FIGURE 3a

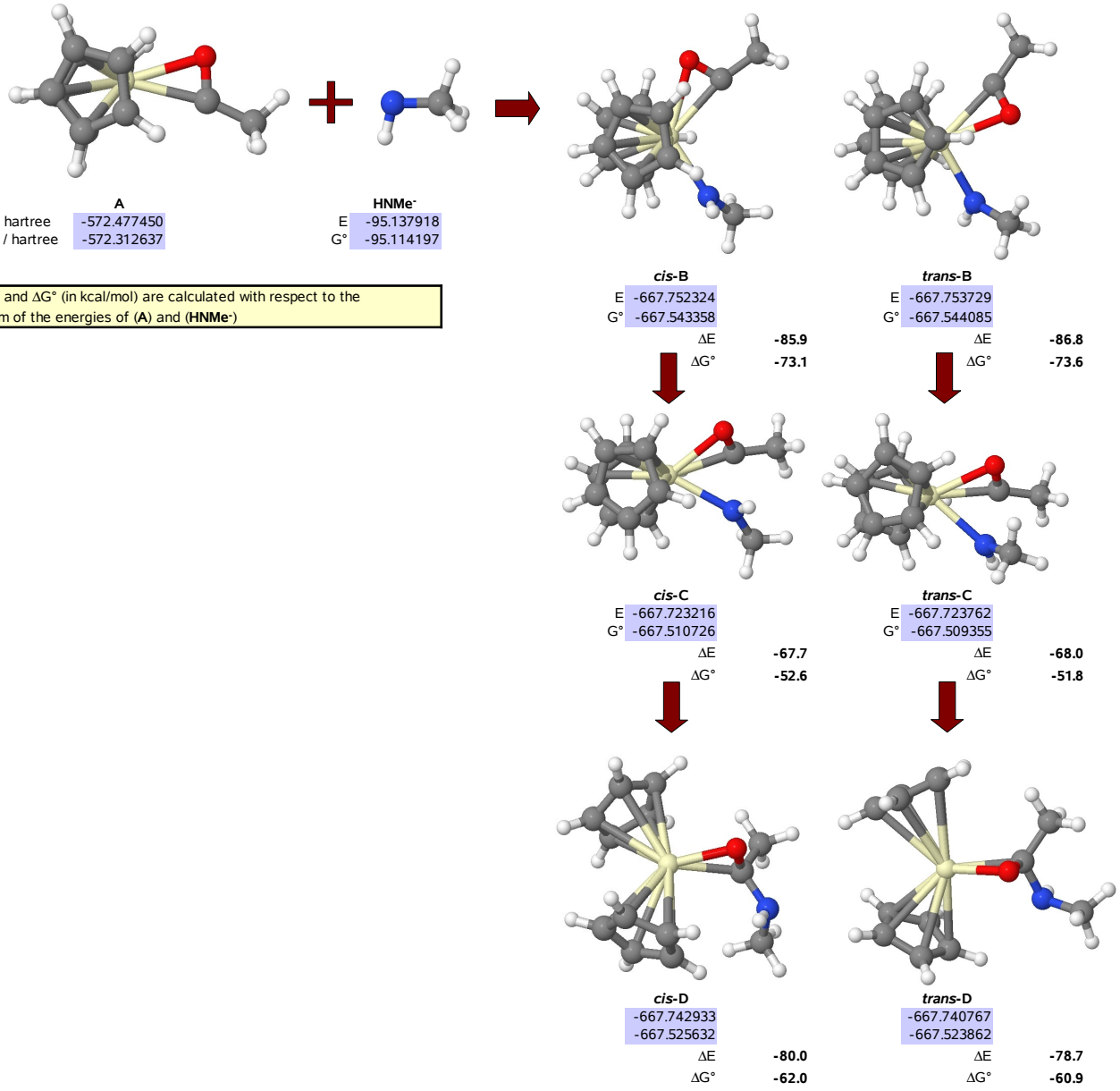
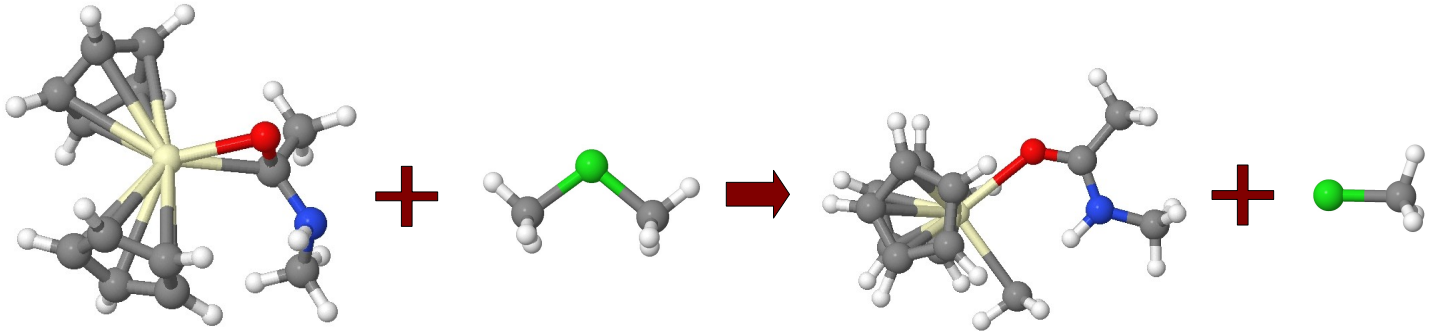

