

Electronic Supplementary Informations

Bis(phosphinimino)methanide Borohydride Complexes of the Rare-Earth

Elements as Initiators for the Polymerization of Methyl Methacrylate:

Combined Experimental and Computational Investigations

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All coordinates of all optimized complexes are given in the following.

Yttrium complexes

Add A

C	-10.505846	3.280860	-0.822810
P	-10.022785	3.036729	0.946520
C	-10.866511	1.460415	1.395590
N	-8.392225	2.991873	1.127869
Si	-7.264704	2.108139	0.134154
C	-10.615957	4.234706	2.099746
P	-10.386705	5.974593	1.883693
C	-11.075595	6.719301	0.335320
C	-11.372030	6.785280	3.208622
Si	-7.929512	7.723260	1.681123
N	-8.767128	6.223130	2.005590
Y	-8.032475	4.270174	3.128878
O	-8.148117	2.063716	4.060396
C	-8.098512	1.136894	4.868539
O	-6.989857	0.454858	5.102911
C	-5.803776	0.866525	4.394529
C	-9.251944	0.654946	5.671215
C	-9.104714	-0.629369	6.435714
C	-10.347537	1.426091	5.696287
B	-5.549747	4.410969	2.878544
H	-6.003852	3.393052	2.339620
H	-4.360858	4.501087	2.740198
H	-6.147927	5.371001	2.370258
H	-5.883199	4.370169	4.067483
B	-8.646881	5.077078	5.458145
H	-8.140933	5.980994	4.787807
H	-9.605701	4.629458	4.803266

H	-9.012433	5.458965	6.538940
H	-7.814234	4.172572	5.539909
H	-10.384308	2.368893	5.159803
H	-11.214321	1.142242	6.285971
H	-8.297310	-0.557327	7.171123
H	-10.031824	-0.869047	6.961177
H	-8.854683	-1.463499	5.771897
H	-5.549919	1.897550	4.646438
H	-5.962035	0.788028	3.317277
H	-5.023435	0.182362	4.723978
H	-10.660484	1.243539	2.445541
H	-10.466855	0.655098	0.773964
H	-11.945304	1.541920	1.236370
H	-10.191985	2.414756	-1.411436
H	-11.588571	3.406814	-0.902596
H	-9.998764	4.167178	-1.208719
H	-11.535958	3.956730	2.609589
H	-11.015331	6.415924	4.172184
H	-12.436171	6.564716	3.086623
H	-11.214333	7.865278	3.151583
H	-12.134895	6.467117	0.238962
H	-10.525839	6.344154	-0.529347
H	-10.963450	7.806289	0.379558
H	-8.897947	8.873143	1.581643
H	-7.184371	7.672333	0.382391
H	-6.963089	8.033431	2.773505
H	-7.981838	1.352938	-0.955521
H	-6.266834	3.003948	-0.522676
H	-6.517494	1.078959	0.926877

Energy = - 770.625308 H

TSAB Nucleophilic attack

C	-10.524858	3.394647	-1.150181
P	-10.006814	3.062165	0.593731
C	-10.749508	1.415319	0.949155
N	-8.373799	3.102979	0.785295
Si	-7.161981	2.447409	-0.291358
C	-10.635797	4.142569	1.836714
P	-10.335742	5.890350	1.865836
C	-10.606335	6.788041	0.273366
C	-11.599998	6.602340	2.994633
Si	-7.941442	7.621404	2.483390
N	-8.791524	6.093460	2.399838
Y	-8.175288	3.903652	3.015265
O	-8.505255	1.828510	3.847025
C	-8.190100	1.127262	4.868857
O	-7.213314	0.213050	4.766819

C	-6.553005	0.086417	3.507567
C	-8.780692	1.257485	6.137268
C	-8.150028	0.620955	7.346467
C	-9.854344	2.161935	6.228856
B	-5.694232	4.041838	3.148878
H	-6.081577	3.294890	2.236568
H	-4.498761	4.119220	3.189919
H	-6.227454	5.142955	2.946533
H	-6.179787	3.597949	4.196563
B	-9.241234	4.621823	5.552468
H	-8.035479	4.613010	5.353763
H	-9.921932	4.442747	4.553683
H	-9.633063	5.519322	6.250672
H	-9.412161	3.501462	6.250796
H	-10.494407	2.281937	5.360788
H	-10.384449	2.221834	7.178759
H	-7.177840	1.066604	7.595678
H	-8.798879	0.729137	8.220529
H	-7.977644	-0.448690	7.190168
H	-6.044148	1.013916	3.234322
H	-7.261564	-0.181699	2.719187
H	-5.823996	-0.712983	3.643036
H	-10.459767	1.128127	1.962132
H	-10.354396	0.686091	0.237099
H	-11.838998	1.453014	0.864007
H	-10.162249	2.597434	-1.803820
H	-11.615965	3.440579	-1.199410
H	-10.101016	4.343330	-1.483380
H	-11.592902	3.850968	2.263858
H	-11.504169	6.115374	3.966890
H	-12.603971	6.450767	2.589333
H	-11.406276	7.671769	3.107252
H	-11.605299	6.579854	-0.117938
H	-9.848019	6.473093	-0.446190
H	-10.499213	7.862877	0.446440
H	-8.911455	8.773890	2.498745
H	-7.044172	7.831428	1.301892
H	-7.122246	7.687547	3.726442
H	-7.780652	1.999443	-1.588430
H	-6.123158	3.470096	-0.611564
H	-6.482853	1.249360	0.295259

Energy = - 770.602067 H

Add B

C	-10.605203	3.332134	-1.107972
P	-10.001897	3.042017	0.615834
C	-10.670709	1.379849	1.032991
N	-8.362425	3.140090	0.735343

Si	-7.172286	2.500748	-0.377328
C	-10.605058	4.124120	1.870516
P	-10.313411	5.873863	1.881655
C	-10.534592	6.738701	0.264485
C	-11.615556	6.600443	2.958004
Si	-7.951327	7.632297	2.536534
N	-8.788730	6.097415	2.461909
Y	-8.113380	3.881948	2.966116
O	-8.484464	1.921861	3.873679
C	-8.216114	1.162475	4.894145
O	-7.294861	0.181723	4.737490
C	-6.646075	0.074028	3.477973
C	-8.802906	1.302247	6.133227
C	-8.317434	0.568506	7.352404
C	-9.822361	2.327194	6.255103
B	-5.639532	4.075427	3.064409
H	-6.031428	3.244034	2.227868
H	-4.444585	4.162209	3.086986
H	-6.182450	5.149105	2.766583
H	-6.113591	3.718888	4.151084
B	-9.167443	4.670563	5.594900
H	-7.970486	4.585774	5.426734
H	-9.879663	4.519404	4.631402
H	-9.551060	5.442294	6.426922
H	-9.322768	3.442135	6.321380
H	-10.510472	2.413267	5.416365
H	-10.361493	2.325848	7.205697
H	-7.816012	1.242466	8.062660
H	-9.140229	0.086144	7.895666
H	-7.600070	-0.207053	7.079068
H	-6.073488	0.974711	3.238543
H	-7.362247	-0.118260	2.672864
H	-5.966850	-0.774776	3.573233
H	-10.308169	1.120572	2.030423
H	-10.297922	0.652693	0.306906
H	-11.764003	1.383552	1.015482
H	-10.248444	2.535625	-1.765619
H	-11.698364	3.343698	-1.107200
H	-10.227883	4.287954	-1.474716
H	-11.547949	3.828597	2.325665
H	-11.569209	6.113277	3.933745
H	-12.603514	6.459056	2.511972
H	-11.415226	7.667595	3.079850
H	-11.522043	6.526644	-0.152868
H	-9.754852	6.404138	-0.422851
H	-10.427105	7.816725	0.416915
H	-8.930490	8.774302	2.619823
H	-7.105791	7.881976	1.324674
H	-7.082248	7.675555	3.746506
H	-7.808443	2.136920	-1.691581

