573
C	-6.345212	10.083429	1.776784
H	-5.490667	9.613648	2.276112
H	-6.220007	11.168843	1.890002
H	-7.241578	9.810433	2.344920
H	-3.272657	8.835776	-0.796289
H	-3.493959	10.502580	-0.275482
H	-3.719009	9.186384	0.872452
H	-5.590381	8.438092	-3.865454
H	-4.781763	9.970774	-3.563468
H	-4.110353	8.483556	-2.905452
H	-9.239932	9.067489	-2.694596
H	-8.283289	10.343137	-3.433685
H	-7.894058	8.660264	-3.764588
H	-9.168906	9.726577	1.099800
H	-9.216155	11.070310	-0.034048
H	-9.809960	9.489652	-0.526699

Ring Opening TS to 2a

49

scf done: -1479.765801

Ca	-7.030342	7.315944	-1.008491
O	-8.405576	5.718148	-1.603825

C	-9.069978	5.303759	-2.749412
H	-8.360176	4.969997	-3.536729
H	-9.616689	6.146867	-3.211481
C	-10.074223	4.166613	-2.510640
H	-10.340172	3.729829	-3.483719
H	-11.000784	4.581871	-2.093624
C	-9.589787	3.072138	-1.553640
H	-9.588793	3.482214	-0.537193
H	-10.339875	2.271378	-1.536952
C	-8.228248	2.423014	-1.843856
H	-8.078244	1.615017	-1.116228
H	-8.249458	1.939346	-2.828362
C	-7.003473	3.350114	-1.801840
H	-6.079951	2.762722	-1.764655
H	-6.931079	3.954615	-2.710683
C	-7.007419	4.315744	-0.656592
H	-7.811194	4.320894	0.072416
O	-6.054507	5.253387	-0.555804
B	-5.348878	4.353216	0.504709
H	-4.299702	3.951114	0.075214
H	-6.137649	3.360664	0.477258
H	-5.426422	4.848890	1.601710
C	-5.493770	9.412602	-0.536366
C	-6.653749	9.588454	0.277328
C	-7.767625	9.813985	-0.585914
C	-7.296982	9.775612	-1.932850
C	-5.892229	9.525677	-1.902430
C	-4.081004	9.274704	-0.038954
C	-4.970660	9.524143	-3.091570
C	-8.112302	10.079829	-3.159398
C	-9.164037	10.164737	-0.150340
C	-6.671660	9.668195	1.779495
H	-5.886805	9.055613	2.237343
H	-6.511268	10.696865	2.129696
H	-7.628160	9.340857	2.203742
H	-3.447962	8.711841	-0.734152
H	-3.605296	10.255537	0.095484
H	-4.028781	8.764465	0.929229
H	-5.462428	9.158067	-4.000483
H	-4.605730	10.534604	-3.320273
H	-4.083619	8.901397	-2.928613
H	-9.159859	9.777856	-3.047588
H	-8.117324	11.155193	-3.383314
H	-7.723534	9.576724	-4.052204
H	-9.424849	9.711927	0.813137
H	-9.287932	11.249526	-0.029988
H	-9.919790	9.841197	-0.875158