A
E / hartree -572.477450
G° / hartree -572.312637
HNMe⁻
E -95.137918
G° -95.114197
ΔE and ΔG° (in kcal/mol) are calculated with respect to the sum of the energies of (A) and (HNMe⁻)
cis-B
E -667.752324
G° -667.543358
ΔE -85.9
ΔG° -73.1
trans-B
E -667.753729
G° -667.544085
ΔE -86.8
ΔG° -73.6
cis-C
E -667.723216
G° -667.510726
ΔE -67.7
ΔG° -52.6
trans-C
E -667.723762
G° -667.509355
ΔE -68.0
ΔG° -51.8
cis-D
-667.742933
-667.525632
ΔE -80.0
ΔG° -62.0
trans-D
-667.740767
-667.523862
ΔE -78.7
ΔG° -60.9

FIGURE 3b



***Cis*-D**
E -667.742933
G° -667.525632

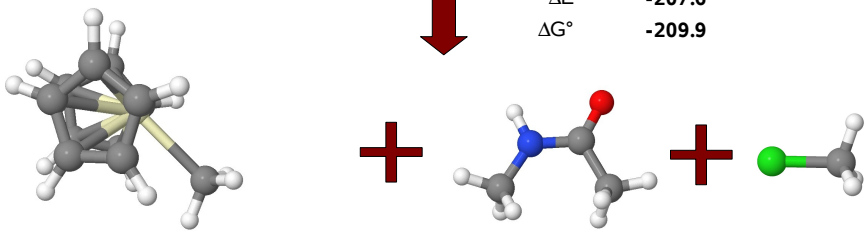
MeClMe⁺
E -94.499278
G° -94.450370

***Cis*-E**
E -707.647397
G° -707.399238

ClMe
E -54.925608
G° -54.911297

ΔE and ΔG° (in kcal/mol) are calculated with respect to the
Sum of the energies of (*cis*-**D**) and (**Me_2Cl^+**)