H	-6.112407	3.515926	-0.644142
H	-6.522413	1.257718	0.145909

Energy = -770.602147 H

TSBC Trapping

C	-10.619179	3.483674	-1.291561
P	-10.068891	3.075919	0.424915
C	-10.659716	4.109917	1.721930
P	-10.361062	5.849266	1.870408
C	-11.777825	6.550637	2.807221
Y	-8.163708	3.764150	2.823333
O	-8.457004	2.006670	3.985049
C	-8.211166	1.294189	5.065929
O	-7.421157	0.190039	4.908781
C	-6.505031	0.190186	3.826348
C	-10.823796	1.425550	0.733262
N	-8.429218	3.094205	0.576747
Si	-7.246905	2.423123	-0.530321
B	-5.702887	4.089792	2.743993
N	-8.919970	6.040606	2.661528
Si	-8.054959	7.555941	2.841012
C	-10.346246	6.784059	0.279998
C	-8.708889	1.561107	6.304517
C	-8.282107	0.793857	7.524516
C	-9.720695	2.639313	6.466679
B	-9.288576	4.972439	5.121003
H	-6.068279	3.029386	2.209142
H	-4.513276	4.230717	2.701459
H	-6.304327	5.003643	2.163624
H	-6.132368	4.048166	3.907273
H	-8.092174	4.855659	5.063516
H	-10.009470	4.341582	4.405925
H	-9.750897	5.828821	5.811575
H	-9.277176	3.681168	6.324215
H	-10.554622	2.573665	5.762428
H	-10.124019	2.671632	7.483748
H	-7.949450	1.471522	8.323559
H	-9.099625	0.189688	7.944914
H	-7.457406	0.117141	7.294229
H	-5.801103	1.028217	3.888875
H	-7.014589	0.228037	2.858195
H	-5.953965	-0.749331	3.905525
H	-10.544416	1.100877	1.738247
H	-10.432869	0.714328	0.001025
H	-11.912546	1.475119	0.645274
H	-10.262374	2.718773	-1.985721
H	-11.711296	3.522324	-1.318623
H	-10.208702	4.449643	-1.589636

H	-11.587270	3.783269	2.186436
H	-11.878810	6.001248	3.745072
H	-12.697539	6.467571	2.222815
H	-11.571259	7.600468	3.028339
H	-11.282433	6.632010	-0.262504
H	-9.500700	6.443131	-0.321440
H	-10.215839	7.849442	0.491356
H	-8.988873	8.668667	3.234061
H	-7.388611	7.987430	1.568928
H	-7.025299	7.396363	3.903806
H	-7.888481	2.071733	-1.845521
H	-6.162454	3.412026	-0.794513
H	-6.637697	1.166896	0.006864

Energy = - 770.596327 H

Add C

C	-10.605346	3.057055	-0.813904
P	-9.832919	2.971241	0.864351
C	-10.518001	4.048896	2.081889
P	-10.465697	5.793816	1.978601
C	-11.880503	6.476670	2.917956
Y	-7.873271	4.107093	3.064975
O	-8.176894	2.434402	4.234139
C	-8.488378	1.315511	4.876599
O	-8.329955	0.168791	4.117498
C	-7.001699	-0.050042	3.659253
C	-10.219444	1.260314	1.406917
N	-8.228918	3.346890	0.839008
Si	-7.040034	2.831253	-0.343219
B	-5.442750	4.524254	2.787375
N	-8.999701	6.365624	2.642565
Si	-8.182412	7.856927	2.092584
C	-10.581940	6.492054	0.285263
C	-8.980575	1.227111	6.129293
C	-9.279290	-0.094250	6.777074
C	-9.269250	2.454033	6.943924
B	-8.930114	6.195787	4.241556
H	-5.797960	3.424411	2.329332
H	-4.265418	4.707098	2.659369
H	-6.117368	5.387168	2.200635
H	-5.795202	4.529210	3.976683
H	-7.741185	6.031371	4.513054
H	-9.536650	5.160391	4.520277
H	-9.381336	7.128616	4.860680
H	-8.683188	2.458700	7.873865
H	-9.039981	3.371871	6.399261
H	-10.326325	2.492604	7.245663
H	-8.724054	-0.206927	7.719151

H	-10.344815	-0.178473	7.036761
H	-9.023946	-0.931590	6.125861
H	-6.308351	-0.145717	4.505129
H	-6.654568	0.759256	3.007343
H	-7.014712	-0.986416	3.096824
H	-9.700105	1.047025	2.345511
H	-9.869408	0.566367	0.637693
H	-11.298544	1.138398	1.535726
H	-10.181101	2.278953	-1.453264
H	-11.682831	2.899581	-0.716723
H	-10.413091	4.028612	-1.270728
H	-11.306446	3.649357	2.712918
H	-11.846768	6.077702	3.933098
H	-12.814940	6.188334	2.431228
H	-11.793592	7.564595	2.959184
H	-11.507036	6.140851	-0.176669
H	-9.722151	6.163140	-0.301533
H	-10.590400	7.584399	0.329743
H	-9.097189	9.033987	2.256265
H	-7.831353	7.744366	0.645620
H	-6.965506	8.033422	2.920747
H	-7.704059	2.504173	-1.653320
H	-6.064094	3.931783	-0.581023
H	-6.297211	1.603948	0.084182

Energy = - 770.644992 H

Add D (2nd insertion)

C	-8.933476	5.886018	-0.627879
P	-9.698946	6.322492	0.978429
C	-10.388676	8.008275	0.755262
N	-8.413534	6.438055	2.151530
B	-9.004144	6.752479	3.618938
Y	-7.805950	4.236920	3.135229
B	-6.570690	3.392129	1.108482
C	-10.997458	5.276154	1.416904
P	-10.925567	3.534585	1.610846
C	-10.709181	2.715629	-0.025346
Si	-7.033288	7.562296	1.883869
O	-6.150777	4.824231	4.297475
C	-5.271043	4.623083	5.259315
C	-5.333394	5.135146	6.515157
C	-6.466308	6.018354	6.946381
N	-9.805327	2.960034	2.701561
Si	-9.869912	1.289334	3.226163
O	-8.000241	2.866254	5.022024
C	-7.652935	2.510905	6.157558
O	-8.329949	2.884610	7.234617
C	-9.479718	3.720352	7.026246