Product from 2a

49

scf done: -1479.828268

Ca	-7.134798	7.211527	-1.710517
O	-8.604527	5.953731	-2.464848
C	-9.514813	5.045084	-2.940755
H	-9.027625	4.260227	-3.562891
H	-10.258281	5.511314	-3.617440
C	-10.305910	4.322027	-1.833910
H	-10.893607	3.512321	-2.291869
H	-11.029861	5.025571	-1.400223
C	-9.466404	3.759632	-0.679125
H	-9.029620	4.608821	-0.136513
H	-10.145590	3.276763	0.034738
C	-8.360776	2.756608	-1.050271
H	-8.115595	2.143379	-0.171178
H	-8.743605	2.055258	-1.802228
C	-7.073173	3.394557	-1.596697
H	-6.421927	2.631235	-2.039155
H	-7.344237	4.111988	-2.375378
C	-6.298153	4.162608	-0.533951
H	-6.965780	4.574762	0.228598
O	-5.625202	5.314681	-1.127034
B	-4.291702	5.307407	-1.380143
H	-3.621713	4.369988	-1.057576
H	-5.540910	3.552702	-0.032044
H	-3.857811	6.274012	-1.935244
C	-5.773010	9.000141	-0.286543
C	-7.124397	9.071113	0.166004
C	-7.917812	9.595132	-0.896855
C	-7.060852	9.835000	-2.010837
C	-5.733990	9.467753	-1.634714
C	-4.581439	8.642110	0.557266
C	-4.494222	9.692062	-2.456439
C	-7.464713	10.482425	-3.306935
C	-9.382020	9.928120	-0.825424
C	-7.604117	8.776417	1.560895
H	-6.985509	8.021884	2.061214
H	-7.578974	9.671572	2.197237
H	-8.637731	8.411140	1.576552
H	-3.748962	8.258642	-0.043651
H	-4.195874	9.513892	1.103480
H	-4.816598	7.881901	1.312016
H	-4.681241	9.583002	-3.531343
H	-4.090578	10.703540	-2.311592
H	-3.690338	8.994353	-2.195379
H	-8.490678	10.227332	-3.595742
H	-7.418182	11.578222	-3.243366

H	-6.812301	10.190224	-4.138026
H	-9.916027	9.291051	-0.111672
H	-9.544452	10.966500	-0.505515
H	-9.881004	9.813454	-1.794164

3a

36

scf done: -1037.216091

Ca	-10.238266	2.444112	-0.652777
B	-9.160581	3.794256	1.113340
H	-8.702922	4.065156	-0.011001
H	-10.386751	3.996759	1.072135
H	-8.996005	2.571848	1.291398
H	-8.631775	4.442280	1.975890
Si	-8.663437	2.511347	-4.098408
H	-7.212553	2.173342	-4.310580
H	-9.362961	2.206989	-5.395808
H	-8.764613	3.984201	-3.854416
N	-9.374399	1.699609	-2.724765
P	-9.528900	0.075837	-2.517704
C	-10.139310	-0.745023	-4.060517
H	-9.402870	-0.622908	-4.860004
H	-11.072922	-0.274204	-4.373395
H	-10.304386	-1.809669	-3.877570
C	-7.925075	-0.776477	-2.198791
H	-7.495199	-0.380295	-1.276367
H	-8.074419	-1.855250	-2.102678
H	-7.241779	-0.574769	-3.027256
C	-10.484328	-0.204048	-1.054952
H	-10.133857	-1.053130	-0.471047
P	-12.223845	0.080197	-0.896693
N	-12.475185	1.704556	-0.843738
C	-13.301774	-0.722260	-2.170061
H	-13.146419	-0.231651	-3.132655
H	-13.060591	-1.784994	-2.251850
H	-14.352480	-0.608152	-1.887966
Si	-14.022506	2.515594	-0.853956
H	-13.762190	3.988086	-0.799553
H	-14.832224	2.233201	-2.090757
H	-14.896587	2.153305	0.316295
C	-12.700021	-0.785839	0.659609
H	-12.076158	-0.411216	1.473832
H	-12.563498	-1.865534	0.556078
H	-13.747611	-0.569968	0.882912