ΔE **-207.6**
ΔG° **-209.9**



Cp2CeMe
E -459.165187
G° -459.009152

***Cis*-NMA**
E -248.434068
G° -248.361740

ClMe
E -54.925608
G° -54.911297

ΔE **-177.4**
ΔG° **-192.1**

COORDINATES

A

C	0.114879	1.611048	1.720947
C	-1.110832	0.988957	2.076158
C	-0.838956	-0.363440	2.392677
C	0.555365	-0.578592	2.238522
C	1.145450	0.643613	1.829616
Ce	-0.387245	-0.179171	-0.401322
C	0.040845	0.437568	-3.133088
C	0.350391	-0.939728	-3.031130
C	1.542804	-1.066671	-2.272097
C	1.971512	0.234299	-1.907405
C	1.039085	1.164227	-2.432221
C	-2.804143	0.045304	-0.956534
O	-2.599539	-1.181179	-0.776804
H	1.108250	2.244080	-2.360318
H	-0.792162	0.864752	-3.678056
H	2.872229	0.477544	-1.355870
H	2.065666	-1.992205	-2.055095
H	-0.207470	-1.751935	-3.483229
H	0.248202	2.656841	1.466752
H	2.202447	0.817378	1.665158
H	1.085749	-1.501040	2.450468
H	-1.564451	-1.096601	2.726459
H	-2.078270	1.473344	2.128850
C	-4.195111	0.479108	-1.311195
H	-4.900061	-0.357887	-1.375375
H	-4.537581	1.206728	-0.565775
H	-4.161953	1.020605	-2.264114

HNMe-

N	0.044555	0.000000	-0.058026
C	-0.024050	0.000000	1.346923
H	1.004321	0.000000	1.782570
H	-0.517214	0.883674	1.907058
H	-0.517214	-0.883674	1.907058
H	-0.940751	0.000000	-0.372582

---

cis-B

C	0.763895	-0.190579	1.915894
C	-0.027498	0.817234	2.519171
C	-1.341775	0.311586	2.662980
C	-1.364089	-1.006863	2.148954
C	-0.063611	-1.317337	1.684046
Ce	-0.995922	0.639153	-0.235074
O	-2.088541	-1.538281	-1.157239
C	-2.987077	-0.671286	-1.264851
N	-1.942528	2.726908	0.376381
C	-2.538664	3.805980	-0.369925
C	0.189745	0.249006	-2.891180
C	1.279733	0.204294	-1.993901
C	1.467787	1.510203	-1.468231
C	0.497051	2.359149	-2.049628
C	-0.300222	1.578712	-2.920448
H	-2.126306	2.867081	1.366944
H	0.367162	3.413521	-1.838226
H	-1.130128	1.937918	-3.519175
H	2.235615	1.810500	-0.763253
H	1.871906	-0.672277	-1.753473
H	-0.215921	-0.592146	-3.440887
H	1.821309	-0.117913	1.685529
H	0.241614	-2.254023	1.231048
H	-2.225712	-1.663364	2.108496
H	-2.184899	0.841246	3.092390
H	0.312536	1.802774	2.816248
C	-4.315052	-1.153163	-1.825068
H	-3.642991	3.881966	-0.279523
H	-2.146909	4.814049	-0.115007
H	-2.338618	3.672138	-1.442528
H	-4.317898	-2.229119	-2.056507
H	-5.109687	-0.920654	-1.104609
H	-4.546890	-0.575484	-2.729363

---

trans-B

C	0.753029	-0.990975	1.336318
C	0.635670	0.215908	2.067841
C	-0.648778	0.239909	2.669483
C	-1.326666	-0.942398	2.296627
C	-0.461707	-1.703208	1.470737

Ce	-1.175511	0.657393	-0.159063
O	-3.480736	-0.504590	-0.219012
C	-2.864349	-1.002301	-1.187666
N	-2.410495	2.610219	0.330678
C	-3.615201	2.806834	1.100635
C	-0.154145	1.088768	-2.847672
C	0.955509	0.569742	-2.132789
C	1.397150	1.565814	-1.229482
C	0.552015	2.691498	-1.372276
C	-0.403004	2.398155	-2.377441
H	-2.037651	3.513214	0.047862
H	0.630545	3.621131	-0.819127
H	-1.196066	3.055813	-2.713390
H	2.233053	1.478511	-0.544865
H	1.400844	-0.409589	-2.271870
H	-0.712135	0.570428	-3.618800
H	1.620321	-1.308751	0.767824
H	-0.689313	-2.667135	1.029236
H	-2.338330	-1.212705	2.575973
H	-1.043060	1.031659	3.296217
H	1.403294	0.974625	2.175870
C	-3.630680	-2.017002	-2.019251
H	-3.472253	3.345593	2.061612
H	-4.413396	3.359056	0.562828
H	-4.050422	1.832309	1.359105
H	-4.650516	-2.191149	-1.645559
H	-3.668313	-1.667842	-3.059170
H	-3.070468	-2.960769	-2.034195