O	-4.232226	3.774523	4.945521
C	-3.582214	4.042734	3.710079
C	-12.635956	3.086203	2.128849
C	-6.532111	1.599703	6.456688
C	-5.845082	1.094624	5.421282
C	-6.227610	1.292281	7.895165
C	-4.251866	4.893927	7.528091
H	-6.484405	2.616516	2.074061
H	-5.969529	2.988298	0.150181
H	-7.776162	3.516719	0.873523
H	-6.153702	4.494492	1.481515
H	-9.099614	5.675331	4.249731
H	-10.121589	7.220962	3.593080
H	-8.220213	7.467938	4.206197
H	-6.091962	6.991378	7.295675
H	-7.168692	6.211091	6.132647
H	-7.017530	5.584196	7.794767
H	-4.650452	4.423059	8.439539
H	-3.462551	4.253409	7.132541
H	-3.796999	5.841218	7.853229
H	-3.130702	5.044427	3.715066
H	-4.266364	3.961156	2.861199
H	-2.791104	3.295976	3.612286
H	-12.848665	3.576177	3.081906
H	-12.713854	2.003834	2.255591
H	-13.349897	3.423531	1.374628
H	-10.829204	1.636561	0.099239
H	-11.448701	3.095966	-0.733015
H	-9.699541	2.910229	-0.392096
H	-11.601366	5.730383	2.201830
H	-10.827403	8.334856	1.699127
H	-11.155251	7.970630	-0.020859
H	-9.595882	8.702783	0.466768
H	-9.733346	5.744907	-1.356993
H	-8.342660	4.974059	-0.526390
H	-8.275693	6.694966	-0.950709
H	-7.481127	8.978458	2.055994
H	-6.542009	7.407248	0.477679
H	-5.952679	7.222637	2.838720
H	-10.468271	1.127877	4.593864
H	-10.724245	0.455750	2.306877
H	-8.512196	0.667479	3.237973
H	-9.908321	3.869800	8.016347
H	-9.183207	4.675608	6.590215
H	-10.192343	3.220776	6.366490
H	-5.980371	2.204661	8.446111
H	-7.086031	0.834680	8.397377
H	-5.379321	0.607799	7.964392
H	-5.006498	0.425360	5.584346
H	-6.093709	1.343735	4.396487

Energy = - 1116.190829 H

TSDP 2nd insertion

C	-9.013749	6.121949	-0.453012
P	-9.700289	6.366907	1.228958
C	-10.456356	8.039073	1.204231
N	-8.353216	6.417430	2.339114
B	-8.850542	6.667386	3.850444
Y	-7.757717	4.144019	3.186745
B	-6.658326	3.493228	0.995637
C	-10.940258	5.236945	1.628285
P	-10.827726	3.486588	1.607751
C	-10.611137	2.870137	-0.114818
Si	-6.973978	7.533683	2.038375
O	-5.815908	4.632019	4.066589
C	-4.840736	4.513084	4.901562
C	-4.930966	4.688709	6.278893
C	-6.124562	5.394702	6.839042
N	-9.688201	2.837670	2.627963
Si	-9.624926	1.118802	2.957028
O	-8.125654	2.977138	5.104691
C	-8.041064	2.672030	6.327341
O	-9.150301	2.635063	7.078913
C	-10.365758	3.089403	6.481599
O	-3.635531	4.130745	4.416637
C	-3.527560	3.904207	3.014403
C	-12.512819	2.913331	2.079174
C	-6.840643	2.346954	7.029007
C	-5.662505	2.376459	6.316362
C	-6.896412	2.065823	8.509394
C	-3.701480	4.617912	7.145203
H	-6.565998	2.621010	1.878031
H	-6.164262	3.127182	-0.037665
H	-7.864030	3.715421	0.864542
H	-6.142247	4.523158	1.424753
H	-8.874990	5.573666	4.453212
H	-9.977382	7.106125	3.917243
H	-8.046893	7.381357	4.414235
H	-5.814621	6.178427	7.541106
H	-6.731600	5.859556	6.058585
H	-6.781786	4.706754	7.397834
H	-3.956400	4.242718	8.143893
H	-2.934360	3.967188	6.720361
H	-3.250445	5.610938	7.287219
H	-3.759876	4.809581	2.447078
H	-4.192245	3.104601	2.677809
H	-2.487894	3.618070	2.847279
H	-12.733963	3.266439	3.088949

H	-12.543471	1.820573	2.067290
H	-13.250572	3.311231	1.379428
H	-10.680394	1.779711	-0.109525
H	-11.385061	3.291621	-0.759739
H	-9.620423	3.148035	-0.477426
H	-11.527893	5.588977	2.475391
H	-10.907121	8.239172	2.176768
H	-11.220946	8.059363	0.425383
H	-9.691402	8.792378	1.001139
H	-9.849800	5.959137	-1.135546
H	-8.337899	5.265426	-0.462967
H	-8.461123	7.013587	-0.754834
H	-7.400265	8.949040	2.265886
H	-6.534618	7.409225	0.613585
H	-5.858666	7.165984	2.942190
H	-10.460591	0.711656	4.137131
H	-10.136774	0.303360	1.799718
H	-8.217356	0.698772	3.222061
H	-11.124601	2.985138	7.257632
H	-10.277511	4.136471	6.178356
H	-10.625793	2.485017	5.610679
H	-7.333607	2.892864	9.079250
H	-7.501965	1.178155	8.725555
H	-5.889725	1.884717	8.895534
H	-4.732150	2.080015	6.789978
H	-5.687317	2.323097	5.235161

Energy = -1116.181270 H

Add E

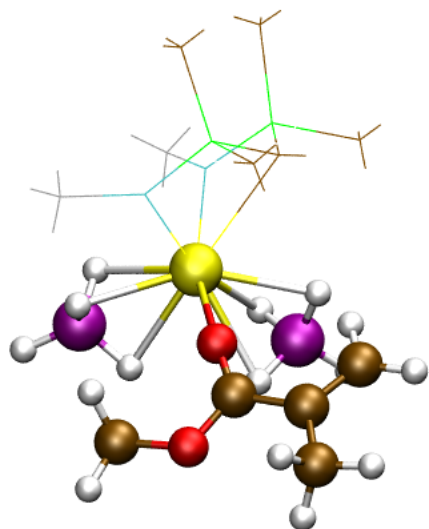
Y	-7.794878	4.994017	2.851874
O	-7.834418	4.161724	4.744456
C	-8.009898	3.498756	5.878947
C	-7.066135	2.808488	6.555174
C	-5.674003	2.683724	5.994756
C	-4.538151	3.466279	6.723144
C	-4.293941	2.902750	8.119941
C	-4.880835	4.951733	6.841464
C	-3.239209	3.289239	5.911606
N	-8.870672	6.873102	1.481887
Si	-8.100568	7.756453	0.130710
B	-8.502618	7.523137	2.907933
B	-5.486839	4.889660	1.949887
N	-8.652113	3.234374	1.523133
Si	-7.753915	1.936511	0.751872
O	-4.327348	3.529481	9.157615
O	-3.994468	1.583758	8.084383
C	-3.730311	0.990088	9.354637
O	-9.322341	3.490648	6.325536

