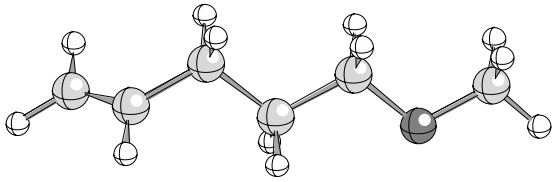
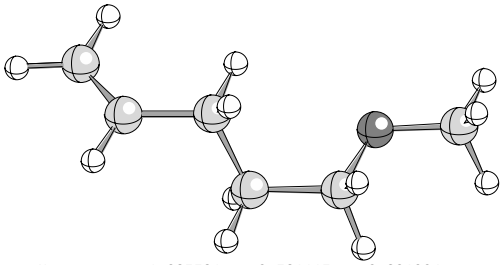
N-methyl-*N*-pent-4-enylaminyl(*E*)



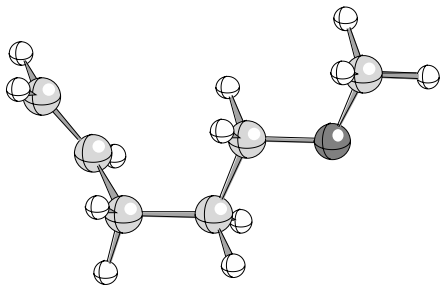
N	2.337736	-0.572232	-0.175275
C	-3.647545	0.033295	-0.487412
C	-2.622766	-0.239462	0.320830
C	-1.309403	0.494407	0.339987
C	-0.110861	-0.419430	0.028006
C	1.230850	0.313005	0.100334
C	3.606753	0.111166	-0.132141
H	-3.604260	0.844515	-1.211898
H	-4.570206	-0.540175	-0.456948
H	-2.712455	-1.065730	1.028835
H	-1.159958	0.944762	1.334373
H	-1.342425	1.326715	-0.376251
H	-0.087566	-1.261677	0.731792
H	-0.226913	-0.855279	-0.971594
H	1.360169	0.772541	1.100037
H	1.241172	1.163931	-0.608721
H	3.778942	0.588484	0.848894
H	3.653863	0.920408	-0.882393
H	4.423316	-0.590758	-0.326822

N-methyl-*N*-pent-4-enylaminyl(G_{12})



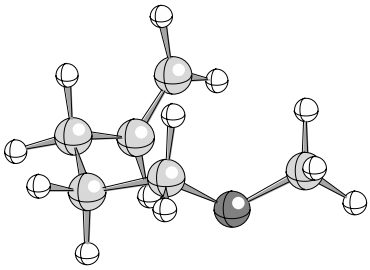
N	-1.835521	-0.531115	-0.281004
C	3.291876	-0.810675	-0.243538
C	2.504583	0.169388	0.201456
C	1.040948	0.030134	0.519084
C	0.149507	0.930139	-0.356012
C	-1.338248	0.799143	-0.017705
C	-3.220917	-0.680314	0.088374
H	2.912359	-1.818134	-0.403437
H	4.343707	-0.647237	-0.463611
H	2.929692	1.165487	0.343123
H	0.870145	0.292174	1.575855
H	0.723657	-1.011608	0.395736
H	0.449329	1.980947	-0.239787
H	0.297709	0.671219	-1.411471
H	-1.925491	1.532073	-0.603357
H	-1.513969	1.067981	1.042501
H	-3.863296	0.046022	-0.440491
H	-3.370857	-0.497569	1.167236
H	-3.570834	-1.690443	-0.145219

N-methyl-*N*-pent-4-enylaminyl(G_{23})



