Supporting Information for:

Comparison of the mechanism of borane, silane and beryllium hydride ring insertion into N-heterocyclic carbene C-N bonds: a computational study

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Cartesian coordinates for precursor NHC optimized geometries

Me_2NHC

M062x/def2-TZVP optimized geometry (Å).
E_e = -304.776887626 (Hartrees)

0 1

C	-0.674417	1.204753	-0.000014
N	-1.055682	-0.122724	-0.000002
C	0.000000	-0.978476	-0.000033
C	-2.433266	-0.565397	0.000023
H	-2.427118	-1.651394	-0.000048
H	-2.952441	-0.204462	0.888646
H	-2.952502	-0.204344	-0.888516
N	1.055682	-0.122723	-0.000003
C	0.674417	1.204753	0.000015
H	1.378772	2.018562	0.000031
C	2.433266	-0.565397	-0.000001
H	2.952464	-0.204434	-0.888599
H	2.952479	-0.204373	0.888563
H	2.427118	-1.651394	0.000035
H	-1.378772	2.018562	-0.000010

Ph_2NHC

M062x/def2-TZVP optimized geometry (Å).
E_e = -688.242854546 (Hartrees)

0 1

C	-0.671911	-1.838655	0.004946
C	0.671911	-1.838655	-0.004947
C	0.000000	0.351030	0.000000
H	-1.368747	-2.656405	0.033056
H	1.368747	-2.656405	-0.033057
N	1.058610	-0.504615	-0.009686
N	-1.058610	-0.504615	0.009686
C	-2.409472	-0.063418	0.023576
C	-2.722568	1.157999	0.607826
C	-3.407447	-0.843250	-0.545804
C	-4.037806	1.591493	0.620143
C	-4.723609	-0.403850	-0.518600
C	-5.044396	0.812805	0.063411
H	-4.278135	2.543205	1.076181
H	-5.497155	-1.013792	-0.966813
H	-6.070763	1.154664	0.079893
C	2.409472	-0.063418	-0.023576
C	3.407447	-0.843250	0.545804
C	2.722569	1.157999	-0.607826
C	4.723609	-0.403850	0.518601
C	4.037806	1.591493	-0.620143
C	5.044396	0.812805	-0.063411
H	5.497155	-1.013792	0.966814
H	4.278136	2.543204	-1.076181
H	6.070763	1.154664	-0.079893
H	1.925700	1.749164	-1.036315
H	3.158220	-1.776364	1.033302
H	-3.158221	-1.776364	-1.033301
H	-1.925700	1.749164	1.036314

Cartesian coordinates for precursor silicon optimized geometry

Ph_2SiH_2

M062x/def2-TZVP optimized geometry (Å).
E_e = -753.950242086 (Hartrees)

0 1

Si	0.000000	0.000000	1.548782
H	-1.167494	0.267033	2.420418
H	1.167494	-0.267033	2.420418
C	0.267002	1.516048	0.487584
C	0.970985	1.447628	-0.717794
C	-0.217171	2.760249	0.897290
C	1.187966	2.583596	-1.484237
H	1.348331	0.492275	-1.067403
C	0.000000	3.900766	0.136606
H	-0.776449	2.840707	1.823149
C	0.703770	3.812770	-1.056178
H	1.734122	2.511313	-2.416294
H	-0.382818	4.856280	0.472204
H	0.873129	4.700004	-1.653175
C	-0.267002	-1.516048	0.487584
C	-0.970985	-1.447628	-0.717794
C	0.217171	-2.760249	0.897290
C	-1.187966	-2.583596	-1.484237
H	-1.348331	-0.492275	-1.067403
C	0.000000	-3.900766	0.136606
H	0.776449	-2.840707	1.823149
C	-0.703770	-3.812770	-1.056178
H	-1.734122	-2.511313	-2.416294
H	0.382818	-4.856280	0.472204
H	-0.873129	-4.700004	-1.653175

Cartesian coordinates for precursor boron optimized geometries

BH_3

M062x/def2-TZVP optimized geometry (Å).
E_e = -26.5950570853 (Hartrees)

0 1

B	0.000000	0.000000	0.000000
H	0.000000	1.186940	0.000000
H	1.027920	-0.593470	0.000000
H	-1.027920	-0.593470	0.000000

BH_2NHMe

M062x/def2-TZVP optimized geometry (Å).
E_e = -121.327126394 (Hartrees)

0 1

B	-1.354648	0.253568	-0.000046
H	-1.345401	1.445803	0.000007
N	-0.144862	-0.421473	-0.000016
H	-0.142072	-1.429917	0.000042
C	1.178345	0.171869	0.000025
H	1.075266	1.255138	-0.000089
H	1.746904	-0.121287	0.884917
H	1.747023	-0.121462	-0.884733
H	-2.364513	-0.377020	0.000050

BCl_3

M062x/def2-TZVP optimized geometry (Å).
E_e = -1405.56984654 (Hartrees)

0 1

B	0.000000	0.000000	0.000000
Cl	0.000000	1.739262	0.000000
Cl	1.506245	-0.869631	0.000000
Cl	-1.506245	-0.869631	0.000000

Cartesian coordinates for precursor beryllium optimized geometries

BeH_2

M062x/def2-TZVP optimized geometry (Å).
E_e = -15.8968123856 (Hartrees)

0 1

Be	0.082677	0.203071	-0.395724
H	0.069235	0.356832	-1.715583
H	0.096119	0.049310	0.924134

$BeCl_2$
M062x/def2-TZVP optimized geometry (Å).
E_e = -935.289572982 (Hartrees)

0 1

Be	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	1.799789
Cl	0.000000	0.000000	-1.799789

Cartesian coordinates for optimized silicon complexes

Me_2NHC/Ph_2SiH_2

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).

E_e = -1058.72615285 (Hartrees)

0 1

Si	0.089850	-0.213159	-0.024862
C	1.894429	-0.861709	-0.132605
C	2.621662	-1.166018	1.020094
C	2.524662	-1.048728	-1.363372
C	3.924408	-1.641931	0.951191
H	2.148427	-1.026153	1.987522
C	3.830499	-1.516384	-1.445770
H	1.973672	-0.824564	-2.270824
C	4.532740	-1.815295	-0.285890
H	4.466345	-1.881143	1.858320
H	4.300182	-1.651550	-2.412729
H	5.549283	-2.184412	-0.345208
C	-1.544667	-1.198639	0.155308
C	-2.149598	-1.805097	-0.947303
C	-2.183236	-1.319079	1.390187
C	-3.342003	-2.506099	-0.826845
H	-1.669387	-1.723404	-1.917956
C	-3.384284	-2.005897	1.521729
H	-1.721890	-0.868210	2.262780
C	-3.965342	-2.602965	0.411140
H	-3.786941	-2.977850	-1.694747
H	-3.864212	-2.082772	2.490057
H	-4.898094	-3.144636	0.509718
C	-0.219610	1.746353	-0.077460
C	-0.056271	3.936947	0.341157
C	-1.148022	3.749686	-0.434273
H	0.376208	4.833767	0.747132
H	-1.863153	4.448950	-0.829266
N	0.496264	2.695066	0.549091
N	-1.224214	2.399472	-0.684813
C	-2.280917	1.749011	-1.448447
H	-3.054783	1.378330	-0.777749
H	-2.701573	2.471265	-2.144241
H	-1.848749	0.911323	-1.990690
C	1.672061	2.433217	1.368587
H	2.264014	3.344003	1.422520
H	1.366980	2.119040	2.365078
H	2.259867	1.639458	0.913601
H	-0.033830	-0.197153	-1.580561
H	0.216311	-0.026067	1.520806

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).

E_e = -1058.70420901 (Hartrees)

0 1

Si	-0.000024	-0.065580	-0.646475
C	-1.598148	-0.951288	-0.189933
C	-2.431731	-1.396918	-1.218164
C	-1.968347	-1.245066	1.124632
C	-3.608060	-2.084732	-0.946956
H	-2.157193	-1.199229	-2.248866
C	-3.134915	-1.942971	1.402836
H	-1.337761	-0.908646	1.939505
C	-3.961767	-2.357950	0.366378
H	-4.245022	-2.409982	-1.760094
H	-3.400522	-2.164457	2.429190
H	-4.875043	-2.897970	0.582857
C	1.598008	-0.951442	-0.189947
C	1.968128	-1.245293	1.124625
C	2.431603	-1.397099	-1.218157
C	3.134626	-1.943300	1.402857
H	1.337537	-0.908842	1.939483
C	3.607867	-2.085012	-0.946919
H	2.157123	-1.199360	-2.248865
C	3.961494	-2.358306	0.366421
H	3.400173	-2.164839	2.429216
H	4.244836	-2.410286	-1.760042
H	4.874719	-2.898404	0.582919
C	0.000113	1.770372	-0.291367
C	-0.670027	3.800321	0.413066
C	0.670515	3.800238	0.413051
H	-1.371567	4.565497	0.693750
H	1.372153	4.565328	0.693726
N	-1.089287	2.599938	-0.148133
N	1.089620	2.599804	-0.148155
C	2.447365	2.125382	-0.049217
H	2.689813	1.487812	-0.897047
H	3.116025	2.983894	-0.046015
H	2.583196	1.547747	0.871588
C	-2.447093	2.125692	-0.049196
H	-3.115646	2.984289	-0.046034
H	-2.689611	1.488119	-0.897003
H	-2.583007	1.548109	0.871631
H	0.000058	0.786388	1.055498
H	-0.000057	-0.251001	-2.144794

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -1058.75214088 (Hartrees)

0 1			
Si	0.090443	-0.016144	0.986195
C	-0.960847	1.391125	0.357352
C	-0.729677	2.675070	0.860185
C	-1.956333	1.227033	-0.608931
C	-1.468674	3.762817	0.419109
H	0.040432	2.830182	1.609722
C	-2.697430	2.314739	-1.053038
H	-2.154426	0.243127	-1.016259
C	-2.456465	3.581402	-0.540084
H	-1.277791	4.748824	0.823689
H	-3.466460	2.171782	-1.801782
H	-3.037540	4.427396	-0.885478
C	1.873569	0.221459	0.468661
C	2.214039	1.040142	-0.610291
C	2.893868	-0.490028	1.106592
C	3.529921	1.138879	-1.043629
H	1.439445	1.603075	-1.119934
C	4.209602	-0.396508	0.676610
H	2.658345	-1.127350	1.953193
C	4.528042	0.418202	-0.402452
H	3.776963	1.777390	-1.882447
H	4.987458	-0.954034	1.183024
H	5.553982	0.494305	-0.739885
C	-0.549786	-1.685951	0.336227
C	-2.511755	-2.535172	-0.476891
C	-1.657221	-2.492056	-1.495154
H	-3.521782	-2.911771	-0.455915
H	-1.796105	-2.829480	-2.509529
N	-1.984134	-1.847287	0.636700
N	-0.489294	-1.778853	-1.136136
C	0.757881	-2.318528	-1.645573
H	0.968384	-3.311052	-1.218860
H	0.693218	-2.407238	-2.729775
H	1.584307	-1.651651	-1.404365
C	-2.260346	-2.397836	1.945685
H	-3.336599	-2.510899	2.072366
H	-1.779164	-3.377780	2.086981
H	-1.897239	-1.717925	2.716701
H	0.009054	-2.550744	0.771352
H	0.052982	-0.065903	2.470251

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -1058.70422546 (Hartrees)

0 1			
C	0.500650	-1.933677	0.090837
C	2.238035	-1.309855	-1.268529
C	2.748825	-0.829052	-0.113579
H	0.119868	-2.835473	0.576112
H	2.673054	-1.214290	-2.249587
H	3.719349	-0.343542	-0.080695
C	1.345972	-3.547786	-1.510050
H	1.665229	-3.542081	-2.551111
H	2.117643	-4.033139	-0.904837
H	0.409559	-4.097247	-1.432945
C	2.744932	-1.149997	2.270916
H	3.280963	-2.102440	2.307875
H	3.475343	-0.344418	2.411686
H	2.039306	-1.113215	3.101528
N	1.137786	-2.169007	-1.073463
N	2.020884	-0.961123	1.028761
Si	-0.037206	-0.293357	0.814437
H	-0.033451	-0.337385	2.298299
C	0.539790	1.338625	0.070919
C	1.580325	2.061152	0.660610
C	-0.091979	1.897229	-1.040236
C	1.981780	3.289582	0.159775
H	2.085765	1.651543	1.528785
C	0.322601	3.115796	-1.565911
H	-0.925933	1.378931	-1.500601
C	1.358447	3.815322	-0.965280
H	2.781290	3.837444	0.643218
H	-0.171104	3.522867	-2.439507
H	1.675573	4.769921	-1.366256
C	-1.914950	-0.273155	0.457019
C	-2.793494	0.398175	1.311113
C	-2.466988	-0.909139	-0.657951
C	-4.159151	0.438381	1.066660
H	-2.401794	0.898983	2.191797
C	-3.832868	-0.875697	-0.914848
H	-1.817793	-1.443232	-1.346750
C	-4.682387	-0.200743	-0.050166
H	-4.817708	0.965215	1.746437
H	-4.234768	-1.376822	-1.787105
H	-5.747435	-0.174684	-0.243352

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -1058.73198804 (Hartrees)

0 1			
C	-0.111702	1.987495	-1.243397
C	0.868702	3.135380	0.587002
C	0.630297	2.117648	1.475914
H	1.346345	4.054223	0.876791
H	0.941855	2.303192	2.504013
H	-0.513897	2.143029	-2.241167
C	0.440774	4.330242	-1.454937
H	-0.134501	5.082810	-0.919028
H	1.478622	4.651817	-1.526586
H	0.032260	4.177904	-2.448429
C	-0.204505	0.080663	2.333918
H	0.512038	0.255480	3.140970
H	-1.215787	0.225519	2.720428
H	-0.116658	-0.958925	2.017989
N	0.389772	3.065606	-0.708983
N	0.053203	0.963053	1.202763
Si	-0.039879	0.176904	-0.609965
C	-1.736885	-0.591906	-0.261060
C	-2.016824	-1.876887	-0.730293
C	-2.758213	0.092454	0.399411
C	-3.255316	-2.468879	-0.527374
H	-1.249457	-2.424339	-1.267660
C	-4.011796	-0.479611	0.582856
H	-2.569900	1.092516	0.777901
C	-4.259674	-1.766140	0.126148
H	-3.441889	-3.473371	-0.886809
H	-4.794148	0.076215	1.085353
H	-5.232158	-2.218760	0.275137
C	1.531826	-0.878554	-0.269694
C	2.463781	-0.694461	0.756590
C	1.769604	-1.941440	-1.148481
C	3.565064	-1.528529	0.904560
H	2.341797	0.121121	1.458979
C	2.850268	-2.798402	-0.995520
H	1.095457	-2.090429	-1.984308
C	3.756549	-2.592034	0.034361
H	4.274443	-1.348593	1.703280
H	2.992301	-3.618584	-1.688415
H	4.609236	-3.248868	0.153328
H	-0.030161	-0.241464	-2.088726

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -1058.72288155 (Hartrees)

0 1			
C	0.320746	-2.133005	-0.853051
C	2.134357	-2.479740	0.625104
C	1.698327	-1.573422	1.526789
H	-0.261074	-2.525200	-1.681927
H	3.053123	-3.020987	0.777535
H	2.319748	-1.428755	2.405985
H	0.488546	-0.606568	-1.824931
C	2.002924	-3.808407	-1.416929
H	2.882575	-3.397999	-1.917767
H	2.296763	-4.681262	-0.834916
H	1.269025	-4.098898	-2.164003
C	0.372611	0.136051	2.532905
H	0.421827	-0.382535	3.492451
H	1.114282	0.942545	2.522985
H	-0.616481	0.585918	2.442240
N	1.415236	-2.805585	-0.539372
N	0.569701	-0.809110	1.441818
Si	0.028293	-0.383130	-0.242339
C	0.912458	1.303797	-0.305873
C	0.333341	2.472018	0.198015
C	2.219436	1.393597	-0.794604
C	1.025786	3.677364	0.209942
H	-0.680064	2.446889	0.586255
C	2.925659	2.587734	-0.766787
H	2.691293	0.512996	-1.220532
C	2.327185	3.737187	-0.266769
H	0.548782	4.570128	0.595688
H	3.939050	2.626801	-1.147274
H	2.870209	4.673727	-0.255601
C	-1.818408	-0.118885	-0.232831
C	-2.629667	-0.908808	0.585098
C	-2.428759	0.848804	-1.033242
C	-4.007535	-0.738298	0.605428
H	-2.171121	-1.662844	1.217118
C	-3.806227	1.020293	-1.022103
H	-1.815089	1.477434	-1.670029
C	-4.596391	0.226642	-0.200334
H	-4.622433	-1.356988	1.247230
H	-4.263980	1.772959	-1.651697
H	-5.670696	0.361776	-0.187746

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -1058.80661076 (Hartrees)

0 1

C	0.755010	-1.491882	-1.276933
C	2.064685	-2.585951	0.447017
C	1.298369	-2.224737	1.482718
H	0.040231	-2.305608	-1.488909
H	2.806497	-3.357306	0.599208
H	1.450560	-2.719144	2.434158
H	0.899652	-0.942822	-2.211734
C	2.700697	-2.813101	-1.855309
H	3.682756	-3.128039	-1.502576
H	2.118244	-3.707225	-2.122977
H	2.836467	-2.211005	-2.754289
C	-0.153463	-0.773679	2.766545
H	-0.468366	-1.617123	3.388002
H	0.625822	-0.221912	3.302990
H	-1.013437	-0.112891	2.642709
N	2.041928	-2.017813	-0.837861
N	0.300993	-1.239491	1.469320
Si	0.016794	-0.344812	0.020140
C	0.865302	1.322888	0.000414
C	0.242016	2.472539	0.493812
C	2.184255	1.431669	-0.452534
C	0.907527	3.690158	0.530739
H	-0.782012	2.419619	0.849599
C	2.851656	2.648164	-0.422682
H	2.695136	0.547999	-0.823041
C	2.213937	3.778969	0.069695
H	0.407811	4.569666	0.916962
H	3.871426	2.714766	-0.780682
H	2.734923	4.727849	0.095235
C	-1.824028	-0.113541	-0.209968
C	-2.721067	-1.007034	0.381867
C	-2.342266	0.895067	-1.026622
C	-4.088419	-0.894302	0.172125
H	-2.338764	-1.800222	1.016140
C	-3.708418	1.009272	-1.244830
H	-1.669615	1.605317	-1.496138
C	-4.583087	0.115233	-0.642460
H	-4.768752	-1.593674	0.641679
H	-4.091048	1.796417	-1.882138
H	-5.649339	0.205423	-0.807932

Cartesian coordinates for optimized boron complexes

Me_2NHC/BH_3

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.462889052 (Hartrees)

0 1			
C	0.778489	-1.512874	-0.001856
C	-0.568174	-1.593011	0.003983
C	-0.021548	0.587136	-0.003582
H	1.532950	-2.278907	-0.001090
H	-1.224617	-2.444465	0.008837
N	-1.038019	-0.299631	0.004618
N	1.094774	-0.169565	-0.006966
C	-2.433402	0.098171	-0.003796
H	-3.045204	-0.770120	0.229478
H	-2.583425	0.877367	0.740171
H	-2.702561	0.496543	-0.980931
C	2.454448	0.338334	0.001109
H	2.409239	1.421193	-0.045134
H	2.959624	0.029023	0.915475
H	2.995671	-0.047228	-0.862122
B	-0.219642	2.174528	0.001315
H	-0.759249	2.444368	1.059268
H	0.836831	2.746999	-0.115081
H	-0.977216	2.430415	-0.914158