---

cis-C

C	1.173434	-0.013233	1.858550
C	0.189274	0.824872	2.428406
C	-0.989831	0.055449	2.611104
C	-0.736367	-1.251169	2.141634
C	0.599822	-1.291995	1.662557
Ce	-0.916534	0.321718	-0.290569
O	-3.019000	-0.830904	-0.336942
C	-3.126828	0.165926	-1.184020
N	-2.890767	1.792838	0.061476
C	-3.269329	3.054101	-0.520249
C	0.702409	-0.117779	-2.671907
C	1.677384	0.250616	-1.707044
C	1.505779	1.620100	-1.415267
C	0.424187	2.103143	-2.197500
C	-0.060374	1.032892	-2.985731
H	-3.514706	1.538517	0.824614
H	0.054928	3.123237	-2.214863
H	-0.887558	1.077717	-3.682378
H	2.097375	2.201745	-0.716568
H	2.424910	-0.404493	-1.273638
H	0.589051	-1.098862	-3.122901
H	2.184758	0.276963	1.597085
H	1.107300	-2.164178	1.262000
H	-1.446478	-2.070008	2.132486
H	-1.924224	0.409949	3.030643
H	0.319665	1.865075	2.709176
C	-4.510044	0.380139	-1.746268
H	-4.361810	3.191571	-0.626895
H	-2.896802	3.942199	0.026518
H	-2.848280	3.121719	-1.535517
H	-5.298759	0.239385	-0.987285
H	-4.617929	1.365172	-2.210316
H	-4.675605	-0.374599	-2.528102

---

trans-C

C	1.231465	-0.290369	1.755683
C	0.506267	0.793598	2.295195
C	-0.794418	0.329110	2.626958
C	-0.871333	-1.038885	2.287096
C	0.376977	-1.420208	1.730156
Ce	-0.915565	0.272811	-0.290748
O	-2.976232	-0.978554	-0.331672
C	-3.105858	0.024341	-1.172286
N	-2.960678	1.654930	0.036803
C	-3.921190	1.535491	1.104181
C	0.658165	0.045976	-2.730481
C	1.641904	0.395524	-1.767176
C	1.423937	1.736827	-1.388205
C	0.304227	2.220605	-2.114042
C	-0.157487	1.180706	-2.955253

H	-3.198020	2.416992	-0.590078
H	-0.106116	3.223760	-2.059634
H	-1.002006	1.233009	-3.630287
H	2.008926	2.298283	-0.668047
H	2.429399	-0.251556	-1.396754
H	0.573147	-0.909247	-3.239358
H	2.258122	-0.260152	1.408591
H	0.647131	-2.417970	1.397506
H	-1.742403	-1.673937	2.395755
H	-1.589260	0.919384	3.068290
H	0.884324	1.798037	2.455911
C	-4.485716	0.192918	-1.761837
H	-3.666726	2.106514	2.015867
H	-4.943897	1.837726	0.814933
H	-3.974937	0.473204	1.396857
H	-5.282775	0.068971	-1.009165
H	-4.603156	1.161083	-2.261517
H	-4.631106	-0.593177	-2.515955