Adduct of ϵ -CL to monomer 3a

54

scf done: -1422.185576

B	-8.718172	2.585021	5.132565
H	-9.111610	3.034016	4.069474
H	-8.442788	1.415195	5.138317
H	-8.070918	3.360429	5.786075
Ca	-11.354868	2.954189	3.183468
O	-11.681681	1.735240	5.070131
C	-11.151823	2.549404	5.903868
C	-11.386976	2.318363	7.393295
C	-10.611793	3.221680	8.355886
C	-10.630376	4.716805	8.004545
C	-11.979920	5.239252	7.505925
C	-12.385784	4.655752	6.131561
O	-11.318241	3.950139	5.491120
N	-12.967468	4.400675	2.193326
Si	-14.695240	4.556526	2.359783
P	-12.014068	5.219258	1.130643
C	-10.395572	4.514127	1.148556
P	-9.960207	2.978284	0.392432
C	-10.242658	2.861490	-1.435359
C	-12.826519	5.335475	-0.529709
C	-11.763958	6.983909	1.605459
C	-8.123606	2.887569	0.528477
N	-10.736892	1.778934	1.200727
Si	-10.824082	0.100621	0.731298
H	-9.883248	2.520930	5.874409
H	-11.537788	-0.112219	-0.577981
H	-15.144051	5.947455	2.730649
H	-15.462649	4.192442	1.117088
H	-15.134671	3.633866	3.454166
H	-9.478144	-0.558623	0.581593
H	-11.582333	-0.632993	1.791416
H	-9.599333	5.255682	1.135627
H	-7.651096	3.692481	-0.041105
H	-7.851108	2.969126	1.582681
H	-7.786306	1.921870	0.144225
H	-9.771882	3.709240	-1.939783
H	-9.815675	1.929349	-1.817072
H	-11.315246	2.862491	-1.637138
H	-13.749953	5.917129	-0.454250
H	-12.152759	5.811545	-1.246189
H	-13.077201	4.328470	-0.869525
H	-11.182589	7.510060	0.843731
H	-12.737390	7.466252	1.721634
H	-11.232121	7.013217	2.558924
H	-13.261468	3.999940	6.213752
H	-12.765378	5.020966	8.240841
H	-12.651786	5.454159	5.433294
H	-11.923902	6.331448	7.432765

H	-10.331777	5.292541	8.888554
H	-9.878768	4.916405	7.234729
H	-11.032421	3.072666	9.358534
H	-9.569165	2.887431	8.410003
H	-12.469030	2.415183	7.550997
H	-11.152720	1.265523	7.575427

Nucleophilic Attack TS to 3a

54

scf done: -1422.172309

B	-9.540411	-0.019627	6.046982
H	-8.889031	0.440304	5.155161
H	-10.427650	-0.780948	5.813946
H	-9.233313	0.212412	7.181120
Ca	-11.619902	2.961941	3.150254
O	-11.877584	1.902022	5.033504
C	-11.204505	2.627033	5.914837
C	-12.018641	3.074320	7.131518
C	-11.253412	3.780767	8.278287
C	-9.860653	4.318713	7.922026
C	-9.845090	5.426843	6.863855
C	-10.782902	5.153476	5.693183
O	-10.652567	3.849872	5.147892
N	-13.429686	4.053398	2.049614
Si	-15.160267	3.853704	2.142002
P	-12.626320	5.123508	1.095472
C	-10.888236	4.850624	1.242041
P	-9.986655	3.517935	0.518331
C	-10.119608	3.354349	-1.322969
C	-13.301477	5.102353	-0.629298
C	-12.867238	6.878579	1.613397
C	-8.213818	3.972749	0.756162
N	-10.405806	2.120492	1.271164
Si	-9.933818	0.509122	0.796863
H	-10.260431	2.141532	6.260423
H	-10.386809	0.136520	-0.590644
H	-15.880239	5.089259	2.618757
H	-15.797625	3.487921	0.827179
H	-15.446935	2.753760	3.114044
H	-8.443645	0.287578	0.818417
H	-10.556337	-0.452995	1.757325
H	-10.316006	5.774197	1.304272
H	-7.969127	4.883743	0.203368
H	-8.034521	4.128073	1.822133
H	-7.585025	3.151791	0.403289
H	-9.890213	4.310364	-1.800435
H	-9.421558	2.591698	-1.680527
H	-11.133772	3.046593	-1.583897

H	-14.348268	5.419674	-0.623584
H	-12.720574	5.769382	-1.270937
H	-13.252643	4.082037	-1.014865
H	-12.378617	7.559178	0.911211
H	-13.937131	7.097202	1.650841
H	-12.441351	7.009474	2.610262
H	-11.821921	5.338508	6.000882
H	-10.148711	6.383901	7.310966
H	-10.568173	5.848646	4.871447
H	-8.820389	5.561185	6.496359
H	-9.378729	4.690482	8.834574
H	-9.235371	3.489529	7.572824
H	-11.866782	4.600575	8.675292
H	-11.129664	3.077553	9.109967
H	-12.854677	3.680703	6.762909
H	-12.476596	2.151794	7.501520