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.398958279 (Hartrees)

0 1			
C	-0.665954	-1.491816	-0.125321
C	0.666040	-1.491776	-0.125348
C	-0.000018	0.668127	0.011248
H	-1.344597	-2.328765	-0.131112
H	1.344731	-2.328686	-0.131184
N	1.144798	-0.176943	-0.308524
N	-1.144780	-0.177019	-0.308476
C	2.377911	0.180797	0.352565
H	3.136530	-0.568706	0.130484
H	2.733719	1.144030	-0.010063
H	2.250418	0.241446	1.445356
C	-2.377917	0.180729	0.352544
H	-2.733744	1.143918	-0.010178
H	-3.136490	-0.568832	0.130516
H	-2.250475	0.241471	1.445339
B	-0.000070	2.173881	-0.340500
H	1.028890	2.764660	-0.399998
H	-1.029109	2.764527	-0.400056
H	-0.000022	0.826891	1.158265

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.422444569 (Hartrees)

0 1			
C	0.874892	1.180308	0.377822
C	-0.439133	1.344094	0.249225
C	0.060967	-0.938054	0.120988
H	1.609725	1.950302	0.561302
H	-1.033847	2.238003	0.334338
N	-1.083555	0.076383	0.042255
N	1.272737	-0.149934	0.286912
B	-1.049759	-1.009321	1.232200
H	0.094313	-1.602698	-0.739842
H	-0.829849	-0.524713	2.298177
H	-1.903891	-1.832678	1.089492
C	-2.049937	0.009730	-1.050285
H	-2.388910	-1.018576	-1.151411
H	-2.907375	0.638151	-0.807156
H	-1.595054	0.350101	-1.982724
C	2.368221	-0.442413	-0.619318
H	2.089393	-0.296339	-1.672373
H	3.208697	0.211140	-0.386339
H	2.691259	-1.473223	-0.479217

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.415361529 (Hartrees)

0 1			
B	0.979040	-1.112147	-1.052239
H	-0.379381	-1.747044	0.742673
H	1.742922	-2.003172	-0.802834
C	-0.275840	-1.081100	-0.113346
C	0.463182	1.243282	-0.328920
C	-0.844870	1.089105	-0.571614
H	1.002050	2.179678	-0.362722
H	-1.536213	1.857180	-0.880493
N	-1.321761	-0.190495	-0.256314
N	1.145934	0.068415	-0.012896
C	-2.387834	-0.208850	0.739049
H	-2.030692	0.142449	1.713651
H	-3.196595	0.440261	0.405570
H	-2.777486	-1.220541	0.834748
C	2.227640	0.136671	0.956585
H	3.109309	0.594057	0.498274
H	1.936021	0.712143	1.836448
H	2.489315	-0.875397	1.255792
H	0.882681	-0.738966	-2.185963

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.433756034 (Hartrees)

0 1			
H	1.427233	2.056576	-0.172639
H	-0.091253	1.498847	1.123210
C	0.785232	1.180966	-0.194254
C	0.632702	-1.175992	-0.101864
C	-0.706070	-1.131597	-0.091363
H	1.179410	-2.104553	-0.110422
H	-1.246487	-2.071606	-0.051109
N	-1.459885	0.012693	-0.186803
N	1.424729	0.013005	-0.183194
C	-2.844978	-0.062987	0.219243
H	-3.302846	-0.981734	-0.154546
H	-2.967046	-0.037967	1.310651
H	-3.388053	0.784243	-0.198902
C	2.804541	-0.103643	0.245523
H	2.859516	-0.333537	1.314735
H	3.296303	-0.902520	-0.309741
H	3.323905	0.832407	0.051242
B	-0.718822	1.301842	-0.074978
H	-1.279044	2.330270	-0.301324

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.453744709 (Hartrees)

0 1			
C	-0.685033	-1.176162	-0.000090
C	0.679447	-1.147905	-0.000096
C	-0.797268	1.192475	-0.000032
H	-1.268788	-2.077875	-0.000170
H	1.202917	-2.099926	-0.000093
N	1.410540	-0.047856	-0.000143
N	-1.394020	0.043972	-0.000022
C	2.849305	-0.117901	0.000220
H	3.194501	-1.152852	-0.000394
H	3.248414	0.393345	-0.880959
H	3.247986	0.392166	0.882286
C	-2.848797	-0.087603	0.000119
H	-3.302869	0.898562	0.000146
H	-3.154925	-0.640716	-0.887097
H	-3.154759	-0.640697	0.887403
B	0.785758	1.383607	-0.000116
H	1.118287	2.010381	-0.991906
H	1.118308	2.010330	0.991714
H	-1.479427	2.039010	0.000081

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -331.489397152 (Hartrees)

0 1			
H	1.285842	2.033635	-0.451748
H	1.069279	1.486276	1.199470
C	0.810938	1.251745	0.147434
C	0.610021	-1.160229	0.018322
C	-0.720470	-1.137965	0.132798
H	1.142396	-2.100020	0.078088
H	-1.291400	-2.040982	0.286398
N	-1.442590	0.073180	0.007202
N	1.374693	-0.037808	-0.240857
C	-2.883786	-0.065514	-0.083687
H	-3.160313	-0.663935	-0.955077
H	-3.280218	-0.556911	0.808797
H	-3.334966	0.919652	-0.173335
C	2.799967	-0.147374	-0.042377
H	3.077299	-0.046011	1.017642
H	3.158838	-1.108924	-0.408855
H	3.306512	0.642061	-0.599584
B	-0.763968	1.287751	-0.017967
H	-1.378165	2.304823	-0.111311

Ph_2NHC/BH_3

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.919289014 (Hartrees)

0 1			
C	0.674524	1.847747	-0.149384
C	-0.669534	1.848894	-0.143257
C	0.000867	-0.302458	0.045844
H	1.385237	2.647768	-0.246827
H	-1.383442	2.649832	-0.207775
N	-1.065896	0.528898	-0.015719
N	1.071994	0.526157	-0.032577
C	2.445108	0.134883	-0.018578
C	3.335923	0.854359	0.765206
C	2.878029	-0.924006	-0.801988
C	4.680541	0.514862	0.757484
C	4.222832	-1.259533	-0.795499
C	5.125909	-0.542281	-0.022638
H	5.375974	1.071782	1.371402
H	4.564323	-2.088714	-1.400885
H	6.174309	-0.810415	-0.023984
C	-2.443511	0.144203	0.016245
C	-2.970548	-0.462241	1.145471
C	-3.241339	0.436046	-1.078593
C	-4.317731	-0.784237	1.170749
C	-4.591271	0.116550	-1.042000
C	-5.128946	-0.494384	0.080819
H	-4.735596	-1.263188	2.046186
H	-5.217839	0.338910	-1.895596
H	-6.180524	-0.748535	0.106779
B	-0.007049	-1.904363	0.126717
H	0.048961	-2.290594	-1.028346
H	0.975651	-2.257097	0.736483
H	2.974511	1.660066	1.391631
H	2.161503	-1.480197	-1.389241
H	-2.321563	-0.688814	1.979712
H	-2.800335	0.897152	-1.953303
H	-1.033732	-2.271956	0.638967

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.862912124 (Hartrees)

0 1			
C	-0.693044	1.803368	-0.033744
C	0.632032	1.859124	-0.107967
C	0.044059	-0.345729	-0.390282
H	-1.403397	2.580016	0.186033
H	1.291374	2.700007	0.018015
N	1.132058	0.615582	-0.545210
N	-1.123932	0.503786	-0.369066
C	-2.433347	0.084607	-0.096579
C	-3.489319	0.911087	-0.493430
C	-2.724075	-1.098794	0.579708
C	-4.798180	0.562296	-0.215382
C	-4.042661	-1.446418	0.841700
C	-5.086063	-0.623001	0.450770
H	-5.601222	1.214249	-0.534782
H	-4.249132	-2.369879	1.367701
H	-6.110890	-0.899746	0.658680
C	2.446359	0.224292	-0.179564
C	3.235948	-0.480689	-1.082984
C	2.959626	0.549924	1.072623
C	4.522445	-0.858578	-0.733699
C	4.254332	0.182102	1.412984
C	5.036891	-0.525765	0.513383
H	5.131614	-1.403286	-1.443402
H	4.648275	0.446042	2.386077
H	6.045604	-0.813595	0.779198
B	0.108971	-1.787750	-0.898116
H	0.176537	-0.873889	0.661000
H	-0.869683	-2.451485	-0.933430
H	1.178468	-2.266286	-1.071671
H	2.833215	-0.710800	-2.060483
H	2.337838	1.092385	1.774534
H	-1.929795	-1.745748	0.920064
H	-3.270574	1.818231	-1.042252

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.892653759 (Hartrees)

0 1			
C	0.587069	-1.022930	1.543278
C	-0.724919	-1.240878	1.480556
C	0.054951	-0.701129	-0.674887
H	1.226447	-1.165582	2.398455
H	-1.411124	-1.569801	2.239973
N	-1.203424	-1.024241	0.131781
N	1.101494	-0.631510	0.326725
C	2.352683	-0.100010	0.070105
C	3.219015	0.275708	1.103312
C	2.767773	0.068079	-1.255046
C	4.467670	0.793767	0.808127
C	4.016080	0.601535	-1.531773
C	4.878091	0.965599	-0.507803
H	5.123136	1.079205	1.621211
H	4.319605	0.721682	-2.563986
H	5.853344	1.377063	-0.728789
C	-2.360648	-0.164420	0.011441
C	-3.507951	-0.633399	-0.603870
C	-2.306191	1.118675	0.538263
C	-4.617269	0.197418	-0.694019
C	-3.414516	1.944329	0.439464
C	-4.571747	1.483647	-0.176494
H	-5.518559	-0.163833	-1.171712
H	-3.375257	2.947655	0.842929
H	-5.437361	2.128761	-0.251529
B	-0.697520	-2.036846	-1.029670
H	-0.035979	0.212507	-1.256827
H	-0.298912	-3.067470	-0.587862
H	-1.401042	-1.999026	-1.990659
H	-3.518728	-1.636116	-1.009138
H	-1.396058	1.457244	1.019522
H	2.120398	-0.247483	-2.062310
H	2.910664	0.183725	2.135613

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.887217585 (Hartrees)

0 1			
C	-0.666468	-0.998772	1.616633
C	0.666373	-1.092663	1.621802
C	0.249117	-1.311967	-0.627535
H	-1.303787	-0.900068	2.482102
H	1.304980	-1.148438	2.488353
N	1.221324	-1.062088	0.340732
N	-1.260176	-1.071204	0.339398
C	-2.308410	-0.148194	0.052843
C	-3.412963	-0.541946	-0.694955
C	-2.226102	1.153760	0.539582
C	-4.429370	0.366727	-0.946141
C	-3.250806	2.053196	0.290586
C	-4.354837	1.663570	-0.455090
H	-5.289768	0.056275	-1.524929
H	-3.180931	3.063584	0.672218
H	-5.151931	2.367677	-0.654361
C	2.337613	-0.246636	0.053005
C	2.811372	0.702036	0.957099
C	2.987635	-0.415063	-1.168752
C	3.924869	1.464869	0.636961
C	4.083527	0.369301	-1.487857
C	4.562760	1.308992	-0.585041
H	4.285381	2.199066	1.346092
H	4.576528	0.230719	-2.441360
H	5.426608	1.911696	-0.831278
B	-0.883406	-2.381781	-0.488934
H	-0.726054	-3.335543	0.213662
H	0.322227	-0.649681	-1.487836
H	2.643397	-1.181298	-1.851651
H	2.298420	0.861894	1.895538
H	-1.349917	1.453624	1.101774
H	-3.467448	-1.555425	-1.065508
H	-1.544570	-2.495398	-1.477900

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.920922301 (Hartrees)

0 1			
C	0.676505	-1.033381	-0.328640
C	-0.676704	-1.059510	-0.361048
C	-0.801410	1.298213	-0.201058
H	1.189877	-1.985723	-0.391746
H	-1.253759	-1.964069	-0.409767
N	-1.402695	0.147712	-0.193035
N	1.423153	0.077420	-0.231263
C	2.807079	-0.027321	-0.036348
C	3.636510	1.016568	-0.455695
C	3.391014	-1.134362	0.590154
C	5.008766	0.935549	-0.280455
C	4.764375	-1.207341	0.752928
C	5.585397	-0.176483	0.316230
H	5.633078	1.753464	-0.617567
H	5.193976	-2.071125	1.244651
H	6.656991	-0.233738	0.452993
C	-2.827911	0.037964	-0.016022
C	-3.576844	-0.662652	-0.949328
C	-3.427095	0.638699	1.079301
C	-4.950678	-0.749406	-0.784658
C	-4.802548	0.546387	1.234563
C	-5.564714	-0.146109	0.305010
H	-5.542916	-1.284862	-1.514778
H	-5.275811	1.009783	2.089985
H	-6.636967	-0.218373	0.430279
B	0.755308	1.482625	-0.449698
H	1.190155	2.299637	0.330250
H	-1.474270	2.141044	-0.064148
H	-2.816276	1.158087	1.806468
H	-3.086137	-1.116455	-1.800645
H	2.769256	-1.924013	0.990385
H	3.195574	1.882417	-0.927961
H	0.887035	1.903976	-1.589428

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.905148122 (Hartrees)

0 1			
C	0.689498	-1.055357	-0.404152
C	-0.646176	-1.099771	-0.428532
C	-0.797992	1.255778	-0.513132
H	1.219188	-1.996385	-0.476537
H	-1.183733	-2.028331	-0.499303
N	-1.438433	0.096041	-0.394691
N	1.455513	0.090345	-0.367969
C	2.823827	-0.004260	-0.078995
C	3.699255	1.003562	-0.498931
C	3.354876	-1.084330	0.633737
C	5.054099	0.917938	-0.232027
C	4.716609	-1.165336	0.886048
C	5.578755	-0.168974	0.456051
H	5.709662	1.708823	-0.574589
H	5.099745	-2.011792	1.442430
H	6.638977	-0.232136	0.660258
C	-2.824946	0.020546	-0.090169
C	-3.617174	-0.964668	-0.671141
C	-3.391160	0.941547	0.784465
C	-4.971568	-1.015232	-0.383122
C	-4.749521	0.888547	1.058390
C	-5.544425	-0.088501	0.477902
H	-5.584637	-1.778338	-0.844653
H	-5.181986	1.606121	1.743438
H	-6.602739	-0.131298	0.697443
B	0.706077	1.399880	-0.410434
H	0.151478	1.731468	0.753690
H	-1.437500	2.131049	-0.560271
H	1.213459	2.400200	-0.807380
H	2.699112	-1.849639	1.026276
H	3.309894	1.847621	-1.049342
H	-3.181371	-1.670166	-1.365961
H	-2.763240	1.679761	1.266946

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -714.961411435 (Hartrees)

0 1			
C	-0.694114	-1.066810	-0.208593
C	0.639317	-1.069861	-0.216266
C	0.797631	1.357511	-0.463108
H	-1.250031	-1.989103	-0.239852
H	1.163342	-2.010316	-0.286057
N	1.422445	0.070966	-0.173024
N	-1.437191	0.138587	-0.114516
C	-2.852179	0.037496	0.004206
C	-3.534208	0.852540	0.901096
C	-3.565466	-0.864395	-0.780093
C	-4.914470	0.773418	1.002954
C	-4.944930	-0.945866	-0.665996
C	-5.626212	-0.128005	0.223881
H	-5.433898	1.411534	1.706229
H	-5.490156	-1.646631	-1.285098
H	-6.702662	-0.193443	0.310759
C	2.806650	-0.012786	-0.023998
C	3.405283	-1.122974	0.588580
C	3.635399	1.025758	-0.463278
C	4.779919	-1.196385	0.724457
C	5.011496	0.941194	-0.312270
C	5.598543	-0.168610	0.274056
H	5.214717	-2.063350	1.205833
H	5.629068	1.757223	-0.665991
H	6.672189	-0.229134	0.388767
B	-0.764796	1.361502	-0.235403
H	1.005350	1.677151	-1.497897
H	1.253548	2.121805	0.174218
H	-1.377277	2.379306	-0.216092
H	-3.041412	-1.483106	-1.497068
H	-2.973124	1.538060	1.522390
H	2.791766	-1.914158	0.995607
H	3.209839	1.896436	-0.939713

Me_2NHC/BH_2NHMe

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.140122071 (Hartrees)

0 1			
B	-0.983546	-1.209735	-0.511694
H	-0.721061	-1.655363	-1.617169
N	-2.344010	-0.529256	-0.475199
H	-3.004418	-0.998058	-1.077783
C	-2.907077	-0.366654	0.850680
H	-2.986093	-1.307118	1.416239
H	-2.264401	0.295592	1.443498
H	-3.896840	0.096843	0.813010
H	-0.849779	-2.111887	0.315202
C	0.242423	-0.187196	-0.182314
C	1.606434	1.556364	0.181705
C	2.351095	0.435670	0.275311
H	1.870275	2.593608	0.284534
H	3.398064	0.295715	0.475990
N	1.498487	-0.620480	0.049426
N	0.317271	1.154373	-0.101714
C	1.877301	-2.022233	0.047741
H	1.462292	-2.504281	-0.834671
H	2.962833	-2.086571	0.034759
H	1.481273	-2.518660	0.931843
C	-0.784609	2.083944	-0.312631
H	-0.988386	2.624490	0.611497
H	-0.508241	2.792066	-1.093018
H	-1.653428	1.500470	-0.616013

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.096546042 (Hartrees)

0 1			
B	0.906450	-1.229531	0.450904
H	0.051093	-0.453625	1.412886
N	2.303257	-0.910106	0.328211
H	2.950642	-1.523331	0.794193
C	2.887622	-0.229088	-0.810351
H	3.354477	-0.926742	-1.513380
H	2.107719	0.302229	-1.357209
H	3.648051	0.500182	-0.511619
H	0.543816	-2.324914	0.763170
C	-0.197934	-0.251702	0.046412
C	-1.453659	1.615515	-0.195613
C	-2.282693	0.570714	-0.252712
H	-1.660946	2.669120	-0.261601
H	-3.350087	0.536439	-0.385530
N	-1.513475	-0.593271	-0.258495
N	-0.129994	1.142007	-0.151933
C	-2.043945	-1.895931	0.042707
H	-2.010348	-2.098389	1.120632
H	-3.076643	-1.942096	-0.298585
H	-1.462411	-2.662215	-0.467378
C	0.840938	1.905006	0.604330
H	0.670547	2.964739	0.423460
H	0.725746	1.694988	1.677153
H	1.855597	1.653786	0.316165

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.12661957 (Hartrees)

0 1			
B	0.912633	-1.300641	0.573747
H	-0.674678	-0.084382	1.547919
N	2.164813	-1.210174	-0.015340
H	2.788306	-1.988140	0.137009
C	2.735357	-0.185806	-0.876536
H	3.114756	-0.633864	-1.796382
H	1.965602	0.536179	-1.132232
H	3.563205	0.328716	-0.382278
H	0.692709	-2.298112	1.195200
C	-0.253615	-0.218618	0.514153
C	-1.195292	1.581992	-0.505469
C	-2.008288	0.547692	-0.712392
H	-1.329928	2.615857	-0.779543
H	-2.972554	0.529711	-1.194386
N	-1.365033	-0.656392	-0.352079
N	0.042752	1.122356	-0.005790
C	-2.201268	-1.687727	0.223238
H	-2.593569	-1.390992	1.208432
H	-3.040125	-1.885608	-0.443676
H	-1.632856	-2.609727	0.338859
C	0.735982	1.966987	0.938919
H	0.875976	2.960359	0.512614
H	0.185023	2.061292	1.887353
H	1.719978	1.544262	1.153362