---

cis-D

C	0.144384	1.701406	1.882272
C	-0.960224	1.000508	2.427721
C	-0.553598	-0.329660	2.680478
C	0.805502	-0.453808	2.287962
C	1.237971	0.806654	1.808420
Ce	-0.636028	-0.193809	-0.224557
C	-0.182532	0.712367	-2.943954
C	-0.115019	-0.698750	-3.031235
C	1.075740	-1.121518	-2.389216
C	1.752465	0.030630	-1.916912
C	0.971986	1.161659	-2.252500
N	-4.024702	0.475009	0.529733
C	-4.171599	1.902959	0.712609
C	-3.115582	0.091313	-0.563067
O	-2.634684	-1.191138	-0.350410
H	-3.620919	0.069040	1.369600
H	1.222492	2.195420	-2.038043
H	-0.972229	1.337757	-3.341879
H	2.702933	0.041873	-1.394537
H	1.430846	-2.144480	-2.311802
H	-0.850498	-1.343194	-3.499078
H	0.153947	2.748315	1.598281
H	2.231396	1.041668	1.442545
H	1.420538	-1.342758	2.385697
H	-1.169724	-1.114508	3.106040
H	-1.941218	1.417154	2.620269
C	-3.826931	0.227944	-1.900040
H	-4.759494	2.109996	1.617064
H	-3.204912	2.445194	0.777978
H	-4.719965	2.337892	-0.131869
H	-4.722316	-0.419996	-1.940635
H	-4.147951	1.259768	-2.091770
H	-3.156567	-0.063871	-2.714070