C	-9.827809	4.774423	6.662182
C	-7.388487	2.089403	7.836681
P	-10.466719	6.271252	1.422127
C	-10.598371	4.864972	2.451342
P	-10.242875	3.211202	1.949703
C	-10.661608	2.163884	3.398935
C	-10.869026	5.996512	-0.347311
C	-11.634071	7.547300	2.022719
C	-11.308920	2.522073	0.604912
H	-5.943197	3.768730	2.228038
H	-4.368221	4.830975	1.524630
H	-6.271545	5.400415	1.133785
H	-5.560449	5.558222	2.992414
H	-9.088250	6.861349	3.768449
H	-8.791074	8.690765	3.011550
H	-7.292838	7.360252	3.053992
H	-5.803199	5.099030	7.407979
H	-4.081999	5.498627	7.349914
H	-5.017153	5.377092	5.842476
H	-3.365722	3.729602	4.917146
H	-2.396543	3.792646	6.398214
H	-2.985483	2.232346	5.793138
H	-4.604895	1.062689	10.007102
H	-2.888123	1.483547	9.847419
H	-3.493937	-0.055068	9.151761
H	-10.183717	2.573467	4.294025
H	-10.294032	1.150544	3.216932
H	-11.746422	2.134473	3.536271
H	-11.096524	1.457279	0.481020
H	-12.359779	2.654431	0.875042
H	-11.100347	3.031619	-0.336982
H	-11.268825	4.980838	3.297999
H	-11.417788	7.748186	3.073323
H	-12.658978	7.186419	1.910954
H	-11.490342	8.465034	1.448084
H	-11.881630	5.593280	-0.415522
H	-10.156570	5.290734	-0.778711
H	-10.816819	6.940390	-0.896552
H	-8.903868	8.978155	-0.202300
H	-8.052628	6.890053	-1.084227
H	-6.736457	8.140304	0.565016
H	-6.958241	1.137437	1.733175
H	-8.693610	0.982923	0.064738
H	-6.837780	2.504155	-0.278023
H	-10.858440	4.630444	6.995948
H	-9.245473	5.222521	7.477821
H	-9.814272	5.454927	5.802401
H	-8.457682	2.124320	8.051815
H	-7.083529	1.035774	7.779469
H	-6.861219	2.524328	8.695568

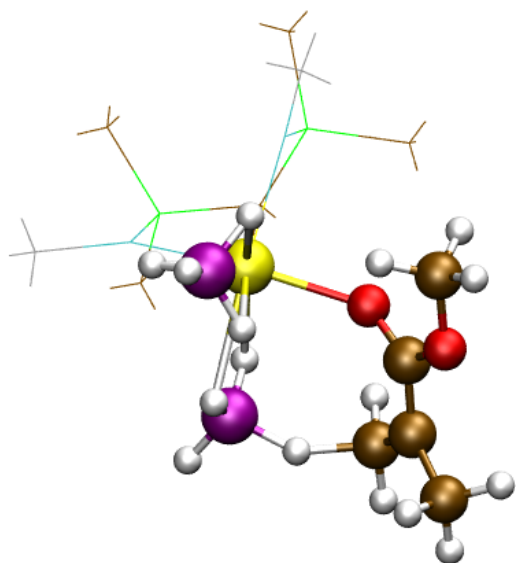
H	-5.670801	3.032987	4.957548
H	-5.383395	1.624281	5.977010

Energy = -1116.214288 H

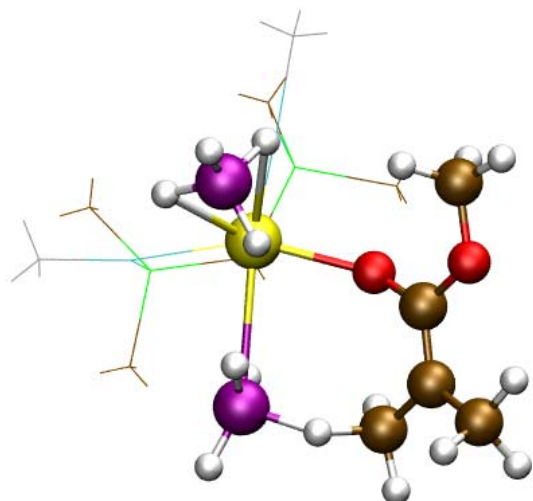
Add A



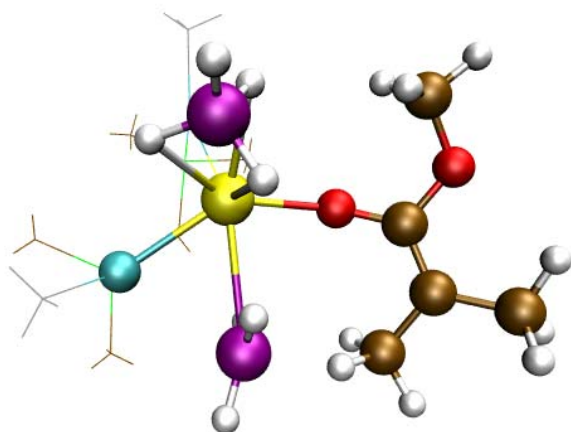
TSAB Nucleophilic attack



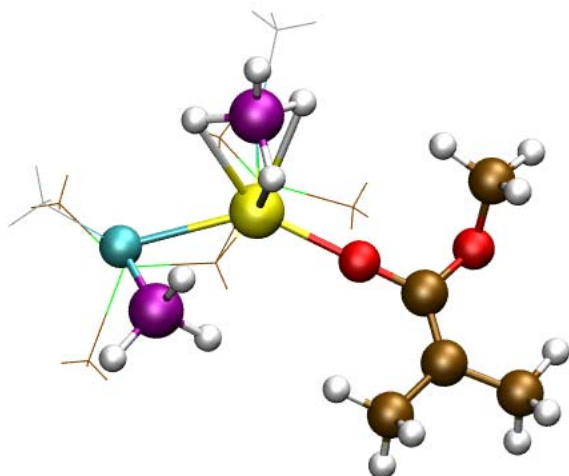
Add B



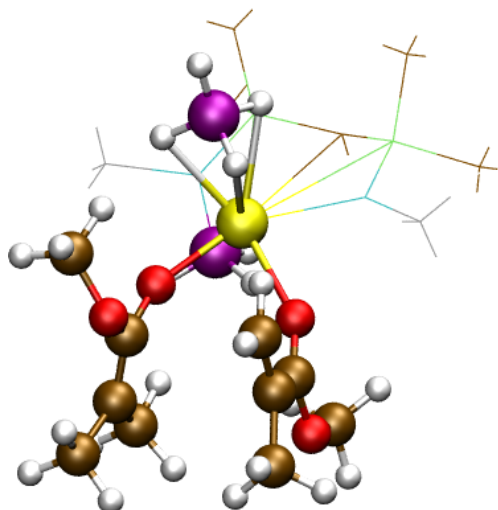
TSBC Trapping



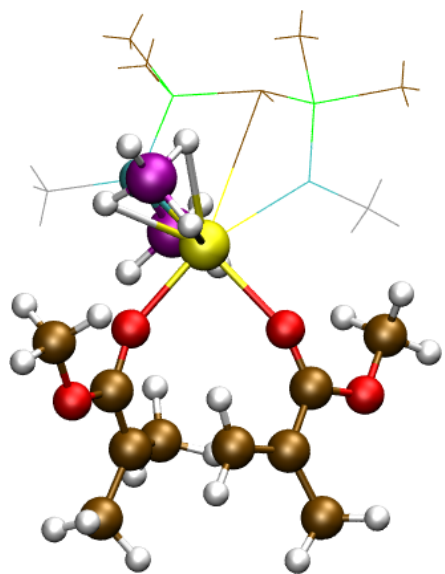
Add C



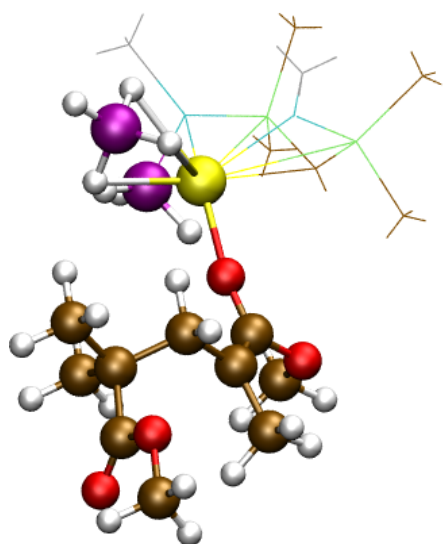
Add D (2nd insertion)