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.097690627 (Hartrees)

0 1			
B	-1.071247	0.317128	-0.913354
H	1.028709	0.260236	-1.908543
N	-2.124628	-0.551434	-0.406107
H	-3.060472	-0.183630	-0.417074
C	-1.991112	-1.776603	0.346272
H	-2.799191	-2.472379	0.102519
H	-1.053505	-2.267633	0.081661
H	-1.992016	-1.637231	1.435477
H	-1.410600	1.076234	-1.787111
C	0.445154	-0.092749	-1.058860
C	0.235730	0.628972	1.282075
C	0.855850	-0.552273	1.148106
H	0.043992	1.114054	2.230029
H	1.182978	-1.201871	1.944587
N	1.171718	-0.865732	-0.182956
N	-0.161171	1.245499	0.103694
C	2.595486	-1.054796	-0.441000
H	3.148181	-0.117136	-0.316079
H	2.988743	-1.791107	0.258744
H	2.734320	-1.431351	-1.452698
C	-0.059773	2.692247	0.023437
H	-0.750141	3.153938	0.736215
H	0.952836	3.042212	0.235231
H	-0.347047	3.002912	-0.978780

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.139816032 (Hartrees)

0 1			
B	0.705942	0.495292	-0.970209
H	-1.437734	1.366820	-1.520284
N	1.261128	1.666081	-0.201496
H	2.151383	2.027272	-0.506506
C	1.114271	1.680196	1.237012
H	1.433720	2.634645	1.661220
H	0.060421	1.545380	1.502804
H	1.668987	0.881163	1.756759
H	1.126508	0.489606	-2.107887
C	-0.907070	0.618857	-0.937445
C	0.144797	-1.467546	0.540977
C	-1.165479	-1.101488	0.664845
H	0.493029	-2.300398	1.146278
H	-1.864845	-1.596687	1.313414
N	-1.666183	-0.071673	-0.142932
N	1.008458	-0.889405	-0.279118
C	-3.108430	0.155089	-0.041366
H	-3.635173	-0.751584	-0.335542
H	-3.356160	0.393685	0.992143
H	-3.389668	0.979603	-0.688788
C	2.381683	-1.339876	-0.304141
H	2.483690	-2.319499	0.165179
H	2.722708	-1.403431	-1.339452
H	3.030976	-0.629439	0.217231

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.114902987 (Hartrees)

0 1			
B	0.613951	-0.449014	0.377048
H	-0.939058	-2.136417	0.310992
N	1.892555	-1.170869	0.472505
H	1.865288	-2.031970	0.996717
C	2.673918	-1.297955	-0.746859
H	2.226811	-1.971260	-1.491841
H	2.766969	-0.318280	-1.219427
H	3.681172	-1.656335	-0.525975
H	-0.075384	-0.667760	1.546320
C	-0.762245	-1.084354	0.100903
C	-0.496613	1.616066	-0.329696
C	-1.694921	1.020890	-0.408813
H	-0.447449	2.680890	-0.533699
H	-2.585536	1.551462	-0.703324
N	-1.849550	-0.378052	-0.181308
N	0.691984	0.988274	-0.054465
C	-3.182354	-0.836117	0.162390
H	-3.479520	-0.451675	1.143265
H	-3.894983	-0.484355	-0.583590
H	-3.196472	-1.923665	0.181640
C	1.753517	1.823687	0.472849
H	1.585183	2.088362	1.525271
H	2.700266	1.291095	0.413825
H	1.830235	2.746208	-0.107186

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -426.192147477 (Hartrees)

0 1			
B	0.772706	-0.147963	0.035258
H	-0.390063	-2.025941	-0.301266
N	2.073790	-0.684627	-0.087648
H	2.849342	-0.066511	-0.261541
C	2.452649	-2.079766	-0.009685
H	3.233022	-2.238832	0.738076
H	1.593952	-2.678873	0.285545
H	2.816478	-2.461900	-0.967474
H	-0.614403	-1.336764	1.301363
C	-0.506139	-1.077023	0.229100
C	-0.776412	1.737321	0.099821
C	-1.831550	0.930838	-0.029904
H	-0.905297	2.801380	0.235117
H	-2.833592	1.335000	-0.000020
N	-1.718825	-0.438034	-0.265587
N	0.544347	1.258019	0.045411
C	-2.913169	-1.219765	-0.050132
H	-3.117054	-1.380840	1.019994
H	-3.773152	-0.722643	-0.499069
H	-2.798720	-2.196562	-0.522588
C	1.597757	2.244893	-0.049839
H	1.297869	3.162300	0.459236
H	2.503006	1.886130	0.442162
H	1.841076	2.497373	-1.087229

Ph_2NHC/BH_2NHMe

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.595377446 (Hartrees)

0 1			
C	-0.803053	-2.172736	-0.641958
C	0.542519	-2.203822	-0.660925
C	-0.069999	-0.174779	0.110983
H	-1.537001	-2.895468	-0.949067
H	1.228279	-2.962816	-0.990427
N	0.976022	-0.974358	-0.201121
N	-1.159709	-0.921772	-0.173753
C	-2.514282	-0.489781	-0.051099
C	-3.416092	-1.274250	0.649593
C	-2.911658	0.688812	-0.661827
C	-4.739461	-0.868057	0.741475
C	-4.232984	1.091100	-0.557458
C	-5.147880	0.314004	0.141265
H	-5.447454	-1.471694	1.293641
H	-4.549893	2.012969	-1.026825
H	-6.179103	0.632088	0.219115
C	2.356572	-0.628266	-0.074611
C	3.240604	-1.569291	0.433402
C	2.789278	0.626504	-0.476920
C	4.586780	-1.251281	0.532838
C	4.136625	0.933308	-0.361938
C	5.036281	-0.000022	0.136095
H	5.280598	-1.978581	0.933429
H	4.483588	1.911479	-0.668415
H	6.086151	0.248576	0.219768
B	-0.027121	1.300097	0.827061
H	-1.058618	1.381617	1.472192
N	0.190487	2.409272	-0.217253
H	-0.683067	2.730455	-0.615004
H	0.929438	1.240334	1.573449
H	-3.076066	-2.180023	1.135646
H	-2.183174	1.269087	-1.211991
H	2.875373	-2.530566	0.772174
H	2.063743	1.340531	-0.855076
C	0.899898	3.567055	0.303377
H	0.438100	4.009673	1.198511
H	1.912691	3.268905	0.590081
H	0.985527	4.349963	-0.455360

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.562041225 (Hartrees)

0 1			
C	0.909677	-2.119240	0.263568
C	-0.418575	-2.197428	0.205886
C	0.134173	0.017357	-0.034876
H	1.649605	-2.874509	0.457240
H	-1.080882	-3.030418	0.353513
N	-0.917832	-0.911218	-0.044111
N	1.276383	-0.788136	0.051399
C	2.625066	-0.374601	0.050893
C	3.550604	-1.106546	-0.689235
C	3.050526	0.703280	0.819766
C	4.891370	-0.759421	-0.661595
C	4.393489	1.049943	0.832054
C	5.317857	0.323674	0.095354
H	5.602597	-1.329910	-1.244769
H	4.717626	1.891294	1.430947
H	6.363977	0.599856	0.109331
C	-2.300809	-0.640797	0.047229
C	-2.790735	0.389630	0.844937
C	-3.189850	-1.473238	-0.630168
C	-4.160822	0.586163	0.946194
C	-4.555455	-1.274193	-0.513943
C	-5.047626	-0.240196	0.271801
H	-4.534351	1.390120	1.567380
H	-5.236435	-1.921770	-1.050871
H	-6.114159	-0.078973	0.355241
B	0.081427	1.528622	-0.272491
H	0.025420	0.929968	1.108868
N	-1.059163	2.211530	-0.798372
H	-1.893922	1.716111	-1.060107
H	1.112031	2.120735	-0.203638
C	-1.233929	3.643395	-0.701412
H	-0.255830	4.114550	-0.602369
H	-1.711370	4.045647	-1.597669
H	-1.835600	3.944123	0.165284
H	3.208170	-1.934833	-1.296853
H	2.334028	1.254347	1.411449
H	-2.799915	-2.262536	-1.260556
H	-2.103617	1.031155	1.378889

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.607046418 (Hartrees)

0 1			
C	0.823716	-0.935065	-1.758925
C	-0.502890	-1.040756	-1.736155
C	0.095888	0.255451	0.116146
H	1.497198	-1.284297	-2.519578
H	-1.143365	-1.484930	-2.476102
N	-1.017775	-0.383450	-0.611004
N	1.275005	-0.211656	-0.648488
C	2.535081	-0.308633	-0.083288
C	3.583445	-0.957185	-0.752868
C	2.800128	0.253061	1.172431
C	4.842085	-1.028478	-0.184435
C	4.066892	0.166988	1.728844
C	5.100942	-0.469656	1.060662
H	5.631901	-1.536399	-0.723805
H	4.240890	0.610292	2.701435
H	6.087194	-0.532911	1.499238
C	-2.247173	-0.607347	-0.023136
C	-2.586260	0.043256	1.171951
C	-3.193134	-1.466011	-0.603302
C	-3.827927	-0.157752	1.753933
C	-4.429446	-1.649158	-0.010212
C	-4.763066	-0.999481	1.171561
H	-4.062657	0.357305	2.676939
H	-5.139317	-2.321149	-0.476233
H	-5.730466	-1.151424	1.629999
B	0.043475	1.856952	0.065970
H	0.139268	-0.151596	1.138107
N	-0.955941	2.462766	-0.665785
H	-1.646642	1.869885	-1.108925
H	0.871053	2.519890	0.608689
C	-1.147684	3.883779	-0.879200
H	-0.355533	4.428187	-0.369286
H	-1.109464	4.131629	-1.941476
H	-2.109058	4.216119	-0.483093
H	3.417740	-1.413823	-1.717797
H	2.022884	0.773363	1.712330
H	-2.956281	-2.006282	-1.508530
H	-1.885319	0.719684	1.641132

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.565638175 (Hartrees)

0 1			
C	-0.498066	0.891049	1.377067
C	0.821974	1.075451	1.282638
C	0.283158	0.942757	-0.941661
H	-1.054072	0.871424	2.303455
H	1.510185	1.277708	2.087223
N	1.312468	0.868301	-0.027756
N	-1.187168	0.723461	0.168594
C	-2.155923	-0.312986	0.109672
C	-3.337232	-0.135066	-0.606605
C	-1.931698	-1.516807	0.776957
C	-4.278218	-1.151256	-0.648898
C	-2.882271	-2.525745	0.736381
C	-4.057600	-2.348515	0.020569
H	-5.196867	-1.002934	-1.201996
H	-2.699667	-3.455410	1.260138
H	-4.797445	-3.137311	-0.016363
C	2.289299	-0.180781	-0.132139
C	3.621715	0.122948	0.105978
C	1.911038	-1.482896	-0.437991
C	4.580148	-0.877999	0.036105
C	2.875604	-2.475686	-0.522791
C	4.210663	-2.176611	-0.284874
H	5.619616	-0.639086	0.219980
H	2.581640	-3.488449	-0.766762
H	4.960410	-2.953969	-0.351359
B	-0.914514	1.966512	-0.943169
H	-1.666591	1.748480	-1.852780
H	0.350487	0.202951	-1.735131
H	0.864519	-1.713453	-0.601905
H	3.895054	1.145570	0.334216
H	-1.005286	-1.653170	1.323026
H	-3.508586	0.802678	-1.114935
N	-0.850476	3.341846	-0.490683
C	0.204710	4.009014	0.235562
H	0.045316	4.044286	1.320745
H	1.152154	3.497857	0.059099
H	0.325904	5.038084	-0.114090
H	-1.671768	3.905704	-0.623626

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.606152182 (Hartrees)

0 1			
C	0.606934	-0.653981	-0.972931
C	-0.749211	-0.646814	-0.996422
C	-0.855464	0.593101	1.015325
H	1.117070	-1.161613	-1.784540
H	-1.331994	-1.123467	-1.762850
N	-1.461347	-0.072325	0.074413
N	1.356793	-0.074833	-0.021659
C	2.735367	-0.346683	0.011617
C	3.627370	0.623678	0.474578
C	3.243503	-1.589215	-0.378483
C	4.986244	0.360346	0.525563
C	4.606012	-1.839117	-0.335878
C	5.487903	-0.867280	0.114508
H	5.660891	1.127404	0.884438
H	4.976676	-2.810157	-0.639240
H	6.550419	-1.066794	0.153008
C	-2.891209	-0.262384	0.083367
C	-3.633908	0.137374	-1.016904
C	-3.497551	-0.830842	1.191330
C	-5.010224	-0.030316	-0.999316
C	-4.875236	-0.993539	1.199358
C	-5.631745	-0.594679	0.106575
H	-5.598308	0.287385	-1.850159
H	-5.355205	-1.441445	2.059298
H	-6.705692	-0.725054	0.115488
B	0.703630	1.008117	0.941245
H	1.219261	0.952698	2.031401
H	-1.518473	0.963421	1.792029
H	-2.890846	-1.150142	2.028924
H	-3.134959	0.589155	-1.864873
H	2.564941	-2.377405	-0.677848
H	3.244024	1.587151	0.777113
N	0.708723	2.410018	0.401181
C	0.386942	2.651485	-0.987578
H	1.099395	2.197705	-1.694075
H	-0.598707	2.235184	-1.222390
H	0.339928	3.721015	-1.200576
H	1.399865	3.047541	0.762823

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.586877687 (Hartrees)

0 1			
C	0.535614	-1.382131	-0.371989
C	-0.806411	-1.386609	-0.382953
C	-0.893889	0.965722	-0.167384
H	1.038236	-2.334757	-0.492182
H	-1.381369	-2.289768	-0.478930
N	-1.549865	-0.171928	-0.267463
N	1.331878	-0.275693	-0.288333
C	2.712199	-0.464907	-0.071199
C	3.641392	0.334135	-0.741750
C	3.177300	-1.448433	0.803782
C	4.999038	0.154451	-0.529770
C	4.538617	-1.635269	0.994347
C	5.457033	-0.832826	0.333762
H	5.706424	0.779092	-1.060721
H	4.881035	-2.403083	1.676768
H	6.518362	-0.975830	0.488086
C	-2.961546	-0.255745	-0.072022
C	-3.723241	-1.063956	-0.907972
C	-3.563930	0.465924	0.949881
C	-5.094522	-1.136557	-0.723872
C	-4.938337	0.391022	1.122165
C	-5.706398	-0.408642	0.288263
H	-5.689101	-1.758472	-1.380207
H	-5.406993	0.949440	1.921941
H	-6.777466	-0.468052	0.428424
B	0.635971	1.046982	0.041886
N	1.365399	2.297146	-0.244702
H	2.276919	2.327783	0.190567
H	0.157152	1.055415	1.298533
H	-1.524465	1.841855	-0.046606
H	-2.953557	1.061907	1.616766
H	-3.242630	-1.611126	-1.708601
H	3.276825	1.077273	-1.438253
H	2.464043	-2.051707	1.351967
C	0.645031	3.534572	-0.027716
H	1.316772	4.389487	-0.103594
H	-0.123164	3.658892	-0.795969
H	0.143543	3.585561	0.952629

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -809.66937058 (Hartrees)

0 1

C	-0.508746	-1.425344	-0.320122
C	0.823059	-1.389755	-0.354950
C	0.910817	1.056933	-0.325982
H	-1.034957	-2.353588	-0.479852
H	1.374275	-2.290316	-0.573971
N	1.569555	-0.230423	-0.171219
N	-1.294721	-0.285550	-0.056816
C	-2.697280	-0.459855	0.038181
C	-3.397872	0.087061	1.111437
C	-3.395381	-1.177258	-0.931636
C	-4.773746	-0.066489	1.201894
C	-4.767885	-1.342394	-0.827198
C	-5.464735	-0.784470	0.236037
H	-5.303857	0.362319	2.042852
H	-5.297202	-1.900103	-1.589272
H	-6.536443	-0.911616	0.312807
C	2.951152	-0.287635	-0.021127
C	3.581784	-1.451174	0.445999
C	3.754004	0.823543	-0.310504
C	4.956519	-1.499989	0.589856
C	5.130549	0.760209	-0.154663
C	5.747875	-0.398232	0.289863
H	5.412709	-2.410084	0.959164
H	5.724934	1.633298	-0.394021
H	6.821792	-0.441176	0.409284
B	-0.664273	1.005023	-0.110199
N	-1.405839	2.196202	-0.037189
H	-2.410236	2.139804	0.036209
H	1.123608	1.492333	-1.316410
H	1.342221	1.750020	0.403528
H	3.307782	1.736342	-0.676876
H	2.989533	-2.308101	0.734095
H	-2.848470	0.616976	1.879653
H	-2.856190	-1.591848	-1.774277
C	-0.900360	3.547667	-0.162679
H	-1.163847	4.156168	0.705446
H	0.184893	3.534643	-0.241325
H	-1.290663	4.041296	-1.055916

Me_2NHC/BCl_3

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -1710.42544332 (Hartrees)

0 1

C	2.830947	0.592817	-0.027575
C	2.750756	-0.753360	-0.018561
C	0.667551	0.047526	-0.028020
H	3.680886	1.250280	-0.026618
H	3.516126	-1.508042	-0.008959
N	1.417038	-1.071389	-0.015820
N	1.541793	1.071113	-0.031223
C	0.936109	-2.450822	-0.010451
H	1.718430	-3.069558	0.422710
H	0.035467	-2.517694	0.591125
H	0.715535	-2.768285	-1.026382
C	1.255132	2.504983	-0.012866
H	0.633536	2.750649	0.842172
H	2.209487	3.020260	0.059620
H	0.739386	2.797212	-0.922086
B	-0.964634	0.041795	-0.001004
Cl	-1.448465	-0.651451	1.660119
Cl	-1.540222	-1.052614	-1.388284
Cl	-1.704282	1.715317	-0.213743

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -1710.33647871 (Hartrees)

0 1

C	-2.011338	0.427512	1.055553
C	-0.958742	0.363988	1.863012
C	-0.386878	-0.505539	-0.257806
H	-2.988097	0.829583	1.274539
H	-0.848105	0.613666	2.902449
N	0.159801	-0.199169	1.133800
N	-1.759690	-0.125997	-0.184036
B	0.760046	0.567535	-0.179505
Cl	0.330490	2.309453	-0.314702
Cl	2.453378	0.125753	-0.580539
Cl	-0.158947	-2.156526	-0.854801
C	-2.411035	0.309431	-1.402266
H	-2.346683	-0.488155	-2.141805
H	-3.461699	0.499924	-1.190163
H	-1.948227	1.215148	-1.804443
C	0.934296	-1.204232	1.873153
H	1.421990	-0.700582	2.706059
H	0.261223	-1.978558	2.239725
H	1.687102	-1.637061	1.223641

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -1710.37950607 (Hartrees)