Borane complex of 3a

54

scf done: -1422.243342

C	-7.196341	7.818970	-1.025467
Ca	-7.921893	5.173446	-1.231789
N	-8.382113	6.512979	-3.159240
Si	-9.128138	6.176840	-4.696205
P	-7.627976	7.909709	-2.731415
C	-8.628049	9.384990	-3.238884
P	-8.320636	7.866197	0.331451
N	-9.159395	6.453284	0.376743
Si	-10.480559	6.089205	1.452757
C	-6.026784	8.170600	-3.607956
C	-7.256337	8.129256	1.814070
C	-9.467126	9.321739	0.375876
O	-9.137430	3.056970	-1.254261
C	-10.429056	2.671578	-1.719555
C	-10.965472	1.399778	-1.077097
C	-10.006102	0.205372	-1.178043
C	-9.233350	0.127771	-2.501167
C	-8.219028	1.274798	-2.749000
C	-7.971899	2.226341	-1.586533
O	-6.971628	3.121990	-1.898841
B	-5.997785	3.510255	-0.776655
H	-6.760626	9.102359	1.765513
H	-10.414701	2.567905	-2.812322
H	-7.719617	1.678927	-0.668010
H	-8.194752	6.308301	-5.871609
H	-10.308389	7.061165	-5.003895
H	-9.624496	4.763556	-4.671085
H	-6.201555	8.151529	-4.686349

H	-5.349034	7.357366	-3.339694
H	-5.584046	9.129626	-3.326039
H	-8.721148	9.413384	-4.328676
H	-9.627459	9.305329	-2.806962
H	-8.147208	10.302494	-2.890452
H	-6.217910	8.236104	-0.797956
H	-10.181754	9.238627	-0.445259
H	-10.021557	9.330673	1.318978
H	-8.898511	10.249983	0.278328
H	-7.875951	8.078504	2.712577
H	-6.508725	7.333968	1.848435
H	-10.127992	6.206779	2.913156
H	-10.908211	4.676521	1.203998
H	-11.686994	6.968856	1.248975
H	-7.231762	0.861796	-2.976608
H	-8.492292	1.876460	-3.623108
H	-8.701524	-0.829562	-2.525088
H	-9.949607	0.088686	-3.331752
H	-9.295183	0.240577	-0.344637
H	-10.574012	-0.722083	-1.040153
H	-11.910242	1.165268	-1.586421
H	-11.212251	1.590380	-0.026540
H	-11.082800	3.517609	-1.485366
H	-6.669417	3.734891	0.250122
H	-5.149856	2.676199	-0.559015
H	-5.509768	4.580103	-1.158076

Ring Opening TS to 3a

54

scf done: -1422.181607

C	-7.377244	7.501213	-1.243664
Ca	-8.938704	5.236456	-1.507192
N	-9.072049	6.766961	-3.321640
Si	-10.033674	6.802904	-4.774676
P	-7.945657	7.878411	-2.867119
C	-8.585876	9.598447	-3.114237
P	-8.260924	7.725400	0.263199
N	-9.509729	6.654698	0.316363
Si	-10.787680	6.620650	1.501999
C	-6.430138	7.834809	-3.916877
C	-7.008481	7.442817	1.585537
C	-8.850178	9.448897	0.603405
O	-9.721160	3.201164	-1.669011
C	-10.420773	2.410397	-2.568239
C	-10.858882	1.053876	-1.993735
C	-9.806775	0.352983	-1.127354
C	-8.405763	0.158062	-1.727235
C	-7.625284	1.434612	-2.074997