TSDP 2nd insertion



Product



Lanthanum complexes

Add A

C	-10.582325	3.426839	-1.039043
P	-10.375351	3.253942	0.791384
C	-11.598015	1.948378	1.233011
N	-8.825163	2.836729	1.172176
Si	-7.864864	1.659618	0.319313
C	-10.809758	4.645086	1.775004
P	-10.244991	6.303275	1.539010
C	-10.442334	6.975389	-0.172413
C	-11.374255	7.345828	2.550029
Si	-7.637344	7.770079	1.913675
N	-8.675972	6.365435	2.026732

La	-8.359154	4.187949	3.296644
O	-7.962480	1.764137	4.209574
C	-7.639459	0.857547	4.978172
O	-6.430543	0.314224	4.976472
C	-5.465873	0.845311	4.049769
C	-8.530175	0.238404	5.993711
C	-8.041065	-0.981701	6.721864
C	-9.711203	0.826197	6.225923
B	-5.697004	4.604876	3.536090
H	-5.960838	3.865514	2.573335
H	-4.515664	4.811246	3.624669
H	-6.327580	5.660086	3.374534
H	-6.149820	4.068267	4.557279
B	-9.840403	4.584067	5.532697
H	-8.694055	4.203579	5.809088
H	-10.354962	3.731086	4.789652
H	-9.738500	5.625820	4.868549
H	-10.496162	4.755210	6.526915
H	-10.008839	1.730026	5.704446
H	-10.391893	0.426599	6.972077
H	-7.127431	-0.765075	7.284409
H	-8.801664	-1.338207	7.420208
H	-7.799304	-1.792504	6.026862
H	-5.330068	1.916174	4.209153
H	-5.795602	0.669599	3.023767
H	-4.545025	0.300672	4.253539
H	-11.592606	1.818754	2.317311
H	-11.307534	1.008965	0.756703
H	-12.599979	2.233226	0.901726
H	-10.431636	2.457022	-1.521783
H	-11.586338	3.794095	-1.265240
H	-9.836795	4.124870	-1.423963
H	-11.796262	4.576437	2.227000
H	-11.332133	6.991080	3.582164
H	-12.398170	7.284098	2.172133
H	-11.030180	8.382240	2.507623
H	-11.477746	6.863255	-0.503772
H	-9.775159	6.436921	-0.848055
H	-10.166790	8.033117	-0.178151
H	-8.367018	8.924997	1.274165
H	-6.430456	7.493550	1.076713
H	-7.192376	8.233645	3.262433
H	-8.425017	0.264892	0.404229
H	-7.729139	1.965753	-1.145446
H	-6.496797	1.642882	0.914221

Energy = - 763.885310 H

TSAB Nucleophilic attack

C	-10.318864	3.760467	-1.379976
P	-10.064795	3.159562	0.350076
C	-11.082618	1.627442	0.424949
N	-8.467956	2.878049	0.648760
Si	-7.390056	2.030827	-0.439850
C	-10.675386	4.190042	1.647481
P	-10.391820	5.931683	1.814097
C	-10.699137	6.949990	0.300480
C	-11.672425	6.525168	2.993581
Si	-8.066028	7.688231	2.551421
N	-8.852786	6.137806	2.358749
La	-8.113925	3.779945	2.978956
O	-8.312088	1.647935	4.077295
C	-8.017073	1.030990	5.160454
O	-6.969122	0.186705	5.172052
C	-6.227812	0.039852	3.963288
C	-8.695249	1.189389	6.374985
C	-8.122704	0.645362	7.656031
C	-9.826765	2.039852	6.352411
B	-5.446621	4.042956	2.915517
H	-5.847159	3.136289	2.163981
H	-4.253731	4.168072	2.861904
H	-6.029138	5.083566	2.569609
H	-5.836872	3.762890	4.060488
B	-9.356167	4.523451	5.685755
H	-8.145760	4.570497	5.530990
H	-10.006057	4.340090	4.666927
H	-9.818896	5.344731	6.430317
H	-9.479552	3.345015	6.343031
H	-10.422120	2.056087	5.443378
H	-10.430291	2.083436	7.259211
H	-7.226269	1.189259	7.983631
H	-8.858145	0.705095	8.464169
H	-7.832714	-0.404460	7.546794
H	-5.767173	0.984774	3.662212
H	-6.863538	-0.326565	3.152178
H	-5.452019	-0.693302	4.187099
H	-11.020437	1.217634	1.435349
H	-10.678517	0.900214	-0.283210
H	-12.124362	1.843708	0.174012
H	-10.011039	2.979129	-2.080910
H	-11.371163	4.004232	-1.546101
H	-9.701868	4.644622	-1.549342
H	-11.651840	3.881091	2.015805
H	-11.570664	5.965121	3.925018
H	-12.672405	6.386946	2.574061
H	-11.500992	7.585580	3.192954
H	-11.689191	6.733931	-0.108784
H	-9.932076	6.733709	-0.445202
H	-10.639340	8.010337	0.563708

H	-9.025896	8.747162	3.025281
H	-7.479235	8.195811	1.266756
H	-6.974840	7.557007	3.557494
H	-8.157602	1.122882	-1.365596
H	-6.599424	2.963062	-1.305134
H	-6.442864	1.184767	0.342375

Energy = -763.859781 H

Add B

C	-10.378053	3.692772	-1.399460
P	-10.064073	3.156393	0.342328
C	-10.664444	4.215164	1.621035
P	-10.389130	5.962923	1.737779
C	-11.697253	6.587004	2.871290
La	-8.083225	3.843188	2.925569
O	-8.343646	1.801824	4.090941
C	-8.089925	1.161091	5.184695
O	-7.081649	0.259099	5.182538
C	-6.339916	0.103953	3.979550
C	-11.040003	1.603868	0.498759
N	-8.452108	2.922400	0.605625
Si	-7.387406	2.102529	-0.517422
B	-5.423054	4.160173	2.873944
N	-8.863542	6.195396	2.307546
Si	-8.089068	7.754599	2.474465
C	-10.669000	6.930684	0.186385
C	-8.774882	1.351767	6.373645
C	-8.305101	0.772252	7.679355
C	-9.869237	2.286191	6.336271
B	-9.312449	4.693688	5.667245
H	-5.800866	3.206459	2.170243
H	-4.231807	4.300930	2.825573
H	-6.018003	5.170563	2.465533
H	-5.821517	3.934942	4.028356
H	-8.105293	4.664189	5.533304
H	-9.980644	4.526941	4.667454
H	-9.752269	5.469189	6.468287
H	-9.462275	3.470257	6.355523
H	-10.472929	2.283918	5.430701
H	-10.491044	2.316419	7.233566
H	-7.813444	1.524738	8.313323
H	-9.137548	0.357329	8.261139
H	-7.584121	-0.029787	7.511490
H	-5.829258	1.030143	3.698604
H	-6.980814	-0.217959	3.152954
H	-5.599827	-0.668959	4.192630
H	-10.929466	1.227739	1.518085
H	-10.643966	0.865072	-0.201791