0 1

C	0.973592	2.173103	-0.000985
C	-0.381272	2.249764	-0.029309
C	0.911977	-0.178688	-0.022503
H	1.611411	3.035845	0.016928
H	-0.829919	3.236437	-0.039241
N	-1.203761	1.204265	-0.049357
N	1.605568	0.921433	-0.011444
C	-2.641976	1.417367	-0.105333
H	-3.037732	1.036847	-1.047275
H	-3.121714	0.880992	0.713655
H	-2.865095	2.479647	-0.019427
C	3.075492	0.919656	-0.012802
H	3.436327	0.390100	0.865939
H	3.435791	0.416672	-0.907241
H	3.417981	1.947934	0.002195
B	-0.696665	-0.221058	0.009368
Cl	1.766272	-1.653164	-0.053007
Cl	-1.217947	-1.056465	1.606546
Cl	-1.313223	-1.213093	-1.446550

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -1710.35329387 (Hartrees)

0 1			
C	-0.500671	2.177407	-0.315762
C	0.831656	2.125465	-0.236753
C	-0.708775	-0.160974	-0.289023
H	-1.031562	3.113580	-0.298732
H	1.396740	3.043760	-0.158816
N	1.554634	0.948250	-0.271514
N	-1.292080	1.027669	-0.448624
C	2.999654	1.068613	-0.125865
H	3.464973	0.107779	-0.321312
H	3.384951	1.800080	-0.836749
H	3.253240	1.384180	0.888195
C	-2.738216	1.173945	-0.301895
H	-3.256678	0.591122	-1.057968
H	-3.026788	0.827964	0.693282
H	-2.991276	2.223151	-0.418280
B	0.845739	-0.275472	-0.232661
Cl	-1.657046	-1.539521	-0.669753
Cl	1.651531	-1.829180	-0.409326
Cl	-0.380488	-0.387324	1.980870

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -1710.35860559 (Hartrees)

0 1			
C	-0.658936	-0.163753	-0.065358
C	-0.349064	2.206180	-0.246464
C	0.971225	2.144155	-0.090500
H	-0.857774	3.157723	-0.264511
H	1.565387	3.038538	0.016426
N	1.658630	0.919642	-0.087691
N	-1.161581	1.091200	-0.432922
C	3.110990	1.021264	-0.030963
H	3.480194	1.569777	-0.898991
H	3.409324	1.552194	0.874725
H	3.550691	0.029448	-0.022284
C	-2.596943	1.324730	-0.344008
H	-2.904772	1.483480	0.693147
H	-2.844148	2.202905	-0.937182
H	-3.131104	0.469415	-0.746508
B	0.933732	-0.267239	-0.110809
Cl	1.708854	-1.847180	-0.121722
Cl	-1.058947	-0.539027	1.737020
Cl	-1.431050	-1.463124	-1.018399

Cartesian coordinates for optimized beryllium complexes

Me_2NHC/BeH_2

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.737389419 (Hartrees)

0 1			
C	-0.676129	-1.493835	-0.000121
C	0.676132	-1.493831	-0.000112
C	-0.000004	0.653384	0.000076
H	-1.382240	-2.305297	-0.000236
H	1.382247	-2.305289	-0.000187
N	1.065698	-0.177470	-0.000021
N	-1.065701	-0.177476	0.000015
C	2.456867	0.250026	0.000254
H	2.956629	-0.132995	-0.888507
H	2.469336	1.336528	-0.001451
H	2.955488	-0.130063	0.890918
C	-2.456868	0.250026	0.000036
H	-2.469328	1.336531	0.000629
H	-2.955949	-0.131035	-0.889951
H	-2.956174	-0.132006	0.889481
Be	0.000001	2.464679	0.000029
H	1.241543	3.047440	-0.002039
H	-1.241524	3.047465	0.000472

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.686341787 (Hartrees)

0 1			
C	-0.668057	-1.459089	0.083210
C	0.668526	-1.458961	0.083112
C	-0.000028	0.681429	-0.180227
H	-1.356325	-2.277417	0.210897
H	1.356965	-2.277154	0.210733
N	1.116896	-0.185488	-0.313527
N	-1.116738	-0.185728	-0.313391
C	2.388267	0.322991	0.123825
H	3.153850	-0.443417	0.016230
H	2.672513	1.179906	-0.489834
H	2.348698	0.640158	1.179094
C	-2.388336	0.322397	0.123743
H	-2.672678	1.179265	-0.489923
H	-3.153669	-0.444244	0.016000
H	-2.349053	0.639529	1.179026
H	-0.000034	1.021103	1.064921
H	-0.001624	3.635340	0.171879
Be	-0.000495	2.323211	-0.020645

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.709106341 (Hartrees)

0 1			
C	-0.662759	1.318933	0.155379
C	0.662825	1.318904	0.155339
C	0.000044	-0.824728	-0.533225
H	-1.363939	2.129945	0.261828
H	1.364020	2.129912	0.261750
N	1.088083	-0.049346	0.132479
N	-1.088041	-0.049348	0.132555
C	2.437144	-0.358663	-0.297116
H	3.152700	0.194110	0.310269
H	2.612064	-1.425108	-0.164035
H	2.586297	-0.104026	-1.351740
C	-2.437078	-0.358574	-0.297224
H	-2.612026	-1.425044	-0.164373
H	-3.152687	0.194090	0.310198
H	-2.586106	-0.103724	-1.351810
Be	-0.000355	-1.210420	1.081393
H	-0.000133	-1.894659	2.234826
H	-0.000125	-0.738191	-1.626644

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.701457482 (Hartrees)

0 1			
C	-0.799302	-0.984829	-0.738528
C	0.517125	-1.109808	-0.521747
C	-0.293250	1.159259	-0.191083
H	-1.458712	-1.749507	-1.120292
H	1.084263	-2.016232	-0.690818
N	1.177034	0.026245	-0.024937
N	-1.324898	0.241236	-0.292920
C	2.122134	-0.196702	1.060718
H	2.938939	-0.841000	0.721343
H	2.551052	0.755842	1.366812
H	1.639668	-0.663311	1.923227
C	-2.260408	0.103464	0.821151
H	-1.758251	-0.275901	1.719277
H	-2.711343	1.070907	1.034953
H	-3.051605	-0.591268	0.539966
Be	1.118162	1.239711	-1.148350
H	1.995269	1.860526	-1.956462
H	-0.384671	1.790435	0.697326

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.707085038 (Hartrees)

0 1			
C	-0.489709	-1.078962	-0.311852
C	0.848813	-0.953666	-0.330107
C	-1.034275	1.257647	-0.462004
H	-0.951593	-2.040019	-0.490359
H	1.427256	-1.852760	-0.538323
N	1.554102	0.216106	-0.108018
N	-1.405775	-0.004607	-0.150442
C	2.882208	0.048384	0.437216
H	3.496665	-0.599680	-0.197885
H	3.383157	1.013295	0.503669
H	2.863302	-0.391400	1.441662
C	-2.629070	-0.302481	0.573661
H	-2.444508	-0.334384	1.651761
H	-3.367643	0.469203	0.363020
H	-3.020771	-1.269821	0.257308
Be	0.584554	1.417678	-0.201274
H	-0.371577	2.070763	0.732300
H	-1.858607	1.958074	-0.550319

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.765251679 (Hartrees)

0 1			
C	-0.625526	-1.077791	-0.002856
C	0.741936	-1.036416	-0.003936
C	-0.903484	1.286162	-0.000437
H	-1.160599	-2.011590	-0.005059
H	1.246828	-2.001150	-0.005456
N	1.489758	0.061135	-0.004205
N	-1.401588	0.075219	0.000107
C	2.935923	-0.105824	0.006311
H	3.217154	-1.159353	-0.062425
H	3.380900	0.432468	-0.830739
H	3.357723	0.309730	0.922662
C	-2.849266	-0.177851	0.004133
H	-3.109643	-0.751355	0.892371
H	-3.376964	0.770123	0.005660
H	-3.114598	-0.751195	-0.882734
Be	0.823856	1.537691	-0.004895
H	1.544243	2.693063	-0.008321
H	-1.695153	2.034332	0.003020

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -320.75249952 (Hartrees)

0 1			
C	0.466057	-1.029009	0.165128
C	-0.871552	-0.934411	0.247554
C	1.095973	1.370126	0.247066
H	0.924534	-1.984151	0.386450
H	-1.437909	-1.802988	0.565268
N	-1.613402	0.244728	-0.008936
N	1.346433	-0.006301	-0.224109
C	-3.026253	0.060898	-0.226217
H	-3.501237	-0.431982	0.629346
H	-3.513724	1.024695	-0.367544
H	-3.222537	-0.550759	-1.113127
C	2.746999	-0.370561	-0.237925
H	2.877722	-1.356728	-0.684185
H	3.302796	0.350852	-0.837905
H	3.180601	-0.377602	0.773760
Be	-0.581956	1.328242	0.055319
H	1.656127	2.055083	-0.392139
H	1.462890	1.509366	1.276477

2 Me_2NHC/BeH_2

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.559727498 (Hartrees)

0 1			
C	3.425933	-0.171181	-0.570856
C	2.724002	-1.184121	-1.122894
C	1.421265	-0.244976	0.469186
H	4.419707	0.189853	-0.768464
H	2.981709	-1.880466	-1.901084
N	1.509494	-1.211280	-0.473912
N	2.612755	0.387362	0.392669
C	0.440786	-2.157362	-0.732243
H	0.864327	-3.075602	-1.135246
H	-0.059517	-2.356175	0.215330
H	-0.277126	-1.744432	-1.442762
C	3.003192	1.494294	1.247843
H	2.153875	1.720618	1.890527
H	3.862893	1.209968	1.854142
H	3.262167	2.361207	0.639156
Be	0.000007	0.000147	1.591477
H	0.142065	1.231269	2.289520
H	-0.142049	-1.230860	2.289725
C	-1.421253	0.245066	0.469142
C	-3.425884	0.170975	-0.570949
C	-2.724069	1.183984	-1.123009
H	-4.419608	-0.190191	-0.768569
H	-2.981845	1.880269	-1.901229
N	-1.509584	1.211328	-0.473990
N	-2.612663	-0.387420	0.392624
C	-0.441001	2.157552	-0.732320
H	-0.864667	3.075747	-1.135295
H	0.059287	2.356412	0.215251
H	0.276954	1.744731	-1.442859
C	-3.002975	-1.494370	1.247832
H	-3.862736	-1.210140	1.854091
H	-3.261809	-2.361345	0.639173
H	-2.153645	-1.720550	1.890549

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.534263629 (Hartrees)

0 1			
C	3.368686	-0.883488	0.334808
C	3.621932	0.225710	-0.394354
C	1.481188	0.341563	0.286421
H	3.997974	-1.714461	0.599955
H	4.515335	0.550766	-0.897246
N	2.458240	0.960225	-0.403671
N	2.054939	-0.791508	0.738769
C	2.271010	2.228643	-1.087371
H	3.187113	2.812364	-1.018634
H	2.018190	2.061694	-2.133971
H	1.455601	2.756608	-0.596833
C	1.374260	-1.765007	1.576152
H	0.312225	-1.524478	1.577990
H	1.522814	-2.765282	1.170609
H	1.762251	-1.722504	2.593226
Be	-0.133612	0.993952	0.663501
H	-1.076790	1.046780	-0.618209
H	-0.136486	2.167995	1.376868
C	-1.506433	0.089618	0.261675
C	-3.682195	-0.140693	-0.364321
C	-2.983801	-1.051286	-1.051642
H	-4.734997	0.084858	-0.391040
H	-3.315322	-1.772180	-1.779403
N	-1.672750	-1.069049	-0.546476
N	-2.836314	0.436857	0.581167
C	-0.592816	-1.468895	-1.403503
H	-0.933142	-2.257929	-2.072983
H	-0.241861	-0.613629	-2.005755
H	0.249274	-1.848395	-0.826669
C	-3.109989	1.726776	1.154271
H	-2.775813	2.530445	0.482440
H	-4.180962	1.822302	1.331158
H	-2.570810	1.835914	2.093154

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.547214057 (Hartrees)

0 1			
C	-2.676827	-1.502438	-0.508404
C	-3.470220	-0.500330	-0.069161
C	-1.400519	0.337419	-0.349769
H	-2.895698	-2.533077	-0.725056
H	-4.515673	-0.482960	0.183076
N	-2.671361	0.615614	0.012329
N	-1.419982	-0.970415	-0.670528
C	-3.123668	1.924797	0.452003
H	-4.103293	2.129303	0.023480
H	-3.188937	1.959929	1.539214
H	-2.406520	2.663870	0.100394
C	-0.278621	-1.740520	-1.149408
H	0.543477	-1.062594	-1.367989
H	0.046123	-2.436098	-0.378538
H	-0.573767	-2.280666	-2.048659
Be	-0.032364	1.504697	-0.330921
H	2.107155	1.518434	0.969118
H	-0.278550	2.750664	-0.854111
C	1.454334	0.853872	0.347900
C	3.037709	-0.687586	-0.291972
C	2.467702	-1.152283	0.821954
H	3.871842	-1.092823	-0.843760
H	2.731598	-2.027041	1.397108
N	1.302020	-0.414472	1.105945
N	2.289998	0.399189	-0.798642
C	0.953002	-0.218194	2.489270
H	0.917015	-1.177063	3.008321
H	1.670823	0.437876	3.007792
H	-0.035542	0.243770	2.553759
C	3.042118	1.469450	-1.416426
H	3.712359	1.958307	-0.692575
H	3.638975	1.078017	-2.241151
H	2.353286	2.218837	-1.806386

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.53517269 (Hartrees)

0 1			
C	-3.343975	-0.117612	0.457223
C	-2.904040	-1.392782	0.389202
C	-1.279279	-0.074523	-0.446861
H	-4.270839	0.291399	0.818885
H	-3.371640	-2.318014	0.675888
N	-1.642963	-1.340601	-0.163222
N	-2.338997	0.666944	-0.061386
C	-0.806698	-2.503884	-0.399172
H	-0.625312	-3.023433	0.541394
H	-1.296880	-3.178963	-1.100416
H	0.139773	-2.162114	-0.809050
C	-2.371476	2.116009	-0.149088
H	-2.076368	2.559627	0.802263
H	-1.672771	2.418011	-0.928214
H	-3.378830	2.440263	-0.404910
Be	0.219877	0.628773	-1.185749
H	2.559259	0.107951	-1.776372
H	-0.050923	1.472480	-2.267907
C	1.760238	-0.179667	-1.084650
C	1.713469	-0.625126	1.170303
C	1.303416	0.655677	1.216137
H	1.799168	-1.296373	2.011537
H	1.057266	1.162950	2.143978
N	1.220987	1.342615	0.023566
N	2.244191	-0.998428	-0.083064
C	1.663499	2.726637	0.034829
H	1.041563	3.322586	0.714954
H	2.706201	2.827915	0.351352
H	1.552147	3.132787	-0.968444
C	3.680253	-1.263313	-0.027540
H	4.236149	-0.355276	0.234629
H	3.879216	-2.027380	0.724742
H	4.018343	-1.631708	-0.994875

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.575813574 (Hartrees)

0 1			
C	-2.673344	-0.583691	1.557736
C	-3.429760	-0.592947	0.438987
C	-1.298861	-0.201119	-0.193110
H	-2.937336	-0.725720	2.590742
H	-4.484908	-0.749269	0.299897
N	-2.572155	-0.357513	-0.612306
N	-1.379895	-0.349317	1.148509
C	-2.988898	-0.296004	-2.003643
H	-3.347523	-1.272617	-2.328140
H	-3.786488	0.438091	-2.114221
H	-2.120077	0.001631	-2.587632
C	-0.245915	-0.223235	2.048966
H	0.653441	-0.578104	1.551664
H	-0.094060	0.819127	2.328440
H	-0.437194	-0.818993	2.939876
Be	0.234814	0.254116	-1.147983
H	1.461654	-2.016356	-1.481799
H	-0.137225	0.561673	-2.483468
C	1.473109	-1.040551	-0.990619
C	2.903435	0.287983	0.392646
C	2.118582	1.415569	0.334692
H	3.851779	0.283526	0.900408
H	2.510630	2.283627	0.868946
N	0.965965	1.536180	-0.286072
N	2.580244	-0.880837	-0.321154
C	0.303661	2.818202	-0.277491
H	0.870785	3.572746	0.277100
H	0.155178	3.169407	-1.302560
H	-0.691429	2.733408	0.175772
C	3.630945	-1.902779	-0.271426
H	4.540088	-1.505179	-0.721670
H	3.835271	-2.157787	0.768448
H	3.301320	-2.783829	-0.813135

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.56025318 (Hartrees)

0 1			
C	3.397115	0.374772	-0.792962
C	3.562865	-0.747160	-0.059982
C	1.373065	-0.224497	-0.005751
H	4.104286	0.976672	-1.335649
H	4.444459	-1.319260	0.169007
N	2.316443	-1.094431	0.410376
N	2.055378	0.675708	-0.744690
C	2.060579	-2.258533	1.242269
H	2.278664	-3.168228	0.683665
H	2.688182	-2.219753	2.131912
H	1.009119	-2.240200	1.522977
C	1.442620	1.795956	-1.441594
H	0.403358	1.864687	-1.122397
H	1.969671	2.715020	-1.188037
H	1.491732	1.633761	-2.517891
Be	-0.403641	-0.178132	0.306198
H	-0.881690	-1.371355	1.122094
H	-1.376118	-2.170203	-0.860559
C	-1.523247	-1.137267	-0.540950
C	-3.221356	0.481927	-0.086573
C	-2.391218	1.402327	0.450077
H	-4.267383	0.702089	-0.229319
H	-2.866070	2.336549	0.753999
N	-1.047277	1.311603	0.618068
N	-2.807288	-0.802760	-0.545384
C	-0.454850	2.254780	1.532671
H	-0.914633	3.247230	1.449921
H	-0.535051	1.941413	2.584509
H	0.613181	2.367230	1.317100
C	-3.869579	-1.790351	-0.622304
H	-4.210296	-2.056971	0.383537
H	-4.714954	-1.388076	-1.182417
H	-3.498650	-2.680639	-1.125238

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -625.610727784 (Hartrees)

0 1			
C	3.505845	0.152748	-0.620390
C	3.454106	-1.025180	0.040120
C	1.369544	-0.182767	-0.004975
H	4.329420	0.667817	-1.082451
H	4.225090	-1.737467	0.274981
N	2.139692	-1.210881	0.400857
N	2.222122	0.648586	-0.636122
C	1.636374	-2.357380	1.139638
H	2.013566	-3.274342	0.690159
H	1.952953	-2.304144	2.180580
H	0.550152	-2.346333	1.085613
C	1.827548	1.888218	-1.288125
H	0.744561	1.972390	-1.225775
H	2.287396	2.738216	-0.785488
H	2.139672	1.866138	-2.331258
Be	-0.406886	-0.018644	0.188282
H	-1.229987	-2.049881	-0.839816
H	-1.788193	-1.899198	0.819616
C	-1.551610	-1.311128	-0.094299
C	-3.205683	0.490567	0.021533
C	-2.408698	1.430253	0.555261
H	-4.273581	0.666425	0.010990
H	-2.874292	2.322339	0.962599
N	-1.013776	1.355645	0.600121
N	-2.783395	-0.692198	-0.598213
C	-0.367500	2.530054	1.127639
H	-0.480272	3.410265	0.475766
H	-0.764779	2.811352	2.111484
H	0.702347	2.346625	1.257533
C	-3.842607	-1.638005	-0.861389
H	-4.163608	-2.164444	0.053444
H	-4.708966	-1.135591	-1.296003
H	-3.490345	-2.387937	-1.571671