---

trans-D

C	1.319181	1.108525	1.769983
C	0.062841	1.682378	2.094656
C	-0.774229	0.654045	2.592883
C	-0.045444	-0.555285	2.558054
C	1.252232	-0.275374	2.047609
Ce	-0.566052	0.041772	-0.239397
O	-2.640568	-0.720845	-0.564415
C	-2.952908	0.637353	-0.555822
N	-3.673117	0.985919	0.682628
C	-5.001903	0.398593	0.830475
C	-0.125862	-0.155247	-3.105034
C	0.991883	-0.822970	-2.546982
C	1.824807	0.148450	-1.936113
C	1.211921	1.411787	-2.101578
C	0.004426	1.225429	-2.824143
H	-3.731151	1.997547	0.744493
H	1.604852	2.361144	-1.753040
H	-0.690723	2.003247	-3.116798
H	2.766060	-0.043173	-1.432457
H	1.198087	-1.886902	-2.613784
H	-0.948810	-0.622107	-3.633456
H	2.181853	1.637617	1.379466
H	2.061613	-0.988971	1.930408
H	-0.408497	-1.524852	2.884799
H	-1.816117	0.762376	2.866695

```
 H    -0.202019     2.730806     2.007541
 C    -3.682701     1.044595    -1.833227
 H    -5.401620     0.614786     1.830881
 H    -5.758937     0.726426     0.091896
 H    -4.898255    -0.686507     0.734633
 H    -4.633660     0.496933    -1.979600
 H    -3.912791     2.119755    -1.844812
 H    -3.058957     0.833024    -2.707842
----------------------------------------
ClMe2+
Cl    -0.056029     0.000000    -0.039443
 C     0.018148     0.000000     1.803956
 C     1.706837     0.000000    -0.584128
 H     1.626195     0.000000    -1.671384
 H     2.152759     0.915165    -0.199217
 H     2.152759    -0.915164    -0.199216
 H    -1.033809     0.000001     2.090412
 H     0.529761    -0.915173     2.095844
 H     0.529762     0.915172     2.095844
----------------------------------------
cis-E
 C     1.257894    -0.222749    -0.893772
 C     0.417607    -0.471678     0.219699
 C     1.127965    -0.110737     1.393034
 C     2.403933     0.363550     1.005875
 C     2.483520     0.299262    -0.407799
Ce     0.598964     2.361094     0.063818
 C    -0.674180     3.481848     3.085598
 C    -1.744323     3.554429     4.141743
 C    -0.859972     4.501380    -1.147782
 C    -1.466738     3.321660    -1.648962
 C    -0.539595     2.684428    -2.509103
 C     0.642231     3.469308    -2.536099
 C     0.440158     4.595150    -1.698742
 N     0.449779     4.178096     3.254718
 C     0.767100     5.020893     4.389104
 O    -0.847289     2.776025     2.061276
 H     1.142153     4.072130     2.485507
 H     1.019137    -0.428382    -1.930701
 H    -0.577561    -0.901468     0.183234
 H     3.347107     0.561583    -1.008901
 H     3.189007     0.701635     1.670982
 H     0.765423    -0.209798     2.409841
 H    -2.475574     2.984188    -1.437522
 H    -0.714869     1.777033    -3.075281
 H     1.526125     3.268546    -3.131435
 H     1.151271     5.392880    -1.522922
 H    -1.324468     5.222668    -0.484933
 H     1.726081     5.502755     4.194595
 H     0.017619     5.805872     4.537214
 H     0.858493     4.445150     5.317406
 H    -1.353506     3.253217     5.118964
 H    -2.121476     4.577842     4.240645
 H    -2.564316     2.895522     3.859665
 C     2.491809     3.870824     1.021032
 H     3.100505     3.639070     0.123970
 H     2.440821     4.970638     1.025344
 H     3.138026     3.568875     1.859610
----------------------------------------
Cp2CeMe
 C     0.861869     1.056978    -1.997580
 C     1.507882    -0.206288    -1.946248
 C     0.609870    -1.175056    -2.454872
 C    -0.588351    -0.509523    -2.828625
 C    -0.430190     0.867962    -2.554385
Ce    -0.519597    -0.312321     0.007851
 C     0.817906    -1.025491     2.410223
 C     1.498426     0.116935     1.927403
 C     0.621757     1.228515     2.041818
 C    -0.594751     0.773622     2.611905
 C    -0.477603    -0.619203     2.829660
 C    -2.814682     0.701590    -0.019873
 H     2.519224     0.145597     1.564632
 H     0.863243     2.256103     1.793751
 H    -1.457823     1.384411     2.843744
 H    -1.228615    -1.255366     3.285814
 H     1.232294    -2.024836     2.493354
 H     2.521345    -0.390168    -1.608763
 H     0.821793    -2.231016    -2.588082
 H    -1.459392    -0.969520    -3.281967
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 H    -1.164088     1.641706    -2.741777
 H     1.303446     2.007672    -1.720447
 H    -3.377459     0.410782    -0.920783
 H    -3.411529     0.387756     0.851248
 H    -2.809911     1.802115    -0.004604
----------------------------------------
cis-NMA
 C     0.747583     1.347623    -0.020668
 C     0.618755    -0.163069    -0.003137
 O     1.589530    -0.905316     0.037964
 N    -0.653752    -0.665216    -0.057679
 C    -1.890663     0.076447     0.036983
 H    -0.688187    -1.671575     0.018718
 H    -1.873422     0.954441    -0.615173
 H     0.208714     1.810022     0.813109
 H     1.806092     1.594926     0.052710
 H     0.345540     1.769424    -0.948336
 H    -2.713325    -0.560128    -0.297472
 H    -2.117104     0.412788     1.058791
----------------------------------------
trans-NMA
 C     1.809507    -0.562652     0.000001
 C     0.478659     0.165821    -0.000004
 O     0.412475     1.387069    -0.000013
 N    -0.624638    -0.638687     0.000003
 C    -1.966597    -0.104359     0.000002
 H    -0.497358    -1.637402     0.000011
 H    -2.523732    -0.416339    -0.890833
 H     2.378363    -0.251351     0.880071
 H     2.378371    -0.251348    -0.880064
 H     1.723813    -1.653084    -0.000001
 H    -2.523723    -0.416311     0.890853
 H    -1.876523     0.983161    -0.000015
----------------------------------------
ClMe
Cl    -0.000006     0.000000    -0.027411
 C    -0.000005     0.000000     1.774451
 H     1.034525     0.000000     2.113996
 H    -0.517257     0.895927     2.113982
 H    -0.517257    -0.895927     2.113982
```