H	-12.095567	1.786489	0.281242
H	-10.078852	2.893199	-2.083567
H	-11.438728	3.914365	-1.541652
H	-9.781625	4.580447	-1.616778
H	-11.636796	3.912799	2.005579
H	-11.624361	6.046484	3.816753
H	-12.686624	6.443476	2.429135
H	-11.526416	7.650621	3.053194
H	-11.647547	6.695530	-0.239572
H	-9.882311	6.696861	-0.533311
H	-10.621568	7.999182	0.417101
H	-9.057915	8.813772	2.929741
H	-7.502185	8.246840	1.184001
H	-7.000551	7.646921	3.486401
H	-8.126615	1.047516	-1.298165
H	-6.786422	3.035813	-1.524842
H	-6.287182	1.435489	0.234430

Energy = -763.860070 H

TSBC Trapping

C	-10.448322	3.885661	-1.526979
P	-10.161450	3.172733	0.155028
C	-10.696965	4.134199	1.531311
P	-10.370118	5.842025	1.872055
C	-11.833540	6.473558	2.787436
La	-8.126753	3.510266	2.777372
O	-8.277439	1.723410	4.202130
C	-7.963073	1.254835	5.391176
O	-6.941714	0.348017	5.448566
C	-6.149628	0.169731	4.289188
C	-11.237844	1.679200	0.168320
N	-8.568062	2.812610	0.381969
Si	-7.544643	2.039323	-0.811102
B	-5.512080	4.060120	2.538965
N	-8.977254	5.949370	2.756474
Si	-8.134314	7.438532	3.140164
C	-10.267603	6.916867	0.375020
C	-8.586568	1.593239	6.556447
C	-8.100076	1.116281	7.896221
C	-9.785141	2.464075	6.505865
B	-9.488913	4.811736	5.115504
H	-5.799678	2.940340	2.079608
H	-4.341451	4.300297	2.423155
H	-6.208692	4.892593	1.937496
H	-5.869083	4.060199	3.729384
H	-8.290342	4.712104	5.156557
H	-10.146311	4.129769	4.380003
H	-10.022948	5.681295	5.734892

H	-9.529492	3.572595	6.368120
H	-10.468990	2.220575	5.688537
H	-10.342400	2.453517	7.448322
H	-7.917790	1.958350	8.579228
H	-8.830728	0.461500	8.393737
H	-7.167093	0.558104	7.801834
H	-5.635102	1.091888	3.994447
H	-6.740350	-0.195376	3.442069
H	-5.404035	-0.582130	4.556510
H	-11.178209	1.211085	1.153309
H	-10.874525	0.976054	-0.584696
H	-12.273852	1.949368	-0.052014
H	-10.187221	3.138893	-2.282882
H	-11.498791	4.164613	-1.642106
H	-9.814592	4.762420	-1.669294
H	-11.649804	3.803767	1.939327
H	-11.985390	5.851510	3.671371
H	-12.720718	6.444046	2.150169
H	-11.637132	7.500129	3.105313
H	-11.161472	6.796347	-0.241270
H	-9.376487	6.651485	-0.197655
H	-10.177608	7.961317	0.686786
H	-9.059953	8.463911	3.735950
H	-7.520134	8.073224	1.927507
H	-7.061196	7.129324	4.124329
H	-8.303339	1.005970	-1.601065
H	-6.985842	3.010896	-1.807026
H	-6.416948	1.359901	-0.113331

Energy = -763.850196 H

Add C

C	-10.932279	2.997629	-0.437000
P	-9.981894	2.987337	1.151872
C	-10.453557	4.195106	2.347851
P	-10.375794	5.926456	2.108801
C	-11.701537	6.709534	3.100249
La	-7.568785	4.155955	3.112364
O	-7.888438	2.358584	4.386377
C	-8.195470	1.157817	4.859907
O	-7.330562	0.148814	4.502297
C	-5.952271	0.434444	4.682613
C	-10.423665	1.362938	1.886472
N	-8.366816	3.201702	0.889432
Si	-7.493129	2.522086	-0.470280
B	-4.982533	4.595379	2.523823
N	-8.858661	6.536423	2.598823
Si	-8.105203	7.984523	1.875289
C	-10.636590	6.474091	0.375916

C	-9.297050	0.856843	5.587027
C	-9.554492	-0.527480	6.108425
C	-10.319435	1.903391	5.921984
B	-8.662626	6.513183	4.196084
H	-5.325401	3.421497	2.297126
H	-3.822485	4.773287	2.271868
H	-5.718636	5.331868	1.844726
H	-5.233219	4.819336	3.721841
H	-7.451485	6.411106	4.398780
H	-9.224429	5.501311	4.627225
H	-9.097631	7.492924	4.754067
H	-10.432032	2.014670	7.009878
H	-10.048251	2.880914	5.516093
H	-11.316771	1.635244	5.539602
H	-9.675572	-0.521999	7.201339
H	-10.485957	-0.947067	5.699669
H	-8.740490	-1.209001	5.857414
H	-5.731603	0.679411	5.730347
H	-5.613530	1.258099	4.045320
H	-5.413020	-0.473931	4.405904
H	-9.967169	1.266440	2.876137
H	-10.039305	0.573503	1.235802
H	-11.510158	1.269759	1.967915
H	-10.665224	2.113696	-1.023994
H	-12.003683	2.974863	-0.221580
H	-10.690423	3.888321	-1.018596
H	-11.178512	3.876095	3.091256
H	-11.578995	6.410010	4.142440
H	-12.675627	6.385284	2.727444
H	-11.609931	7.795575	3.030394
H	-11.603631	6.098945	0.034780
H	-9.839852	6.076666	-0.255991
H	-10.630531	7.565618	0.317247
H	-8.973188	9.189645	2.079227
H	-7.927587	7.786055	0.405440
H	-6.792225	8.176037	2.538338
H	-7.789739	1.061889	-0.670866
H	-7.855965	3.205018	-1.759187
H	-6.035052	2.694744	-0.230179

Energy = -763.899989 H

Add D (2nd insertion)

C	-9.919731	6.264424	-0.375617
P	-10.003619	6.262125	1.453781
C	-11.272801	7.503735	1.915415
N	-8.497418	6.810601	2.051755
B	-8.498740	7.123286	3.623671
La	-7.564442	4.448734	3.123273