2 Ph_2NHC/BeH_2

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.49024197 (Hartrees)

0 1			
C	1.984423	-1.538086	2.123722
C	2.997585	-0.695882	1.860469
C	1.126371	0.204343	0.941441
H	1.955594	-2.450048	2.691235
H	4.032145	-0.722984	2.150385
N	2.456585	0.360637	1.147674
N	0.848753	-0.972844	1.566786
Be	0.000060	1.309682	-0.000188
H	-0.692611	2.064503	0.974177
H	0.692748	2.064346	-0.974635
C	-1.126350	0.204299	-0.941621
C	-1.984623	-1.538365	-2.123399
C	-2.997712	-0.696050	-1.860245
H	-1.955927	-2.450473	-2.690680
H	-4.032308	-0.723192	-2.150029
N	-2.456586	0.360566	-1.147691
N	-0.848853	-0.973048	-1.566727
C	-3.235965	1.462649	-0.690229
C	-2.726537	2.750044	-0.775864
C	-4.505583	1.227010	-0.181827
C	-3.510063	3.809453	-0.347083
H	-1.725548	2.904444	-1.157216
C	-5.282881	2.296852	0.238678
H	-4.874595	0.211958	-0.100565
C	-4.785412	3.589217	0.156234
H	-3.115854	4.815277	-0.405481
H	-6.272455	2.117051	0.638129
H	-5.389518	4.424126	0.486692
C	0.437813	-1.578515	-1.659605
C	0.548148	-2.958624	-1.549778
C	1.562118	-0.791418	-1.872833
C	1.796305	-3.557478	-1.649363
H	-0.334754	-3.555782	-1.359822
C	2.805003	-1.400380	-1.956333
H	1.452703	0.285667	-1.941332
C	2.927995	-2.780144	-1.847650
H	1.881388	-4.633238	-1.563696
H	3.680580	-0.785050	-2.121268
H	3.901193	-3.247776	-1.922580
C	-0.437972	-1.578185	1.659665
C	-1.562209	-0.790913	1.872599
C	-0.548425	-2.958314	1.550193
C	-2.805175	-1.399715	1.956061
H	-1.452668	0.286181	1.940781
C	-1.796654	-3.557011	1.649815
H	0.334452	-3.555601	1.360527
C	-2.928287	-2.779498	1.847751
H	-3.680727	-0.784270	2.120717
H	-1.881841	-4.632786	1.564427
H	-3.901543	-3.247009	1.922690
C	3.236090	1.462599	0.690109
C	2.726846	2.750070	0.775695
C	4.505707	1.226771	0.181783
C	3.510518	3.809355	0.346872
H	1.725875	2.904614	1.157037
C	5.283144	2.296488	-0.238787
H	4.874605	0.211670	0.100649
C	4.785834	3.588918	-0.156436
H	3.116449	4.815236	0.405223
H	6.272711	2.116548	-0.638196
H	5.390062	4.423731	-0.486915

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.46130551 (Hartrees)

0 1			
C	-2.468020	-1.418845	-1.989338
C	-3.274083	-0.377709	-1.710984
C	-1.179327	0.211061	-1.099855
H	-2.670600	-2.369383	-2.448288
H	-4.325371	-0.235163	-1.880939
N	-2.468977	0.612506	-1.177985
N	-1.192714	-1.037757	-1.618939
Be	0.298197	1.040700	-0.502194
H	0.789982	1.980811	-1.371102
H	0.352967	1.418538	1.043639
C	1.154703	0.240958	0.721047
C	1.709584	-1.104843	2.531215
C	2.769998	-0.339807	2.277826
H	1.517693	-1.791524	3.335820
H	3.695205	-0.232401	2.814490
N	2.489690	0.425805	1.145356
N	0.739613	-0.830160	1.559776
C	3.453548	1.271087	0.574062
C	3.119976	2.538227	0.105153
C	4.783383	0.847434	0.521755
C	4.108279	3.361410	-0.414471
H	2.095431	2.871460	0.152057
C	5.762978	1.681871	0.010297
H	5.038153	-0.147355	0.864859
C	5.430269	2.944113	-0.464497
H	3.836986	4.344774	-0.777201

H	6.788845	1.337987	-0.029183
H	6.194025	3.594275	-0.870447
C	-0.541111	-1.394850	1.662919
C	-0.660023	-2.769953	1.869336
C	-1.692559	-0.608642	1.638579
C	-1.908508	-3.351260	2.023806
H	0.236946	-3.377121	1.877603
C	-2.938415	-1.201122	1.781112
H	-1.601459	0.464766	1.533651
C	-3.057087	-2.572186	1.968152
H	-1.984070	-4.420464	2.178189
H	-3.823370	-0.576624	1.774847
H	-4.032270	-3.026839	2.083491
C	-0.050920	-1.888848	-1.712388
C	1.161439	-1.372667	-2.147205
C	-0.175828	-3.222177	-1.352118
C	2.265774	-2.208417	-2.202745
H	1.237734	-0.328573	-2.423798
C	0.932357	-4.052861	-1.428311
H	-1.121173	-3.591012	-0.974011
C	2.154086	-3.546326	-1.847880
H	3.216634	-1.808406	-2.529113
H	0.842006	-5.092483	-1.141782
H	3.020487	-4.192965	-1.894970
C	-2.966977	1.850499	-0.674242
C	-2.216364	3.008818	-0.819929
C	-4.202378	1.875893	-0.040509
C	-2.715907	4.200562	-0.317834
H	-1.251929	2.966066	-1.310130
C	-4.694823	3.077186	0.448023
H	-4.767234	0.960943	0.083870
C	-3.952244	4.240744	0.312399
H	-2.132063	5.105174	-0.425193
H	-5.655748	3.097956	0.945003

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.49793125 (Hartrees)

0 1			
C	-1.391090	-2.197230	-1.914650
C	-2.544098	-1.507707	-1.853769
C	-0.906267	-0.136997	-1.127401
H	-1.179080	-3.189477	-2.267553
H	-3.541951	-1.783952	-2.138559
N	-2.230857	-0.247101	-1.379483
N	-0.400685	-1.341147	-1.471531
Be	0.094822	1.184585	-0.400762
H	0.269495	2.328292	-1.124459
H	0.754198	1.513049	1.954716
C	0.846556	0.735056	1.170595
C	1.299516	-1.437479	1.975710
C	2.471581	-0.909647	1.619437
H	1.111749	-2.388246	2.440977
H	3.445409	-1.352044	1.719050
N	2.283268	0.361342	1.085932
N	0.277602	-0.531555	1.691920
C	3.276105	1.233589	0.721354
C	2.973817	2.572609	0.425875
C	4.619087	0.823749	0.625258
C	3.974208	3.450687	0.042395
H	1.952335	2.916979	0.480795
C	5.603243	1.718715	0.246291
H	4.893939	-0.200609	0.834584
C	5.296526	3.040988	-0.052763
H	3.708646	4.476113	-0.183779
H	6.627908	1.373111	0.182165
H	6.071575	3.733602	-0.350646
C	-1.052989	-0.693994	1.927031
C	-1.620893	-1.963528	2.155020
C	-1.909131	0.423901	1.927783
C	-2.978529	-2.093737	2.374749
H	-0.993509	-2.844783	2.142504
C	-3.267541	0.269332	2.152295
H	-1.500623	1.416051	1.783091
C	-3.820454	-0.983438	2.375427
H	-3.389933	-3.081282	2.546180
H	-3.900072	1.149202	2.147908
H	-4.880887	-1.095622	2.556779
C	0.983734	-1.680791	-1.432756
C	1.933709	-0.730796	-1.775868
C	1.359491	-2.971189	-1.082607
C	3.276656	-1.077540	-1.759823
H	1.631747	0.269936	-2.068554
C	2.701336	-3.314341	-1.092458
H	0.608001	-3.689895	-0.781169
C	3.661561	-2.368284	-1.425795
H	4.018506	-0.331356	-2.011431
H	2.997365	-4.318637	-0.819427
H	4.710182	-2.636251	-1.425167
C	-3.204369	0.780018	-1.188037
C	-2.852703	2.109643	-1.365931
C	-4.499177	0.428631	-0.830772
C	-3.810800	3.093947	-1.169638
H	-1.840577	2.370221	-1.648044
C	-5.451787	1.420112	-0.656656
H	-4.750377	-0.606107	-0.641052
C	-5.110576	2.755300	-0.820806
H	-3.535526	4.131835	-1.302797
H	-6.459107	1.145705	-0.372022
H	-5.854338	3.527592	-0.675845

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.47443987 (Hartrees)

0 1

C	-1.468263	-3.709537	-1.151460
C	-2.680393	-3.236957	-0.806481
C	-1.139470	-1.783369	-0.000851
H	-1.175856	-4.596743	-1.683346
H	-3.670849	-3.608714	-0.997537
N	-2.458030	-2.060524	-0.113012
N	-0.542004	-2.812851	-0.648763
Be	-0.397722	-0.478066	1.037139
H	-0.396873	-0.912215	2.358477
H	-0.330777	1.949423	1.480756
C	-0.518817	1.223838	0.685884
C	1.000644	0.287811	-1.032016
C	0.034602	1.065008	-1.537094
H	1.704911	-0.271049	-1.638438
H	-0.181996	1.225312	-2.581683
N	-0.633044	1.839587	-0.547426
N	1.075549	0.187385	0.360303
C	-0.370088	3.250098	-0.680461
C	0.772942	3.813902	-0.123768
C	-1.261870	4.038554	-1.391091
C	1.009933	5.171501	-0.269908
H	1.469096	3.181615	0.417411
C	-1.014453	5.396802	-1.544443
H	-2.147874	3.579952	-1.812797
C	0.117992	5.965874	-0.980987
H	1.898062	5.610417	0.166366
H	-1.713104	6.011303	-2.097650
H	0.306684	7.025436	-1.094383
C	2.348378	0.320991	0.948537
C	3.429926	0.866778	0.251117
C	2.544248	-0.107544	2.265226
C	4.684798	0.935234	0.841001
H	3.284341	1.247969	-0.752052
C	3.796025	-0.019927	2.849333
H	1.694713	-0.507737	2.804762
C	4.878672	0.490038	2.139993
H	5.512960	1.352467	0.281417
H	3.929558	-0.358171	3.869507
H	5.855941	0.553373	2.600299
C	0.868123	-2.959896	-0.805815
C	1.383348	-3.265917	-2.057962
C	1.701906	-2.763824	0.283344
C	2.757302	-3.364858	-2.220575
H	0.713998	-3.391210	-2.899846
C	3.075182	-2.837177	0.104491
H	1.271991	-2.519301	1.247724
C	3.604000	-3.140316	-1.143057
H	3.165786	-3.596130	-3.195642
H	3.729493	-2.639816	0.944500
H	4.676295	-3.194789	-1.277328
C	-3.507333	-1.249726	0.417209
C	-3.545091	0.102406	0.115832
C	-4.481027	-1.836011	1.211935
C	-4.570911	0.878424	0.632758
H	-2.773817	0.536482	-0.506104
C	-5.510720	-1.053233	1.711803
H	-4.415406	-2.889515	1.452932
C	-5.554610	0.304311	1.426414
H	-4.599977	1.937027	0.409550
H	-6.269768	-1.503022	2.338077
H	-6.353803	0.915056	1.825306

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.51060988 (Hartrees)

0 1

C	2.662995	0.718226	2.240253
C	2.575891	2.026745	1.944156
C	1.026737	0.948070	0.682347
H	3.278679	0.190300	2.945198
H	3.095442	2.880077	2.340484
N	1.573638	2.148726	0.998977
N	1.707312	0.078253	1.471830
Be	-0.112083	0.618719	-0.763916
H	0.105898	1.699520	-1.644113
H	-2.399898	1.289072	0.290379
C	-1.830529	0.543261	-0.270867
C	-0.846443	-1.784271	-1.623329
C	-2.154625	-1.592071	-1.298967
H	-0.649535	-2.703344	-2.169903
H	-2.921925	-2.270392	-1.627063
N	-2.613104	-0.447723	-0.604476
N	0.178751	-0.966607	-1.373834
C	-4.018533	-0.444806	-0.276287
C	-4.797936	0.643155	-0.637824
C	-4.570806	-1.522200	0.400701
C	-6.143910	0.658550	-0.302496
H	-4.347505	1.458191	-1.189949
C	-5.916328	-1.496890	0.735099
H	-3.942767	-2.362325	0.668426
C	-6.704534	-0.408502	0.385011
H	-6.756322	1.503344	-0.589224
H	-6.349727	-2.329342	1.273910

H	-7.755096	-0.394969	0.643937
C	1.473808	-1.425259	-1.620631
C	1.824688	-2.782623	-1.630102
C	2.497278	-0.481831	-1.795007
C	3.140972	-3.173837	-1.814133
H	1.076442	-3.539059	-1.433058
C	3.810653	-0.883396	-1.971223
H	2.229975	0.568424	-1.808879
C	4.147471	-2.232417	-1.981128
H	3.384272	-4.229760	-1.802254
H	4.579425	-0.133056	-2.111690
H	5.174835	-2.543439	-2.117420
C	1.519897	-1.335243	1.516980
C	0.241218	-1.872204	1.521408
C	2.636500	-2.156844	1.576477
C	0.085795	-3.247572	1.585598
H	-0.615879	-1.214146	1.459090
C	2.470370	-3.530142	1.662466
H	3.627299	-1.725811	1.507791
C	1.196501	-4.078632	1.666900
H	-0.911050	-3.668874	1.575217
H	3.341468	-4.171111	1.695200
H	1.067434	-5.151697	1.722709
C	1.200323	3.406793	0.442241
C	-0.138617	3.737192	0.313760
C	2.191630	4.293091	0.050957
C	-0.485888	4.970657	-0.210160
H	-0.889810	3.023216	0.619331
C	1.835801	5.529265	-0.468450
H	3.232394	4.004416	0.125557
C	0.498008	5.869885	-0.599307
H	-1.530789	5.229135	-0.319033
H	2.607427	6.219266	-0.783479
H	0.221150	6.832051	-1.009638

Reaction complex T3

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.50596413 (Hartrees)

0 1			
C	-2.738119	1.932480	-1.678810
C	-2.039496	3.035368	-1.351810
C	-0.838109	1.245029	-0.658549
H	-3.670123	1.812957	-2.200185
H	-2.230250	4.077728	-1.531833
N	-0.881128	2.596532	-0.738685
N	-1.987553	0.851904	-1.258561
Be	0.307602	0.206721	0.305966
H	1.272809	1.011577	1.068795
H	2.557489	0.326940	-0.821107
C	1.822415	-0.305361	-0.321956
C	0.328887	-2.236283	1.175059
C	1.601486	-2.422226	0.767422
H	-0.104579	-3.082272	1.700077
H	2.128112	-3.328000	1.011704
N	2.380227	-1.424613	0.101502
N	-0.423990	-1.112710	1.057551
C	3.793727	-1.638682	0.043223
C	4.651961	-0.616362	0.427151
C	4.304512	-2.854422	-0.396231
C	6.023783	-0.806381	0.353026
H	4.233842	0.309583	0.803551
C	5.677078	-3.035854	-0.466036
H	3.627508	-3.642593	-0.699077
C	6.540830	-2.014127	-0.094168
H	6.690135	-0.011021	0.661095
H	6.072905	-3.979065	-0.820014
H	7.611363	-2.161498	-0.147763
C	-1.732824	-1.132101	1.507396
C	-2.520675	-2.293615	1.572197
C	-2.342617	0.080908	1.874009
C	-3.843068	-2.235651	1.979254
H	-2.113297	-3.240902	1.244294
C	-3.667556	0.129503	2.269191
H	-1.742358	0.983775	1.868141
C	-4.436381	-1.028465	2.324453
H	-4.426410	-3.148778	2.002286
H	-4.101611	1.081053	2.553102
H	-5.471270	-0.990726	2.637740
C	-2.406803	-0.500951	-1.441918
C	-1.478578	-1.463628	-1.807818
C	-3.741029	-0.827755	-1.250235
C	-1.898777	-2.772308	-1.981759
H	-0.439449	-1.187637	-1.932430
C	-4.154288	-2.135485	-1.449255
H	-4.437874	-0.078000	-0.898021
C	-3.235724	-3.109065	-1.812812
H	-1.175418	-3.530182	-2.252674
H	-5.191326	-2.396308	-1.284821
H	-3.558568	-4.132393	-1.953332
C	0.137119	3.485136	-0.285042
C	1.457157	3.236319	-0.622988
C	-0.210759	4.597384	0.466026
C	2.442094	4.113301	-0.200215
H	1.693379	2.362988	-1.214796
C	0.781250	5.473877	0.880712
H	-1.245317	4.760166	0.741036
C	2.106887	5.233061	0.549368
H	3.475335	3.920684	-0.457553
H	0.516413	6.339545	1.473272
H	2.878953	5.915847	0.878695

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -1392.57018005 (Hartrees)

0 1

C	2.499876	-0.358419	2.458357
C	3.065730	0.823053	2.138931
C	1.300859	0.524231	0.768254
H	2.739461	-1.076946	3.221158
H	3.897955	1.349420	2.569530
N	2.310768	1.352169	1.108217
N	1.419386	-0.517890	1.614934
Be	0.072756	0.587425	-0.540782
H	-1.356538	2.491491	-1.102943
H	-1.514403	1.942888	0.555922
C	-1.359336	1.588780	-0.470460
C	-1.199075	-0.858046	-2.142714
C	-2.341949	-0.242749	-1.804356
H	-1.232267	-1.545226	-2.981063
H	-3.228824	-0.461969	-2.383587
N	-2.500451	0.734091	-0.815319
N	0.046847	-0.631923	-1.551105
C	-3.775320	1.009571	-0.341998
C	-4.095719	2.257574	0.213966
C	-4.789046	0.035727	-0.385098
C	-5.371883	2.515583	0.688107
H	-3.346373	3.034274	0.252875
C	-6.059685	0.311379	0.088275
H	-4.564639	-0.950927	-0.766863
C	-6.368940	1.552332	0.630040
H	-5.588203	3.492621	1.103281
H	-6.816143	-0.462853	0.042979
H	-7.362707	1.760893	1.002309
C	0.969707	-1.667326	-1.581611
C	0.596310	-3.012058	-1.727531
C	2.338559	-1.392782	-1.414893
C	1.542958	-4.023799	-1.686010
H	-0.451759	-3.262552	-1.824245
C	3.274458	-2.410254	-1.357195
H	2.659600	-0.358233	-1.364854
C	2.887138	-3.740170	-1.489625
H	1.218530	-5.052461	-1.790841
H	4.321865	-2.161991	-1.232576
H	3.621160	-4.534357	-1.458184
C	0.588669	-1.680567	1.567891
C	-0.779670	-1.534413	1.392527
C	1.176751	-2.932566	1.647257
C	-1.567700	-2.668873	1.281985
H	-1.227737	-0.549024	1.334139
C	0.373821	-4.060208	1.568130
H	2.253689	-3.023621	1.712170
C	-0.994307	-3.930576	1.380410
H	-2.632571	-2.557103	1.126129
H	0.827835	-5.041015	1.617028
H	-1.614849	-4.813521	1.300559
C	2.599655	2.579496	0.441300
C	1.561278	3.430292	0.090150
C	3.917525	2.899679	0.147435
C	1.853218	4.612372	-0.572960
H	0.541098	3.169009	0.339830
C	4.197864	4.092111	-0.502154
H	4.712051	2.209950	0.402075
C	3.167911	4.947889	-0.866144
H	1.046040	5.275932	-0.853078
H	5.223762	4.343385	-0.736989
H	3.389168	5.873531	-1.380318