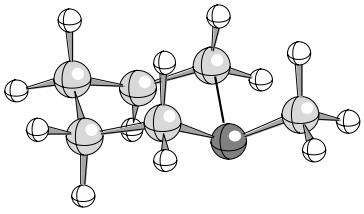
N	-2.202043	0.290997	-0.304069
C	2.734551	-1.274910	0.084205
C	2.210283	-0.161541	-0.430779
C	1.528425	0.929634	0.351433
C	0.076946	1.192283	-0.097026
C	-0.865603	0.015787	0.167219
C	-3.129751	-0.754929	0.049357
H	2.705726	-1.478512	1.153131
H	3.219546	-2.022227	-0.538373
H	2.264333	-0.002804	-1.510068
H	2.096899	1.863708	0.232442
H	1.551645	0.685696	1.422426
H	-0.310648	2.078193	0.420645
H	0.052491	1.425912	-1.169440
H	-0.875780	-0.230199	1.247232
H	-0.481528	-0.895539	-0.328412
H	-3.198052	-0.880733	1.144541
H	-2.811957	-1.732603	-0.354565
H	-4.127477	-0.525810	-0.337532

N-methyl-*N*-pent-4-enylaminyl($G_{12}G_{23}$)



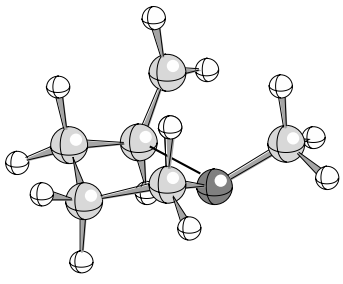
N	1.435585	0.125285	-0.553169
C	1.054750	-0.949216	0.335484
C	-0.230417	-1.643169	-0.130816
C	-1.515320	-0.846069	0.171590
C	-1.554084	0.530502	-0.436939
C	-1.813230	1.654936	0.233980
C	2.276596	1.102014	0.092392
H	1.883729	-1.682332	0.328325
H	0.958104	-0.619770	1.386832
H	-0.145918	-1.821794	-1.210187
H	-0.307345	-2.626204	0.351885
H	-2.368992	-1.429692	-0.206013
H	-1.653238	-0.767499	1.258857
H	-1.361398	0.584021	-1.508360
H	-1.846549	2.622159	-0.260573
H	-2.007227	1.650842	1.305284
H	2.676575	1.806928	-0.643379
H	3.118183	0.640035	0.638168
H	1.695215	1.672325	0.837198

endo TS



N	1.094859	-0.110964	-0.498785
C	0.380812	-1.194040	0.161876
C	-1.104784	-1.261355	-0.219397
C	-1.905223	-0.039650	0.307589
C	-1.269538	1.206483	-0.233969
C	-0.010468	1.555289	0.185592
C	2.409401	0.081957	0.081783
H	0.866948	-2.137266	-0.146888
H	0.476082	-1.159386	1.266703
H	-1.187942	-1.309876	-1.311912
H	-1.537631	-2.186792	0.182887
H	-2.957138	-0.125113	0.011399
H	-1.874402	-0.046738	1.406377
H	-1.635469	1.592069	-1.184138
H	0.532268	2.361845	-0.299452
H	0.303660	1.332029	1.203701
H	2.867286	0.991477	-0.322608
H	3.055494	-0.765917	-0.202067
H	2.425624	0.138314	1.186650

exo TS



N	0.676240	-0.689228	-0.482066
C	-0.310065	-1.426058	0.283282
C	-1.661075	-0.805431	-0.068445
C	-1.473521	0.704518	0.140425
C	-0.142367	1.154045	-0.441689
C	0.682976	2.014123	0.265637
C	2.013675	-0.764514	0.068032
H	-0.137909	-1.384708	1.376202
H	-0.264917	-2.489268	-0.005425
H	-1.891303	-1.017326	-1.119574
H	-2.477955	-1.206669	0.541928
H	-1.489391	0.932814	1.214388
H	-2.291526	1.275309	-0.317687
H	-0.106108	1.219931	-1.526035
H	1.515500	2.524105	-0.210160
H	0.594695	2.119688	1.344249
H	2.660201	-0.025879	-0.416954
H	2.424141	-1.763397	-0.150223
H	2.073154	-0.620101	1.160307