B	-6.444682	4.296293	0.630489
C	-10.477481	4.738538	2.138513
P	-10.275972	3.047007	1.698279
C	-10.249089	2.776105	-0.121524
Si	-7.443150	7.940394	1.160817
O	-5.679838	4.058039	4.274914
C	-4.611543	3.857074	5.032983
C	-4.380952	4.417477	6.244364
C	-5.369295	5.349927	6.879303
N	-8.941696	2.418475	2.429553
Si	-8.394649	0.766420	2.343236
O	-8.615632	3.810509	5.434074
C	-8.732752	3.374734	6.579033
O	-9.654630	3.853714	7.414597
C	-10.469050	4.926937	6.927647
O	-3.716469	2.931086	4.545363
C	-3.310077	3.137811	3.200004
C	-11.806398	2.197729	2.273505
C	-7.922209	2.298407	7.192442
C	-6.844033	1.872642	6.517665
C	-8.330266	1.776266	8.542169
C	-3.128676	4.138482	7.024811
H	-6.223489	3.267212	1.276620
H	-5.973051	4.242257	-0.476017
H	-7.678750	4.433399	0.583386
H	-5.997368	5.257684	1.272680
H	-9.236446	6.300470	4.166024
H	-8.854304	8.246594	3.905154
H	-7.346551	6.936101	4.020242
H	-4.896137	6.305459	7.146623
H	-6.207333	5.571988	6.215241
H	-5.776944	4.936886	7.815443
H	-3.353064	3.662093	7.991299
H	-2.451312	3.482285	6.476322
H	-2.592369	5.069387	7.260941
H	-2.787050	4.098026	3.090515
H	-4.155776	3.112923	2.507035
H	-2.619623	2.326184	2.959209
H	-11.913827	2.371213	3.346601
H	-11.714231	1.122453	2.100524
H	-12.679403	2.588296	1.745730
H	-10.217411	1.699407	-0.307706
H	-11.138201	3.203454	-0.590005
H	-9.341288	3.222577	-0.530916
H	-11.055938	4.854862	3.051873
H	-11.336885	7.539687	3.004432
H	-12.238064	7.221171	1.490461
H	-10.965485	8.486606	1.550472
H	-10.855592	5.860723	-0.766162
H	-9.074986	5.656838	-0.704059

H	-9.787578	7.287951	-0.734036
H	-8.079489	9.298710	1.106012
H	-7.225917	7.477001	-0.238849
H	-6.154627	8.026863	1.894576
H	-9.336679	-0.186494	3.028221
H	-8.233125	0.258360	0.938649
H	-7.072662	0.684875	3.032445
H	-11.082181	5.233660	7.774426
H	-9.849012	5.753870	6.576119
H	-11.101997	4.580538	6.106540
H	-8.310626	2.568250	9.297544
H	-9.349986	1.377123	8.527464
H	-7.652884	0.980293	8.859605
H	-6.202564	1.098166	6.926894
H	-6.563157	2.301794	5.562370

Energy = -1109.454139 H

TSDP 2nd insertion

C	-9.968338	6.369624	-0.331942
P	-10.025981	6.307934	1.497155
C	-11.304679	7.514891	2.018160
N	-8.516753	6.852237	2.090146
B	-8.503141	7.133977	3.667259
La	-7.585010	4.477079	3.109687
B	-6.433740	4.412488	0.620197
C	-10.457343	4.754035	2.143393
P	-10.253383	3.084724	1.619324
C	-10.262625	2.894958	-0.210820
Si	-7.479395	8.006870	1.209039
O	-5.492717	4.177882	4.100750
C	-4.664009	3.812289	5.018226
C	-4.735827	4.158471	6.361092
C	-5.613697	5.293386	6.781683
N	-8.894398	2.451820	2.292535
Si	-8.309950	0.819606	2.151052
O	-8.489210	3.692776	5.306243
C	-8.484152	3.413312	6.529496
O	-9.539412	3.743725	7.295882
C	-10.605060	4.445954	6.663807
O	-3.664916	2.965756	4.656852
C	-3.595191	2.589037	3.286764
C	-11.758775	2.189599	2.188702
C	-7.441679	2.734619	7.248208
C	-6.360753	2.285600	6.533548
C	-7.565133	2.561701	8.740974
C	-3.666790	3.725742	7.327563
H	-6.204096	3.372946	1.247539
H	-5.957355	4.384100	-0.485625

H	-7.670297	4.535826	0.571149
H	-6.003475	5.365232	1.284522
H	-9.220563	6.287224	4.201214
H	-8.872313	8.244152	3.978324
H	-7.343079	6.953141	4.042728
H	-5.047554	6.023826	7.373917
H	-6.043435	5.821276	5.926206
H	-6.452894	4.952811	7.412209
H	-4.093149	3.553842	8.323886
H	-3.168725	2.808892	7.005439
H	-2.891708	4.497438	7.447722
H	-3.542885	3.462696	2.632082
H	-4.454887	1.981516	2.986883
H	-2.682905	1.996872	3.194788
H	-11.841272	2.309506	3.271174
H	-11.656569	1.125315	1.961769
H	-12.649482	2.592075	1.700869
H	-10.236107	1.827330	-0.444488
H	-11.160615	3.341546	-0.643084
H	-9.362680	3.358488	-0.618423
H	-11.040885	4.827855	3.057845
H	-11.354079	7.513718	3.108549
H	-12.271731	7.232054	1.597351
H	-11.016929	8.513654	1.681488
H	-10.906698	5.971696	-0.722438
H	-9.124046	5.779372	-0.691675
H	-9.848755	7.405190	-0.659026
H	-8.135723	9.356421	1.178700
H	-7.265749	7.566823	-0.198410
H	-6.188871	8.100395	1.937702
H	-9.241183	-0.185126	2.771236
H	-8.089026	0.375645	0.733159
H	-7.003773	0.741741	2.874606
H	-11.313677	4.679909	7.459161
H	-10.245821	5.364324	6.192400
H	-11.088807	3.820140	5.907617
H	-7.667797	3.516790	9.267134
H	-8.443165	1.960428	9.004225
H	-6.680511	2.053845	9.134227
H	-5.595312	1.686016	7.014764
H	-6.413716	2.229276	5.453660

Energy = -1109.447822 H

Product

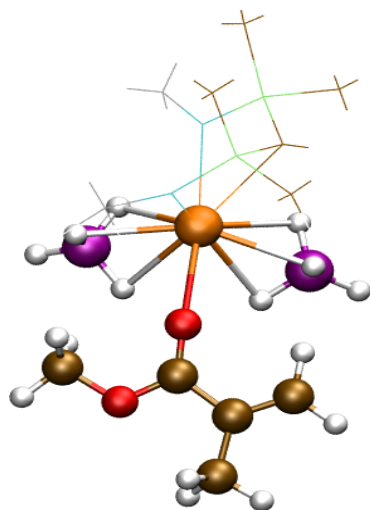
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P	-9.988813	6.328221	1.322496
C	-11.187461	7.673502	1.663295
N	-8.466275	6.794545	1.931784