$Me_2NHC/BeCl_2$

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -1240.14327461 (Hartrees)

0 1			
C	2.668811	-0.647462	-0.190446
C	2.668865	0.647888	0.190897
C	0.527567	0.000498	-0.000556
H	3.478046	-1.325877	-0.394676
H	3.478143	1.326110	0.395599
N	1.351567	1.024332	0.298078
N	1.351495	-1.023535	-0.298695
C	0.936539	2.357737	0.711891
H	1.344966	3.094235	0.021935
H	-0.146823	2.413996	0.686040
H	1.301193	2.554891	1.718837
C	0.936598	-2.356902	-0.712775
H	-0.146976	-2.411288	-0.693637
H	1.307181	-2.556141	-1.717137
H	1.339390	-3.093088	-0.019185
Be	-1.267734	-0.000063	-0.000061
Cl	-2.123353	-1.514405	0.761853
Cl	-2.125817	1.513304	-0.761104

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -1240.02139602 (Hartrees)

0 1			
C	-0.605383	-0.662343	1.732665
C	-0.605400	0.662410	1.732637
C	-0.440345	0.000025	-0.518245
H	-0.823587	-1.368836	2.515167
H	-0.823617	1.368920	2.515122
N	-0.142022	1.080183	0.442743
N	-0.141998	-1.080144	0.442769
C	-0.363033	2.447603	0.002437
H	0.075179	3.132455	0.726151
H	0.125039	2.586231	-0.960987
H	-1.429734	2.654161	-0.106500
C	-0.363095	-2.447566	0.002495
H	0.124893	-2.586226	-0.960968
H	0.075148	-3.132423	0.726185
H	-1.429812	-2.654078	-0.106355
Be	1.198081	-0.000118	-0.266879
Cl	3.036939	-0.000020	-0.459828
Cl	-2.121301	-0.000026	-1.139632

Reaction complex T2

M062x/def2-TZVP optimized geometry (Å).
E_e = -1239.99080918 (Hartrees)

0 1			
C	-1.050499	-0.323883	1.604253
C	-1.913049	0.497239	1.002878
C	-0.458754	0.260355	-0.787247
H	-1.284439	-0.811164	2.544267
H	-2.853855	0.853739	1.389661
N	-1.342444	1.097037	-0.187449
N	0.175136	-0.610672	1.010861
C	-0.797295	2.438848	0.097756
H	-0.081135	2.417363	0.927098
H	-0.321276	2.830866	-0.797197
H	-1.625488	3.089403	0.372614
C	0.579143	-2.011179	1.127948
H	-0.117661	-2.671243	0.599179
H	1.577125	-2.145954	0.710914
H	0.612021	-2.310407	2.178963
Be	1.116134	0.200417	-0.075378
Cl	2.937022	0.463240	-0.272959
Cl	-1.193254	-1.088364	-1.589476

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -1240.07798253 (Hartrees)

0 1			
C	0.734868	2.055047	-0.000123
C	-0.626450	2.119712	-0.000010
C	0.821756	-0.305333	-0.000028
H	1.333257	2.947500	-0.000228
H	-1.050905	3.121756	-0.000026
N	-1.469756	1.085817	0.000117
N	1.443801	0.848804	-0.000105
C	-2.892772	1.406075	0.000298
H	-3.166085	1.983066	-0.886542
H	-3.461997	0.479666	0.000232
H	-3.165913	1.982827	0.887347
C	2.911366	0.960316	-0.000192
H	3.311374	0.470855	0.884636
H	3.311257	0.470960	-0.885133
H	3.180833	2.010166	-0.000145
Be	-0.918937	-0.413227	0.000052
Cl	1.830658	-1.702614	-0.000005
Cl	-1.955775	-1.989805	-0.000001

Reaction complex D

M062x/def2-TZVP optimized geometry (Å).
E_e = -1239.96932875 (Hartrees)

0 1			
C	0.889092	1.588068	-0.046616
C	2.062644	0.942306	0.027082
C	-0.621137	-0.316672	-0.085419
H	0.888470	2.661026	0.071695
H	2.950134	1.537510	0.208230
N	2.264403	-0.448433	-0.089697
N	-0.388781	1.044737	-0.295953
C	3.643586	-0.880872	-0.117300
H	4.173243	-0.574156	0.789731
H	3.696180	-1.966121	-0.185696
H	4.173819	-0.461371	-0.977342
C	-1.504905	1.973198	-0.184579
H	-1.278020	2.875226	-0.750472
H	-2.397029	1.513623	-0.602965
H	-1.697511	2.233371	0.860125
Be	0.898088	-1.049539	-0.117396
Cl	-1.359860	-0.640899	1.619761
Cl	-1.819356	-0.984468	-1.255242

2 $Me_2NHC/BeCl_2$

Reaction complex A

M062x/def2-TZVP optimized geometry (Å).
E_e = -1544.97102012 (Hartrees)

0 1			
C	3.449744	-1.122439	0.253109
C	2.665486	-1.802737	1.117033
C	1.438713	-0.111678	0.268672
H	4.477083	-1.265188	-0.030278
H	2.871623	-2.657064	1.736794
N	1.445363	-1.165821	1.113498
N	2.682529	-0.095292	-0.248766
C	0.310964	-1.557098	1.935211
H	0.678159	-2.111293	2.796424
H	-0.199697	-0.655906	2.270901
H	-0.377707	-2.184935	1.367258
C	3.178327	0.900850	-1.191283
H	2.828928	1.883850	-0.891154
H	4.265599	0.864808	-1.181622
H	2.802968	0.698941	-2.192351
Be	-0.000017	0.998637	-0.000008
C	-1.438728	-0.111697	-0.268707
C	-3.449746	-1.122482	-0.253192
C	-2.665438	-1.802815	-1.117043
H	-4.477098	-1.265226	0.030148
H	-2.871538	-2.657170	-1.736777
N	-1.445309	-1.165911	-1.113445
N	-2.682555	-0.095326	0.248703
C	-0.310838	-1.557254	-1.935026
H	-0.677952	-2.111602	-2.796175
H	0.199794	-0.656086	-2.270823
H	0.377836	-2.184962	-1.366933
C	-3.178389	0.900820	1.191197
H	-4.265661	0.864793	1.181476
H	-2.803086	0.698906	2.192286
H	-2.828960	1.883814	0.891086
Cl	0.169936	2.024585	-1.724601
Cl	-0.169994	2.024556	1.724601

Reaction complex C

M062x/def2-TZVP optimized geometry (Å).
E_e = -1544.89736833 (Hartrees)

0 1			
C	2.793511	0.852172	-1.880901
C	3.485511	-0.071540	-1.181614
C	1.452891	0.106716	-0.224570
H	3.066316	1.440832	-2.738725
H	4.481836	-0.456384	-1.308457
N	2.650463	-0.511356	-0.180511
N	1.556882	0.942397	-1.285392
C	3.036408	-1.550963	0.763246
H	3.193327	-2.486556	0.227394
H	3.959463	-1.258649	1.262337
H	2.242479	-1.669249	1.494461
C	0.511802	1.846821	-1.741448
H	-0.458175	1.360977	-1.672863
H	0.490365	2.747561	-1.129626
H	0.715758	2.110434	-2.777346
Be	-0.095697	-0.005635	0.798340
C	-1.394238	-0.699478	-0.236467
C	-2.727924	1.251137	-0.169871
C	-1.856122	1.953167	0.622679
H	-3.670031	1.668584	-0.472015
H	-2.183541	2.959313	0.886390
N	-0.686672	1.542381	1.072642
N	-2.496047	-0.082779	-0.565278
C	0.080441	2.425754	1.924302
H	-0.403924	3.398593	2.045001
H	0.217725	1.972255	2.908574
H	1.079002	2.586000	1.501010
C	-3.571299	-0.713136	-1.346046
H	-3.949703	-1.577972	-0.805473
H	-4.364202	0.011347	-1.493150
H	-3.182487	-1.042942	-2.306763
Cl	-1.257184	-2.332975	-0.817004
Cl	0.146026	-1.042319	2.506405

Cartesian coordinates for optimized THF complexes

$Me_2NHC\text{-}BeH_2\text{-}THF$

THF

M062x/def2-TZVP optimized geometry (Å).
E_e = -232.430367038 (Hartrees)

0 1			
C	-0.772904	1.009904	-0.050712
C	0.772366	1.010375	-0.050140
C	-1.123854	-0.469602	0.159908
C	1.124168	-0.469150	0.159473
O	0.000205	-1.191783	-0.301244
H	-1.287818	-0.679498	1.225036
H	-1.995478	-0.801612	-0.401243
H	1.288985	-0.679499	1.224369
H	1.995585	-0.800415	-0.402434
H	1.192078	1.639725	0.732985
H	1.157524	1.364177	-1.005047
H	-1.193657	1.639789	0.731424
H	-1.157514	1.362437	-1.006313

Reaction complex B

M062x/def2-TZVP optimized geometry (Å).
E_e = -553.191547889 (Hartrees)

0 1			
C	3.829929	0.188767	-0.090580
C	3.102335	-0.284983	-1.371057
Be	0.208054	-0.541901	1.396827
H	0.291905	0.302071	2.517855
H	0.416307	-1.937617	1.461867
C	-1.259591	-0.079939	0.420120
C	-3.258257	-0.058378	-0.623293
C	-2.802532	1.213312	-0.597880
H	-4.168889	-0.474490	-1.016584
H	-3.233479	2.125979	-0.970023
N	-1.585881	1.176009	0.044050
N	-2.299847	-0.828381	-0.002422
C	-0.741842	2.328797	0.304108
H	-1.369239	3.189627	0.529481
H	-0.114423	2.086991	1.160839
H	-0.116449	2.549240	-0.561110
C	-2.408486	-2.263065	0.201880
H	-3.242471	-2.482003	0.868072
H	-2.568650	-2.759117	-0.755133
H	-1.476691	-2.598992	0.652723
C	2.801289	-0.025357	1.018814
C	1.724498	-0.715712	-0.867347
O	1.537084	0.017849	0.344626
H	2.895600	-1.008968	1.488715
H	2.778791	0.737708	1.791574
H	1.685093	-1.781122	-0.623434
H	0.898657	-0.467376	-1.531990
H	3.615111	-1.109342	-1.863174
H	3.017244	0.529914	-2.088190
H	4.741493	-0.372956	0.104285
H	4.097239	1.241220	-0.170072

Reaction complex T1

M062x/def2-TZVP optimized geometry (Å).
E_e = -553.15919948 (Hartrees)

0 1			
C	-3.843906	0.554947	0.423493
C	-3.648770	-0.370292	-0.778185
Be	-0.188094	1.031854	0.068926
H	0.989050	0.416791	1.087696
H	-0.485144	2.360915	0.162243
C	1.253397	0.199354	-0.155781
C	3.494158	-0.122186	0.026161
C	2.918976	-1.324802	0.122842
H	4.534908	0.147899	0.092817
H	3.367491	-2.291590	0.279571
N	1.557134	-1.197673	-0.211669
N	2.524248	0.805437	-0.370883
C	0.608451	-2.110176	0.361637
H	1.038284	-3.110696	0.394087
H	0.338264	-1.806083	1.387908
H	-0.302638	-2.146099	-0.234778
C	2.664196	2.200858	-0.054769
H	2.396085	2.397779	0.995332
H	3.694881	2.510683	-0.224770
H	2.001394	2.791617	-0.685420
C	-2.536834	0.383418	1.179538
C	-2.193177	-0.122155	-1.123241
O	-1.551716	0.077652	0.160073
H	-2.203092	1.279346	1.699522
H	-2.557169	-0.464129	1.865450
H	-2.065472	0.790988	-1.710171
H	-1.684524	-0.946948	-1.617814
H	-4.309028	-0.138778	-1.611423
H	-3.800394	-1.412108	-0.490833
H	-3.948383	1.587998	0.088898
H	-4.707035	0.295640	1.033085

Reaction complex D

E_e = -553.238582484 (Hartrees)

M062x/def2-TZVP optimized geometry (Å).

0 1			
C	-3.408272	-0.128407	0.938230
C	-3.514040	-1.176259	-0.170226
H	-3.060614	-0.587643	1.864792
H	-3.966629	-2.108867	0.160046
Be	0.171136	0.111944	-0.354488
H	0.820499	-2.209970	-0.074618
H	1.534186	-1.490542	-1.504562
C	1.220969	-1.265942	-0.464643
C	2.895614	0.373770	0.259214
C	2.171429	1.483780	0.047862
H	3.956841	0.482531	0.440561
H	2.691550	2.436250	0.058774
N	0.786363	1.519518	-0.164032
N	2.403851	-0.936601	0.342783
C	0.243551	2.849666	-0.284568
H	0.302280	3.418137	0.654120
H	0.771295	3.435508	-1.048025
H	-0.805082	2.814725	-0.585843
C	3.424913	-1.958163	0.312172
H	3.827268	-2.111119	-0.703049
H	4.249950	-1.696348	0.977016
H	3.001474	-2.905558	0.650388
O	-1.460216	-0.059960	-0.361870
C	-2.348925	0.807779	0.386505
C	-2.060787	-1.364395	-0.566649
H	-4.345477	0.387669	1.135494
H	-4.093495	-0.785839	-1.008324
H	-1.903303	-1.640314	-1.606892
H	-1.542892	-2.073204	0.078714
H	-2.769359	1.534179	-0.309921
H	-1.749512	1.320915	1.135605

Cartesian coordinates for optimized proposed reaction scheme 2 and 3 in main manuscript

Me_2NHC-BeH_2Me-BeH_2Me-Me_2NHC

M062x/def2-TZVP optimized geometry (Å).
E_e = -720.18189565 (Hartrees)

C	-4.358883	-0.791635	-0.354333
C	-4.469301	-0.032378	0.756049
C	-2.390251	0.266492	-0.066344
H	-5.060194	-1.452720	-0.831667
H	-5.285732	0.103635	1.442760
N	-3.257193	0.601124	0.912700
N	-3.084045	-0.595126	-0.838304
C	-2.940635	1.511782	1.998385
H	-3.354035	1.121456	2.927066
H	-1.859692	1.585796	2.080253
H	-3.352850	2.500884	1.799908
C	-2.564317	-1.266917	-2.017983
H	-1.515708	-1.006116	-2.121573
H	-2.649085	-2.345254	-1.890616
H	-3.124068	-0.953440	-2.899133
Be	-0.673281	0.851061	-0.148641
H	0.008064	0.096192	-1.229003
Be	0.656352	-0.755609	-0.203884
C	2.392238	-0.241328	-0.074539
C	4.495725	-0.133062	0.732980
C	4.399239	0.764304	-0.270657
C	2.923009	-1.760230	1.804046
C	2.599478	1.517226	-1.822853
N	3.260552	-0.731311	0.836314
N	3.108797	0.682898	-0.746361
H	-0.000486	0.015987	0.906146
H	1.851186	-1.731406	1.980179
H	3.195099	-2.745095	1.425801
H	3.454830	-1.562969	2.733228
H	2.767685	2.565582	-1.580649
H	3.106446	1.268813	-2.755172
H	1.532107	1.341835	-1.914189
H	5.119946	1.451867	-0.676576
H	5.318464	-0.388321	1.376836
C	-0.334948	2.584924	-0.151616
H	-0.467771	3.017166	-1.151809
H	-0.955862	3.193934	0.515801
H	0.703637	2.790415	0.136191
C	0.252610	-2.471384	-0.341656
H	-0.802348	-2.646553	-0.095171
H	0.393768	-2.839311	-1.366075
H	0.823748	-3.154039	0.298255

Me_2NHC-BeH_2-BeH_2-Me_2NHC

M062x/def2-TZVP optimized geometry (Å).
E_e = -641.543768982 (Hartrees)

C	-4.395512	0.938335	-0.359450
C	-4.672545	-0.130413	0.418636
C	-2.461734	-0.160889	-0.017074
H	-5.033142	1.710638	-0.750791
H	-5.597306	-0.474287	0.846699
N	-3.479241	-0.787539	0.611538
N	-3.043041	0.903253	-0.607220
C	-3.323144	-1.976596	1.430690
H	-4.127922	-2.676439	1.210037
H	-2.361702	-2.423982	1.187641
H	-3.350904	-1.711345	2.487416
C	-2.335090	1.872570	-1.431945
H	-2.206352	1.481544	-2.440501
H	-2.920771	2.789088	-1.465841
H	-1.357660	2.068082	-0.996024
Be	-0.747072	-0.709333	-0.050527
Be	0.749678	0.716964	-0.056866
C	2.462230	0.162427	-0.020090
C	4.393964	-0.941633	-0.358304
C	4.671717	0.125446	0.421806
C	2.333984	-1.868988	-1.437736
C	3.324061	1.974171	1.431968
N	3.042272	-0.902564	-0.609901
N	3.479645	0.785598	0.612057
H	1.356344	-2.065011	-1.002524
H	2.206054	-1.474996	-2.445233
H	2.919069	-2.785792	-1.473973
H	3.346096	1.707629	2.488499
H	4.132228	2.671467	1.215710
H	2.365347	2.425324	1.185061
H	5.596190	0.466270	0.852910
H	5.030584	-1.715220	-0.748741
H	-0.000532	0.001126	-1.122157
H	0.000514	0.009382	1.011492
H	-0.594302	-2.093169	-0.055398
H	0.602707	2.101348	-0.071033

$PhSiH_2Me$

M062x/def2-TZVP optimized geometry (Å).
E_e = -562.22420221 (Hartrees)

C	-0.041346	-0.237972	0.012745
C	0.916073	-1.255804	-0.021234
C	0.408354	1.082625	0.032687
C	2.272204	-0.966686	-0.032590
H	0.598808	-2.293588	-0.040793
C	1.765711	1.380071	0.021457
H	-0.306852	1.897433	0.056625
C	2.699043	0.355195	-0.010578
H	2.997044	-1.770513	-0.060106
H	2.093750	2.411840	0.037311
H	3.757277	0.583649	-0.019603
Si	-1.868161	-0.651754	0.038221
H	-2.173464	-1.555570	-1.095334
H	-2.187858	-1.386232	1.284554
C	-2.899395	0.903179	-0.071756
H	-2.675069	1.456911	-0.984673
H	-3.962106	0.658629	-0.077748
H	-2.711139	1.558339	0.780288

$PhSiH_3$

M062x/def2-TZVP optimized geometry (Å).
E_e = -522.900414565 (Hartrees)

C	0.464638	0.002081	-0.010629
C	-0.254348	1.198753	-0.007747
C	-0.252020	-1.197307	-0.007813
C	-1.642870	1.199929	0.002511
H	0.274665	2.145302	-0.018343
C	-1.639127	-1.202430	0.002690
H	0.278236	-2.143686	-0.018694
C	-2.336352	-0.001599	0.008519
H	-2.183193	2.138041	0.002749
H	-2.177266	-2.141793	0.003272
H	-3.418857	-0.003264	0.014301
Si	2.333472	0.000458	0.004661
H	2.852394	-0.262498	1.364565
H	2.842655	-1.056643	-0.894951
H	2.823227	1.321561	-0.443328

$THF\text{-}BeH_2\text{-}THF$

M062x/def2-TZVP optimized geometry (Å).
E_e = -559.47143086 (Hartrees)

