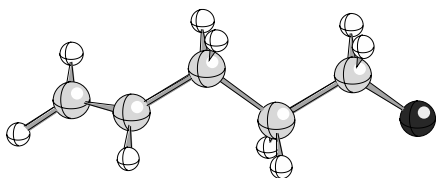
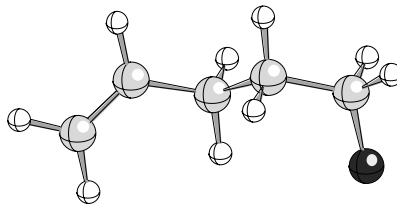


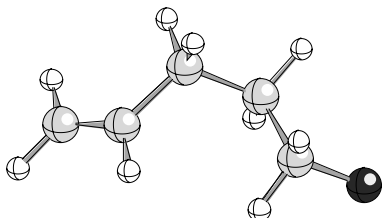
4-penten-1-oxyl(E)



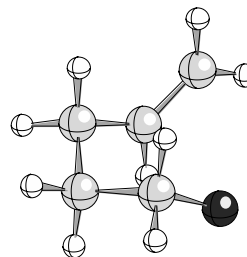
O	3.003638	-0.357069	-0.230923
C	1.881093	0.395243	-0.009248
C	0.560399	-0.383410	0.000675
C	-0.651669	0.509395	0.323651
C	-1.946279	-0.256585	0.356309
C	-2.993455	-0.031252	-0.437616
H	1.851192	1.250572	-0.714195
H	0.642859	-1.196056	0.733697
H	0.421196	-0.855916	0.979487
H	-0.486565	0.987635	1.302479
H	-0.724318	1.322217	-0.411638
H	-2.000330	-1.062966	1.090058
H	-3.901192	-0.624889	-0.370854
H	-2.984594	0.759530	-1.185493
H	2.052121	0.876083	0.980197

4-penten-1-oxyl(G_{12})

O	2.312621	0.998173	-0.069283
C	2.018071	-0.339144	-0.005510
C	0.575957	-0.713062	-0.369323
C	-0.460663	-0.014668	0.528346
C	-1.879138	-0.352361	0.158472
C	-2.796340	0.526303	-0.247337
H	2.236614	-0.624880	1.047932
H	0.468659	-1.805036	-0.302176
H	0.395205	-0.442627	-1.417266
H	-0.274251	-0.310332	1.573357
H	-0.302707	1.068456	0.474302
H	-2.150740	-1.407907	0.225985
H	-3.806728	0.221886	-0.507530
H	-2.571469	1.587796	-0.331850
H	2.757130	-0.915142	-0.596380

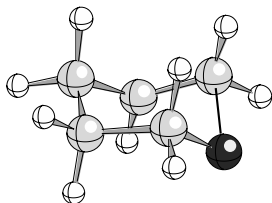
4-penten-1-oxyl(G_{23})

O	2.776319	-0.459764	-0.296157
C	1.553342	-0.321614	0.303125
C	0.633073	0.718649	-0.352080
C	-0.731712	0.875410	0.352274
C	-1.584486	-0.366372	0.323613
C	-2.723725	-0.494296	-0.357990
H	1.658401	-0.152004	1.393593
H	0.485833	0.443021	-1.402833
H	1.154559	1.684117	-0.342632
H	-0.557461	1.175236	1.397170
H	-1.277022	1.701046	-0.120685
H	-1.227607	-1.216362	0.907919
H	-3.297456	-1.417190	-0.349492
H	-3.129775	0.324376	-0.949365
H	1.101033	-1.334790	0.221928

4-penten-1-oxyl($G_{12}G_{23}$)

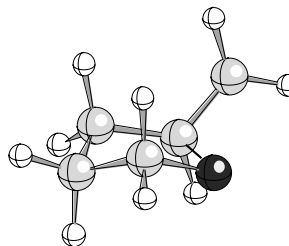
O	-0.934169	-1.454572	-0.294458
C	-1.527044	-0.403898	0.358893
C	-1.088498	0.972148	-0.163137
C	0.401098	1.237804	0.139802
C	1.302649	0.182703	0.436697
C	2.096047	-0.619300	0.280908
H	-2.612658	-0.531992	0.159400
H	-1.413673	-0.471546	1.458086
H	-1.262716	1.001623	-1.245862
H	-1.706300	1.757333	0.292803
H	0.667910	2.222611	-0.270714
H	0.550274	1.296645	1.226240
H	1.279100	0.072004	-1.520858
H	2.718863	-1.375892	-0.187813
H	2.147034	-0.550951	1.365770

endo TS



O	-0.195744	-1.473408	-0.351105
C	-1.209050	-0.727124	0.242872
C	-1.222153	0.749025	-0.195844
C	0.106635	1.438411	0.220976
C	1.246388	0.614262	-0.296700
C	1.552688	-0.582278	0.287637
H	-2.157145	-1.198511	-0.073331
H	-1.183601	-0.780105	1.349979
H	-1.328765	0.789219	-1.286509
H	-2.079868	1.275701	0.245427
H	0.135647	2.463739	-0.165772
H	0.142801	1.497247	1.317409
H	1.621731	0.827491	-1.295726
H	2.270641	-1.260919	-0.160901
H	1.297458	-0.780374	1.324613

exo TS



O	0.223359	-1.340358	-0.323192
C	1.291305	-0.754269	0.348109
C	1.397030	0.710645	-0.087000
C	-0.026399	1.274538	0.078848
C	-1.028237	0.272409	-0.444100
C	-2.070115	-0.196823	0.317216
H	2.197127	-1.317848	0.062165
H	1.201637	-0.828508	1.448622
H	1.693476	0.748969	-1.142192
H	-2.132879	1.280868	0.493478
H	-0.228321	1.471262	1.139368
H	-0.134341	2.227928	-0.454591
H	-1.095834	0.156657	-1.522897
H	-2.837597	-0.837140	-0.105791
H	-2.107410	-0.020323	1.388924