B	-8.478633	7.207631	3.482726
La	-7.831252	4.433507	3.228678
B	-6.365238	4.060475	0.906764
C	-10.556688	4.876365	2.095576
P	-10.524376	3.162220	1.676484
C	-10.576148	2.843179	-0.136494
Si	-7.301827	7.778968	1.008477
O	-5.482763	4.400379	4.236695
C	-4.653381	3.991020	5.053035
C	-4.985807	3.667837	6.492728
C	-5.512286	4.977160	7.110503
N	-9.219659	2.464973	2.378787
Si	-8.743552	0.792846	2.315064
O	-8.383597	3.820006	5.356206
C	-8.387002	3.432065	6.608607
O	-9.512169	3.730161	7.341095
C	-10.695809	3.989551	6.617590
O	-3.390884	3.807215	4.700644
C	-3.055478	4.106342	3.331951
C	-12.104133	2.463485	2.313089
C	-7.363823	2.794658	7.238859
C	-6.105839	2.531525	6.470368
C	-7.447970	2.362867	8.675419
C	-3.759670	3.183241	7.273538
H	-6.301481	3.098567	1.691202
H	-5.689241	3.862219	-0.071554
H	-7.560811	4.213909	0.618780
H	-5.996884	5.072385	1.517237
H	-9.298931	6.490275	4.056753
H	-8.739018	8.373390	3.678985
H	-7.356683	6.942984	3.920710
H	-4.739243	5.754053	7.083498
H	-6.396106	5.338975	6.583491
H	-5.788072	4.803315	8.152845
H	-4.060884	2.951935	8.299854
H	-3.333486	2.276740	6.833948
H	-2.971875	3.941759	7.311817
H	-3.160285	5.177543	3.147168
H	-3.708597	3.562448	2.647603
H	-2.017599	3.796543	3.216947
H	-12.158348	2.659489	3.386136
H	-12.111287	1.382305	2.153456
H	-12.956853	2.921594	1.806502
H	-10.639283	1.762676	-0.291291
H	-11.440677	3.328135	-0.595368
H	-9.647840	3.198253	-0.586828
H	-11.212046	5.081898	2.938583
H	-11.279316	7.783975	2.745599
H	-12.157300	7.424250	1.227598
H	-10.808587	8.609242	1.245373

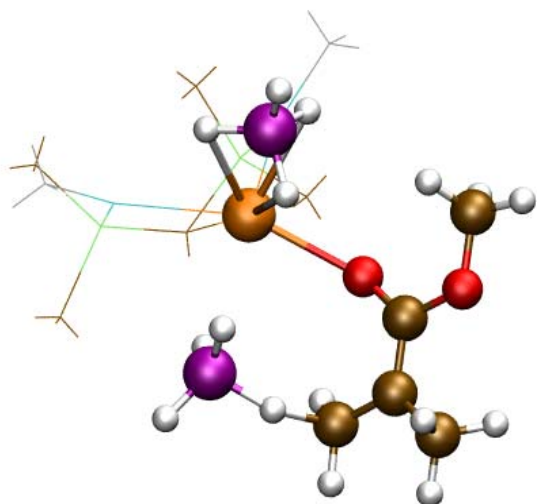
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H	-9.029304	5.525382	-0.755414
H	-9.621227	7.195930	-0.910648
H	-7.847517	9.163368	0.810829
H	-7.049244	7.190452	-0.337708
H	-6.045290	7.854118	1.796153
H	-9.781804	-0.125691	2.898295
H	-8.477147	0.299665	0.921341
H	-7.489913	0.643547	3.114220
H	-11.457361	4.225450	7.365008
H	-10.582453	4.838350	5.934998
H	-11.021765	3.112023	6.042035
H	-6.808068	2.960184	9.344335
H	-8.469650	2.447217	9.051462
H	-7.127372	1.317962	8.796097
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H	-6.365273	2.321832	5.426232

Energy = -1109.474022 H

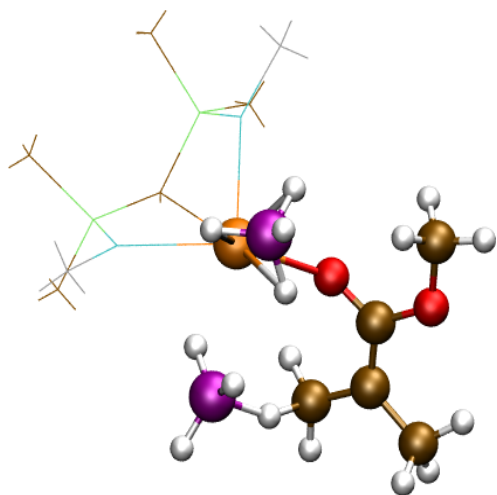
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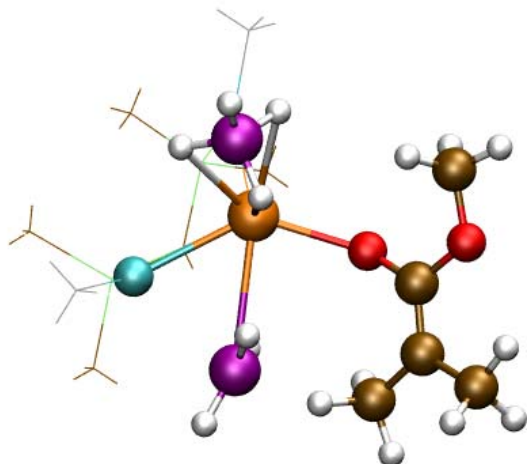
TSAB Nucleophilic attack



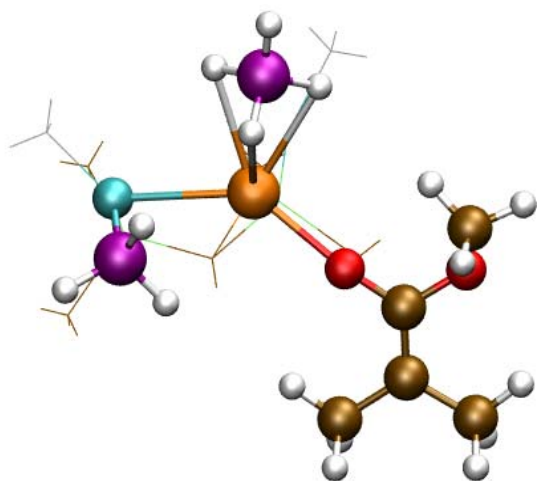
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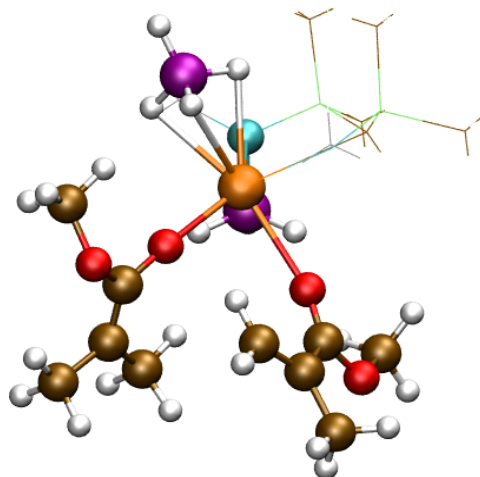
TSBC Trapping



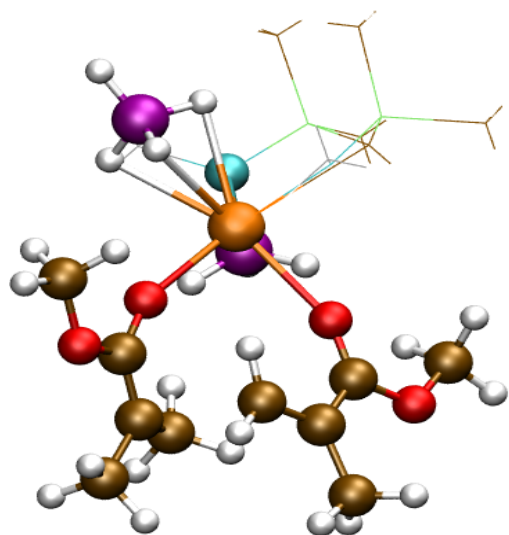
Add C



Add D (2nd insertion)



TSDE 2nd insertion



Add E