C	3.170005	0.815874	-0.542277
C	3.576430	-0.464361	0.187028
C	1.762677	0.473908	-0.991063
C	2.294462	-0.827175	0.920317
O	1.222820	-0.331894	0.078873
H	1.109518	1.336230	-1.105911
H	1.760261	-0.130588	-1.901541
H	2.216587	-0.319586	1.882584
H	2.136789	-1.893995	1.063582
H	4.407874	-0.325033	0.875198
H	3.846834	-1.241767	-0.530201
H	3.130172	1.653645	0.155536
H	3.823582	1.070756	-1.374456
C	-3.489732	0.104485	0.522950
C	-3.184566	-0.867862	-0.615495
C	-2.427489	1.167022	0.309920
C	-1.662810	-0.875045	-0.620623
O	-1.270365	0.436778	-0.156989
H	-2.710360	1.879400	-0.468200
H	-2.133094	1.703278	1.209326
H	-1.221667	-1.027502	-1.604741
H	-1.255992	-1.599753	0.085960
H	-3.573880	-0.482177	-1.559573
H	-3.593176	-1.863894	-0.455598
H	-4.498050	0.512793	0.485768
H	-3.332042	-0.379532	1.487531
Be	0.000672	0.446693	1.027820
H	-0.383471	-0.449485	2.032635
H	0.413922	1.770284	1.211210

Cartesian coordinates for optimized 2,6-diisopropylphenyl substituted NHC complexes

2,6-diisopropylphenyl substituted NHC

M062x/6-31G* optimized geometry (Å).
E_e = -1093.50403247 (Hartrees)

Be	0.249445	0.895579	-1.194281
C	0.533468	-0.296983	0.147953
C	0.340618	-1.946852	1.706216
C	1.655652	-1.650532	1.589687
H	-0.185451	-2.660832	2.320951
H	2.529748	-2.051870	2.078627
N	1.746771	-0.643697	0.640645
N	-0.322592	-1.111123	0.817906
C	-1.729925	-1.182417	0.551812
C	-2.597108	-0.377657	1.295075
C	-2.167448	-2.046554	-0.455633
C	-3.960389	-0.458639	1.013117
C	-3.542702	-2.114289	-0.694908
C	-4.430917	-1.327354	0.030461
H	-4.655517	0.161422	1.573590
H	-3.911434	-2.781183	-1.469145
H	-5.496091	-1.386842	-0.172591
C	2.996171	-0.116457	0.163540
C	3.558770	0.978667	0.820510
C	3.584208	-0.727967	-0.945605
C	4.791134	1.442162	0.362467
C	4.817138	-0.234615	-1.372911
C	5.419350	0.835345	-0.720508
H	5.251296	2.295592	0.852500
H	5.298109	-0.690188	-2.233801
H	6.378097	1.208772	-1.067441
H	1.108103	1.994250	-1.042233
H	0.090104	0.133740	-2.378174
O	-1.374266	1.545365	-0.821782
C	-1.473093	2.907234	-0.398400
C	-2.438913	1.304144	-1.759604
C	-2.971302	3.084239	-0.196278
H	-0.858384	3.017484	0.496078
H	-1.070309	3.560540	-1.182414
C	-3.555280	2.299955	-1.386053
H	-2.046543	1.463180	-2.767905
H	-2.722433	0.256794	-1.650945
H	-3.277852	4.132488	-0.179743
H	-3.269350	2.618408	0.749005
H	-3.765414	2.969175	-2.224710
H	-4.484431	1.788886	-1.123296
C	-1.175991	-2.815810	-1.286023
H	-0.576191	-2.111318	-1.877194
H	-0.489307	-3.396454	-0.660800
H	-1.689622	-3.500813	-1.964621
C	-2.048791	0.557472	2.338308
H	-1.504268	0.013045	3.117153
H	-1.340645	1.257895	1.881964
H	-2.851758	1.124965	2.815433
C	2.806690	1.668100	1.925320
H	1.901177	2.123033	1.504624
H	2.496401	0.970442	2.710337
H	3.415405	2.453021	2.380176
C	2.872684	-1.831508	-1.682113
H	2.537287	-2.624589	-1.004542
H	1.985014	-1.422990	-2.182100
H	3.527199	-2.275645	-2.435833

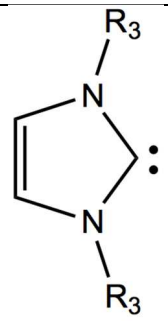
Reaction complex T1

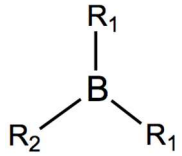
M062x/6-31G* optimized geometry (Å).
E_e = -1093.47138345 (Hartrees)

Be	0.156468	1.178296	-0.825107
C	0.519983	-0.334291	-0.178122
C	0.445426	-2.566346	0.432943
C	1.709998	-2.294894	0.084115
H	-0.014796	-3.490135	0.749272
H	2.579198	-2.934457	0.044141
N	1.803117	-0.924820	-0.212083
N	-0.278092	-1.357119	0.429543
C	-1.689003	-1.276387	0.417652
C	-2.317004	-0.423819	1.343552
C	-2.440282	-1.990224	-0.533761
C	-3.704008	-0.293823	1.305228
C	-3.832253	-1.852582	-0.523169
C	-4.464206	-1.008276	0.381535
H	-4.194142	0.357538	2.025575
H	-4.419177	-2.403497	-1.253807
H	-5.545623	-0.908197	0.370825
C	3.016054	-0.189258	-0.065995
C	3.458591	0.144609	1.220665
C	3.732440	0.174733	-1.210965
C	4.657261	0.845933	1.348638
C	4.927699	0.875691	-1.047872
C	5.389519	1.206489	0.221693
H	5.013222	1.114994	2.339894
H	5.496563	1.165589	-1.927346
H	6.322156	1.751881	0.333595
H	0.946002	2.098025	-1.448400
H	0.062532	-0.265340	-1.456877
O	-1.407107	1.718148	-0.518771
C	-1.531294	3.050997	0.005413

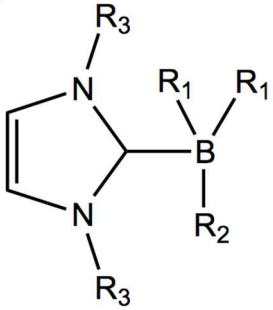
C	-2.478181	1.507850	-1.467062
C	-3.031056	3.176221	0.215101
H	-0.928372	3.098735	0.913758
H	-1.137788	3.760166	-0.732360
C	-3.602961	2.461473	-1.023804
H	-2.095312	1.741089	-2.466322
H	-2.742214	0.451904	-1.407005
H	-3.357953	4.214683	0.297291
H	-3.313771	2.643402	1.127752
H	-3.828396	3.179713	-1.816077
H	-4.516735	1.912117	-0.788796
C	-1.780929	-2.860979	-1.575864
H	-0.886672	-2.382114	-1.983442
H	-1.468155	-3.826956	-1.164362
H	-2.477706	-3.058106	-2.394869
C	-1.490737	0.319275	2.356604
H	-0.903006	-0.379629	2.960817
H	-0.772492	0.981276	1.860632
H	-2.125454	0.911865	3.021777
C	2.626120	-0.231275	2.417853
H	1.612654	0.173487	2.318436
H	2.522649	-1.318102	2.509214
H	3.070025	0.154682	3.339038
C	3.196749	-0.178575	-2.571956
H	3.012157	-1.254363	-2.657748
H	2.241689	0.330053	-2.744251
H	3.897160	0.119649	-3.356524

Diagram of boron optimized geometries

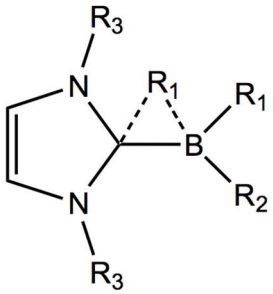




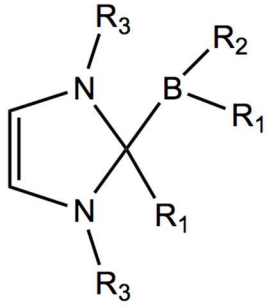
A



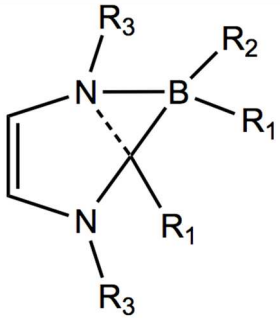
T1



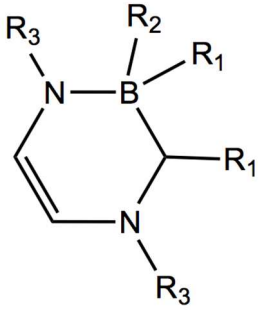
B



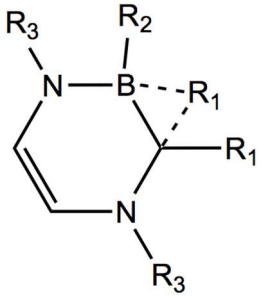
T2



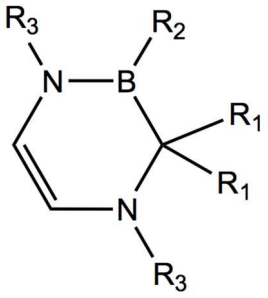
C



T3



D

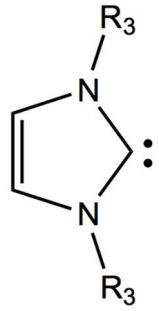


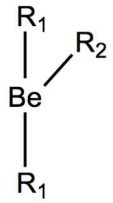
Me_2NHC/BH_3: R_1/R_2 = H, R_3 = Me
Me_2NHC/BH_2NHMe: R_1 = H, R_2 = NHMe R_3 = Me
Me_2NHC/BCl_3* : R_1/R_2 = Cl, R_3 = Me

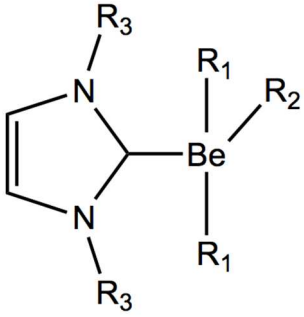
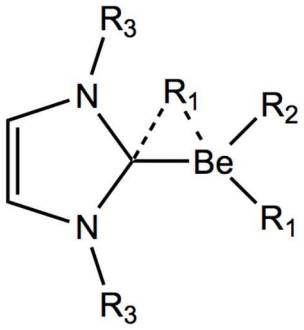
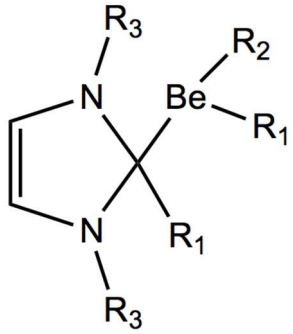
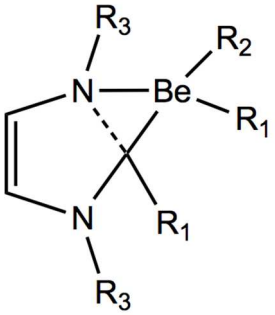
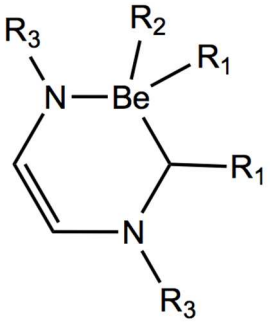
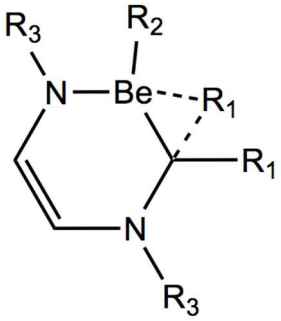
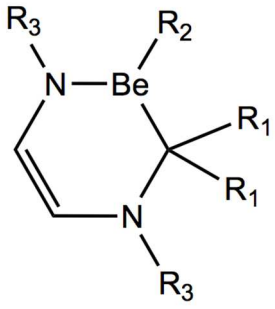
Ph_2NHC/BH_3: R_1/R_2 = H, R_3 = Ph
Ph_2NHC/BH_2NHMe: R_1 = H, R_2 = NHMe R_3 = Ph

* Please note structures **T1** and **T2** are not applicable.

Diagram of beryllium optimized geometries





A		**T1**		**B**	
T2		**C**		**T3**	
D					

Me_2NHC/BeH_2: R_1 = H, R_2 = N.A., R_3 = Me

2 Ph_2NHC/BeH_2: R_1 = H, R_2 = Ph_2NHC, R_3 = Ph

2 $Me_2NHC/BeCl_2$**: R_1 = Cl, R_2 = Me_2NHC, R_3 = Me

2 **Me_2NHC/BeH_2**: R_1 = H, R_2 = Me_2NHC, R_3 = Me

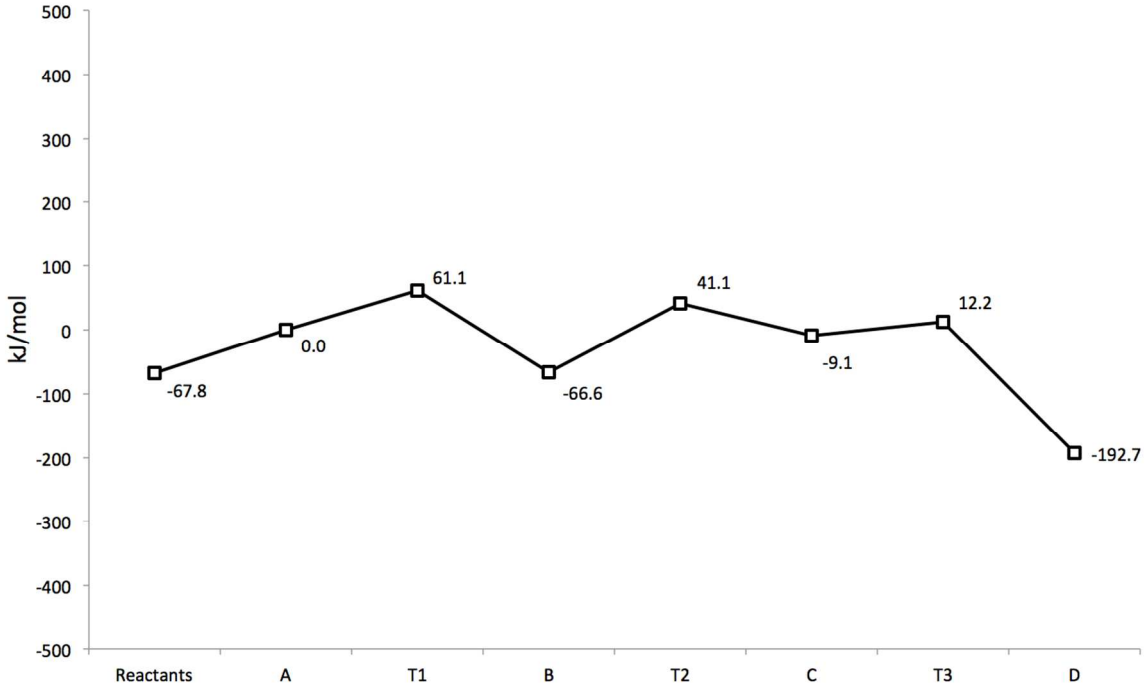
$Me_2NHC/BeCl_2$*: R_1 = Cl, R_2 = N.A., R_3 = Me

* Please note structures **T1** and **T2** are not applicable.