C	-7.709036	2.507450	-1.032199
O	-7.152511	3.701402	-1.248863
B	-5.965481	3.255664	-0.352689
H	-6.228196	8.207670	1.547635
H	-9.829576	2.214239	-3.487545
H	-8.287439	2.365788	-0.125054
H	-9.217572	6.758369	-6.040742
H	-10.914824	8.018493	-4.891777
H	-10.921060	5.596991	-4.766240
H	-6.715996	7.961802	-4.963792
H	-5.949378	6.862192	-3.791558
H	-5.737044	8.628812	-3.626925
H	-8.786716	9.774373	-4.175066
H	-9.520642	9.710492	-2.561165
H	-7.854124	10.326126	-2.755002
H	-6.297617	7.568955	-1.132943
H	-9.634888	9.708667	-0.109701
H	-9.263925	9.510087	1.614384
H	-8.018433	10.151338	0.507571
H	-7.504818	7.475252	2.558488
H	-6.565311	6.455242	1.438947
H	-10.298128	6.449031	2.916993
H	-11.677010	5.459085	1.184738
H	-11.640281	7.862241	1.507257
H	-6.570285	1.202087	-2.255611
H	-7.990773	1.886649	-3.001591
H	-7.812473	-0.429023	-1.013960
H	-8.473131	-0.453745	-2.635754
H	-9.725205	0.900099	-0.181103
H	-10.189261	-0.638498	-0.853006
H	-11.156995	0.404212	-2.829297
H	-11.754460	1.193132	-1.374319
H	-11.325387	2.933465	-2.930121
H	-6.329728	2.066674	-0.098968
H	-4.960507	3.153242	-1.009172
H	-5.958646	3.859011	0.693531

Product from 3a

54

scf done: -1422.243811

C	-7.341346	7.363596	-1.245595
Ca	-8.876553	5.053599	-1.924656
N	-8.851433	6.825024	-3.525060
Si	-9.715513	7.037911	-5.026355
P	-7.843221	7.925169	-2.838222
C	-8.589470	9.621398	-2.886265
P	-8.321082	7.350184	0.214853
N	-9.494422	6.207981	0.083540

Si	-10.838668	6.005117	1.177390
C	-6.268674	8.146166	-3.774786
C	-7.119941	7.004734	1.575199
C	-9.038762	8.982236	0.725847
O	-9.967676	3.365591	-2.396596
C	-10.596819	2.222221	-2.826260
C	-11.074578	1.310114	-1.681616
C	-10.044707	1.037382	-0.578201
C	-8.707409	0.414781	-1.014238
C	-7.706955	1.393322	-1.649611
C	-7.177476	2.421467	-0.661382
O	-6.790398	3.637533	-1.357650
B	-5.496414	3.904954	-1.645665
H	-6.397824	7.820169	1.669156
H	-9.935016	1.611970	-3.480726
H	-7.952205	2.724941	0.047502
H	-8.811736	7.353649	-6.192264
H	-10.731057	8.149930	-4.985281
H	-10.436539	5.766635	-5.337932
H	-6.504268	8.399765	-4.811122
H	-5.715062	7.205229	-3.752659
H	-5.663848	8.941351	-3.331133
H	-8.732560	9.935615	-3.924442
H	-9.565197	9.595992	-2.396794
H	-7.937712	10.334632	-2.375598
H	-6.280482	7.509274	-1.054312
H	-9.806985	9.276058	0.008174
H	-9.500856	8.894712	1.713722
H	-8.254814	9.743127	0.757004
H	-7.667337	6.891241	2.513971
H	-6.595613	6.073803	1.350398
H	-10.414866	5.778026	2.607743
H	-11.622925	4.811038	0.739247
H	-11.772259	7.186521	1.212367
H	-6.863152	0.845095	-2.087380
H	-8.204873	1.951559	-2.445179
H	-8.234998	-0.066325	-0.145339
H	-8.898925	-0.394432	-1.730635
H	-9.860974	1.980204	-0.049499
H	-10.506877	0.370936	0.161491
H	-11.417387	0.357896	-2.114037
H	-11.950764	1.770454	-1.205304
H	-11.480562	2.446515	-3.455369
H	-6.312260	2.057920	-0.096412
H	-4.632324	3.162011	-1.270755
H	-5.279400	4.898185	-2.274041