** Please note structures **T1**, **B**, **T2**, **T3** and **D** and not applicable.

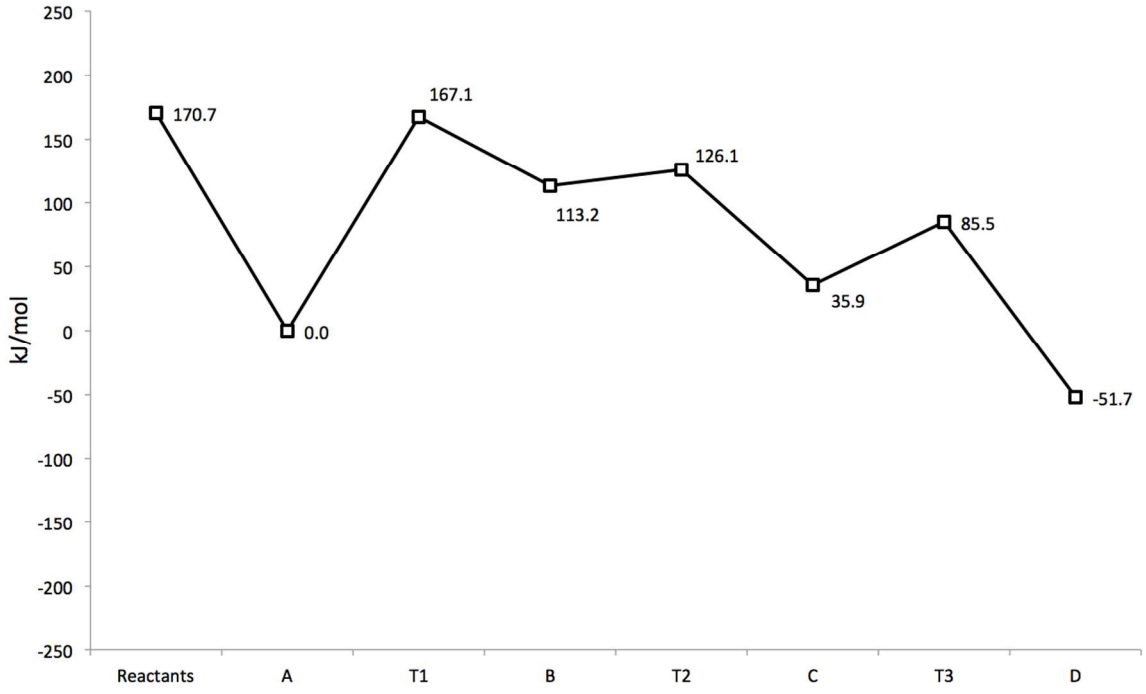
Reaction profile for silicon complex

Me_2NHC/Ph_2SiH_2 Reaction Pathway

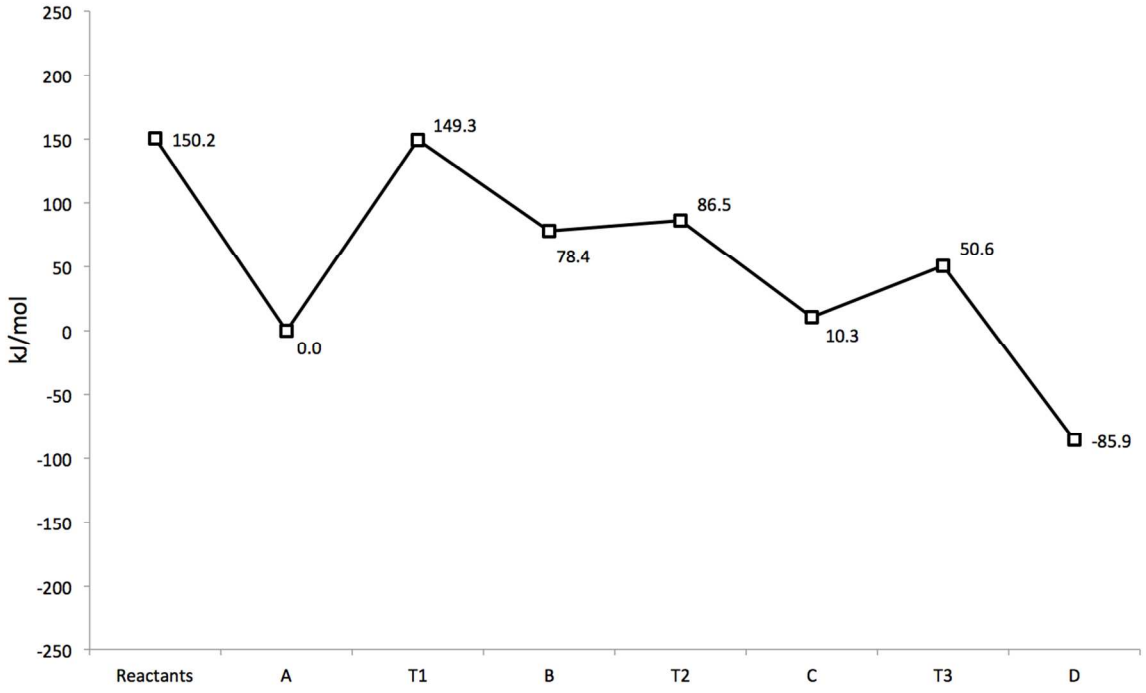


Reaction profile for boron complexes

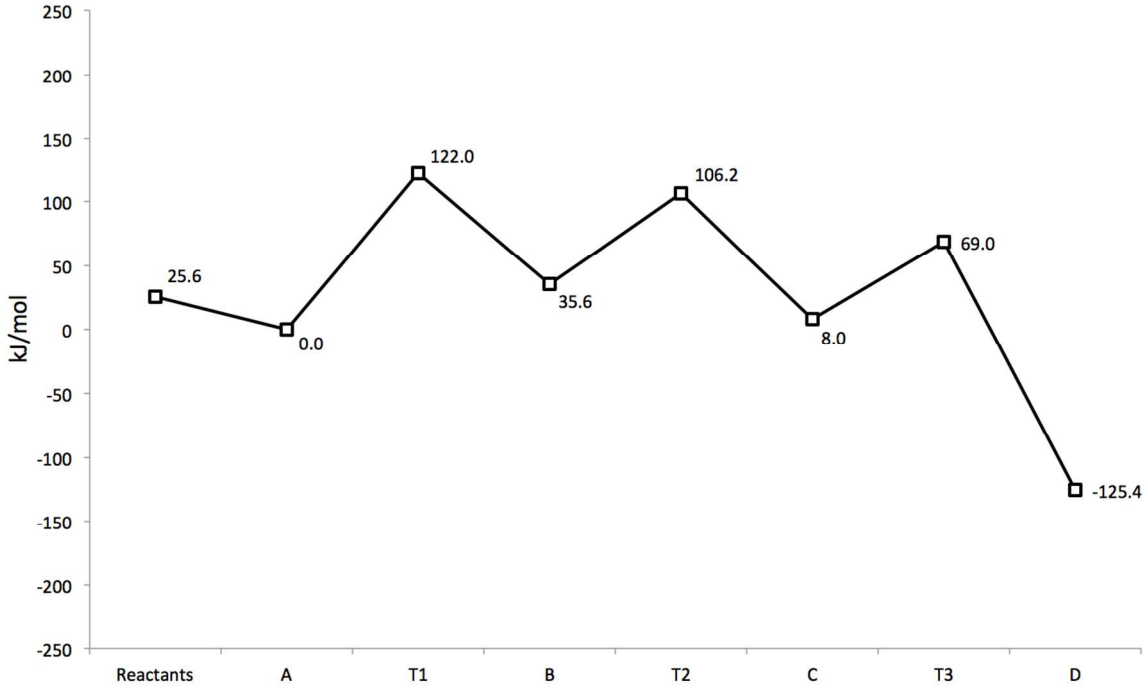
Me_2NHC/BH_3 Reaction Pathway



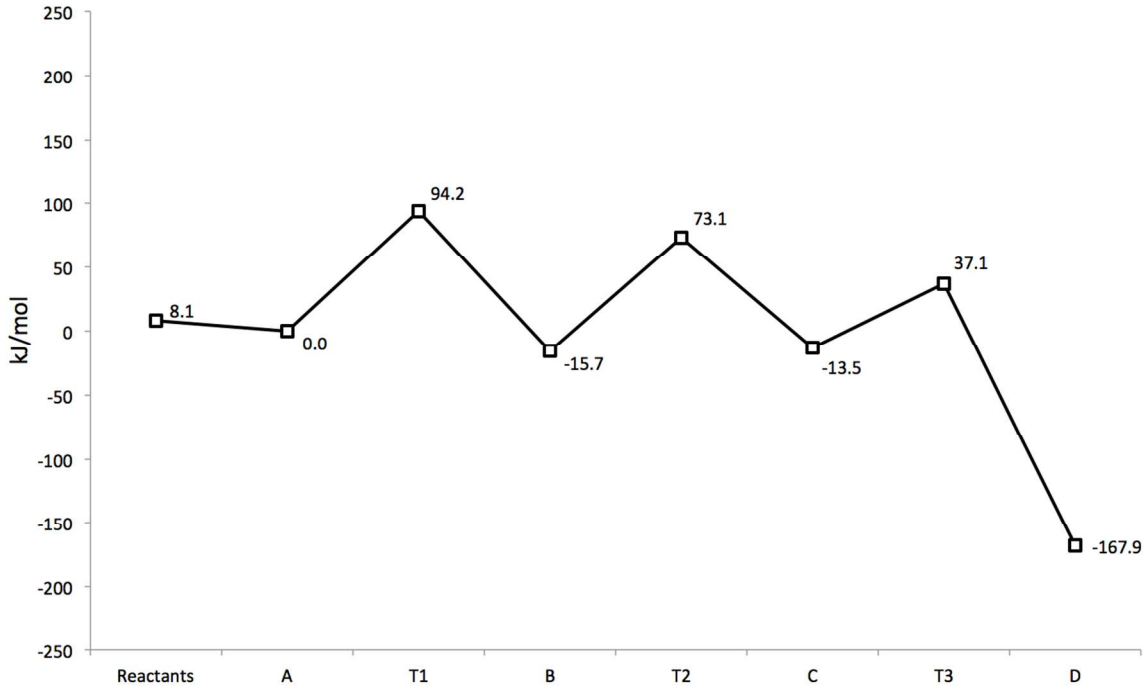
Ph_2NHC/BH_3 Reaction Pathway



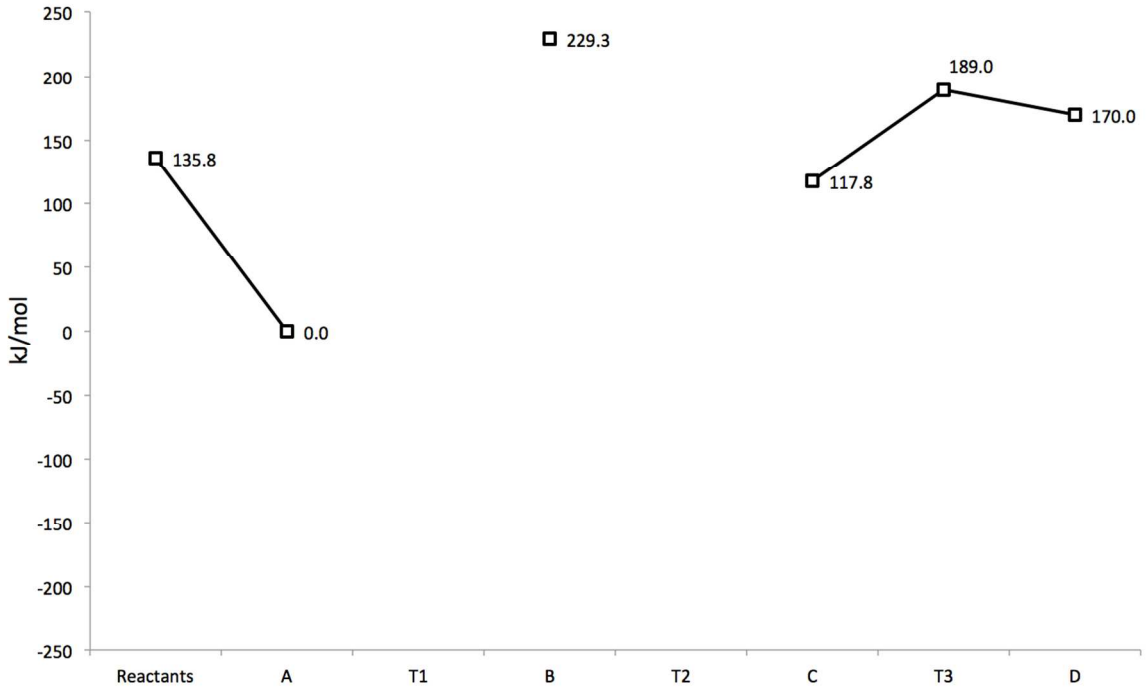
Me_2NHC/BH_2NHMe Reaction Pathway



Ph_2NHC/BH_2NHMe Reaction Pathway

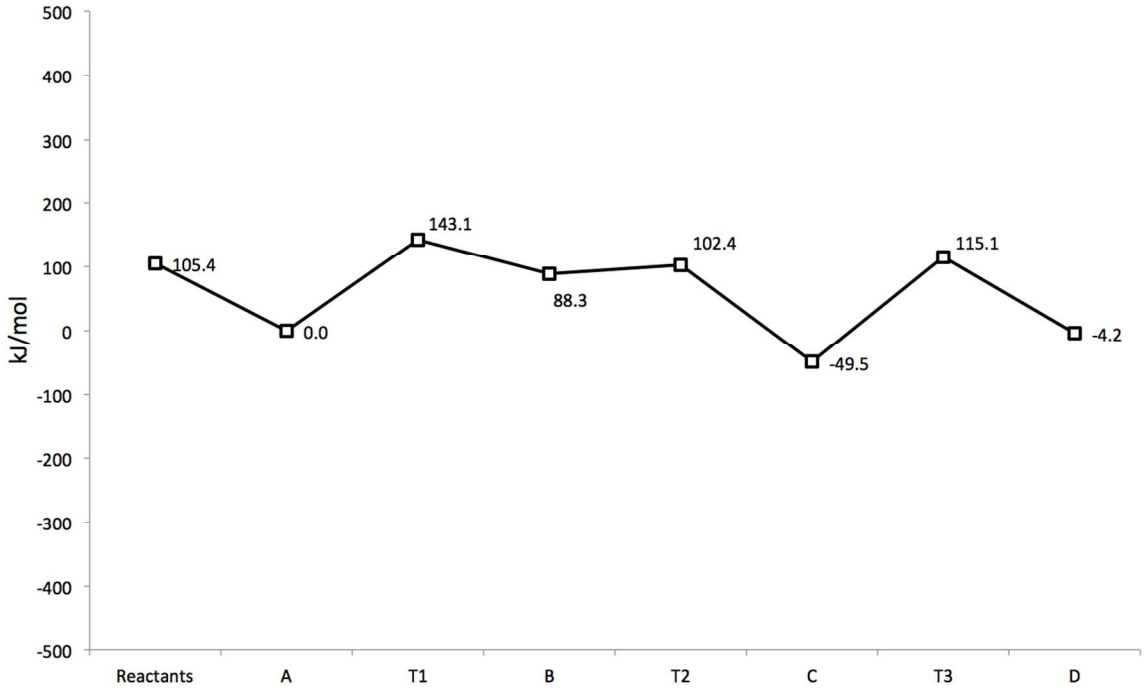


Me_2NHC/BCl_3 Reaction Pathway

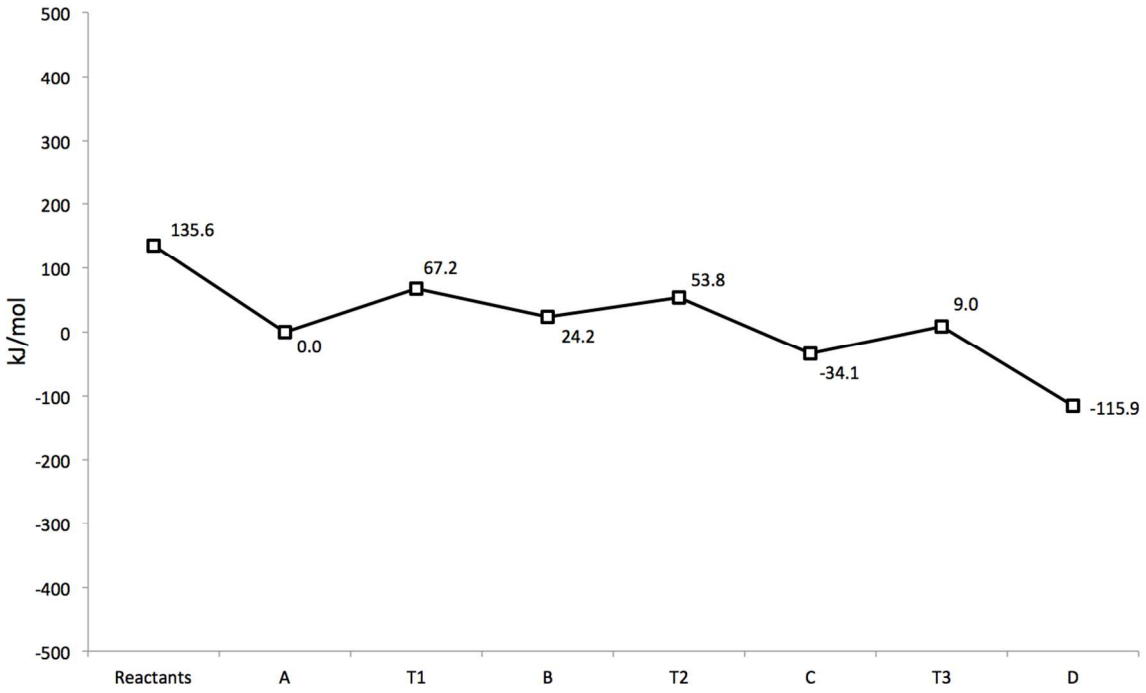


Reaction profile for beryllium complexes

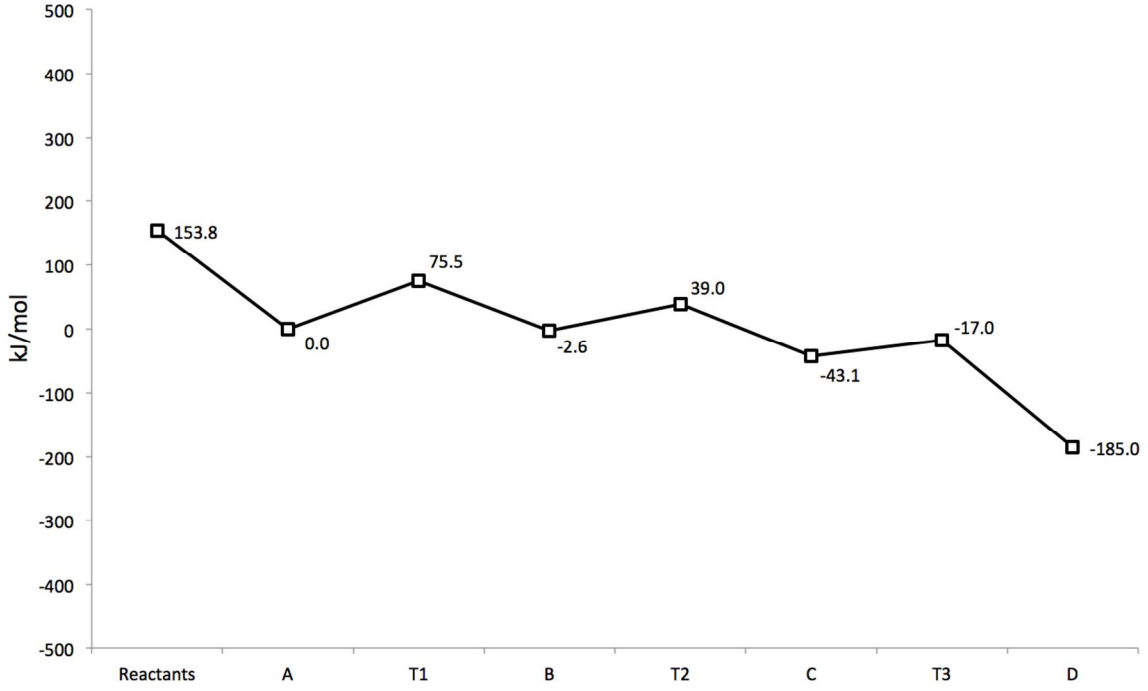
Me_2NHC/BeH_2 Reaction Pathway



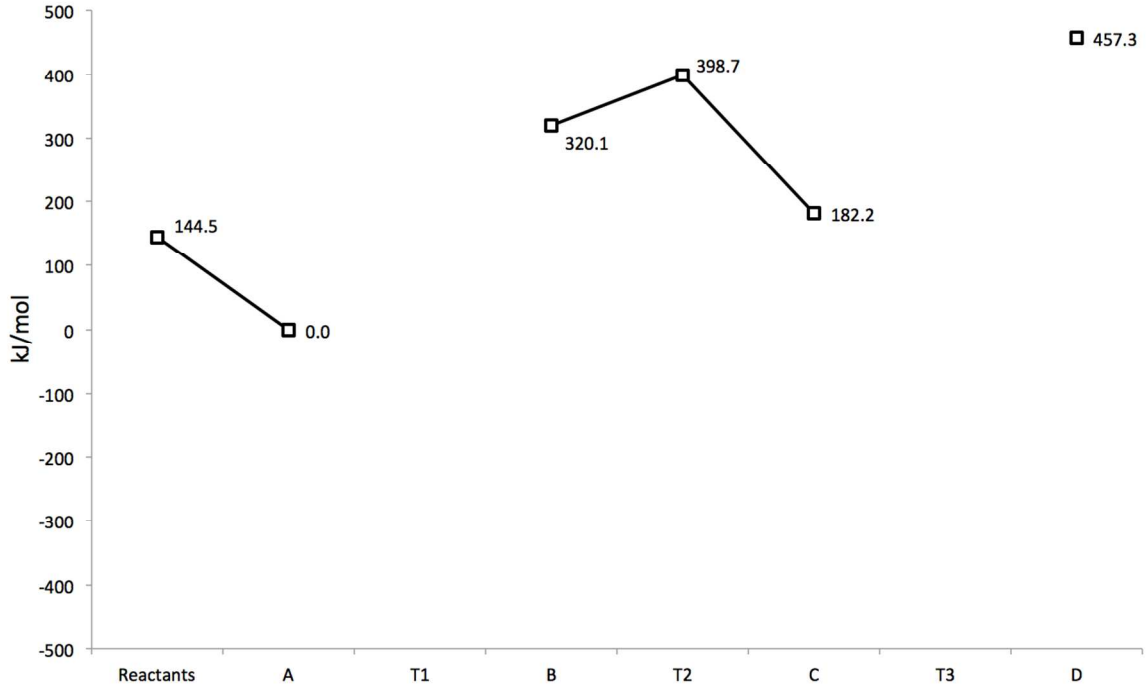
2 Me_2NHC/BeH_2 Reaction Pathway



2 Ph_2NHC/BeH_2 Reaction Pathway



$Me_2NHC/BeCl_2$ Reaction Pathway



2 $Me_2NHC/BeCl_2$ Reaction Pathway

