Electronic Supplementary Material (ESI) for Polymer Chemistry.

DFT Investigations on the Ring-Opening Polymerization of Substituted Cyclic Carbonates Catalyzed by Zinc-{β-Diketiminate} Complexes

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Supplementary Information

Table S1. Selected bond lengths (Å) of the stationary points calculated for the initiation step of the ROP of 7CC-γ(*R*) mediated by [(BDI^{iPr})Zn(OMe)]. The labels refer to the intermediates and transition states shown in Figures 6, 7 and 9.

	$Zn–O_{OMe}$	$Zn–O_{CO}$	$C_{CO}–O_{CO}$	$C_{CO}–O_1$	$C_{CO–}O_{OMe}$	$C_{CO}–O_2$	$Zn–O_1$	$Zn–O_2$
[(BDI^{iPr})Zn(OMe)]	1.816	-	-	-	-		-	-
R-7CC-γMe	-	-	1.199	1.362	-	1.350	-	-
$\mathbf{I}_{7CC\text{-}\gamma(R,re)}$	1.880	2.266	1.224	1.331	2.627	1.332	3.756	3.379
TS($\mathbf{I}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$)	1.947	2.121	1.247	1.345	2.006	1.363	3.624	3.346
$\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$	-	1.853	1.346	1.407	1.407	1.405	3.980	2.827
TS($\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$)	-	2.014	1.271	1.349	1.351	1.864	3.724	2.014
$\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$	-	2.361	1.230	1.323	1.324	2.565	3.769	1.875
TS($\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{IV}^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)	-	2.821	1.219	1.332	1.330	2.630	3.970	1.848
$\mathbf{IV}^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$	-	-	1.207	1.331	1.352	-	-	1.823
TS($\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$)	-	1.851	1.336	1.464	1.400	1.391	2.833	3.607
$\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$	-	1.929	1.313	1.567	1.385	1.379	2.195	3.495
TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$)	-	1.987	1.284	1.780	1.360	1.355	2.057	3.440
$\mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$	-	2.233	1.228	2.814	1.327	1.316	1.880	3.315
TS($\mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{IV}^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)	-	4.261	1.209	3.684	1.347	1.330	1.838	4.394
$\mathbf{IV}^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$	-	-	1.207	-	1.351	1.332	1.821	-
$\mathbf{I}_{7CC\text{-}\gamma(R,si)}$	1.887	2.236	1.226	1.329	2.581	1.331	3.502	3.651
TS($\mathbf{I}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$)	1.951	2.110	1.249	1.344	1.991	1.366	3.385	3.603
$\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$	-	1.854	1.346	1.412	1.410	1.402	3.161	4.050
TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$)	-	2.354	1.323	2.730	1.323	1.324	1.873	3.791
$\mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$	-	2.262	1.223	3.512	1.329	1.322	1.875	4.142
TS($\mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{IV}^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)	-	2.784	1.219	2.708	1.328	1.333	1.852	3.947
TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$)	-	1.837	1.340	1.395	1.398	1.446	3.405	3.205
$\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$	-	1.932	1.315	1.378	1.382	1.568	3.480	2.187
TS($\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$)	-	2.000	1.284	1.354	1.358	1.793	3.449	2.042
$\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$	-	2.261	1.229	1.316	1.328	2.772	3.434	1.878
TS($\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{IV}^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)	-	3.266	1.213	1.328	1.340	3.010	4.181	1.839

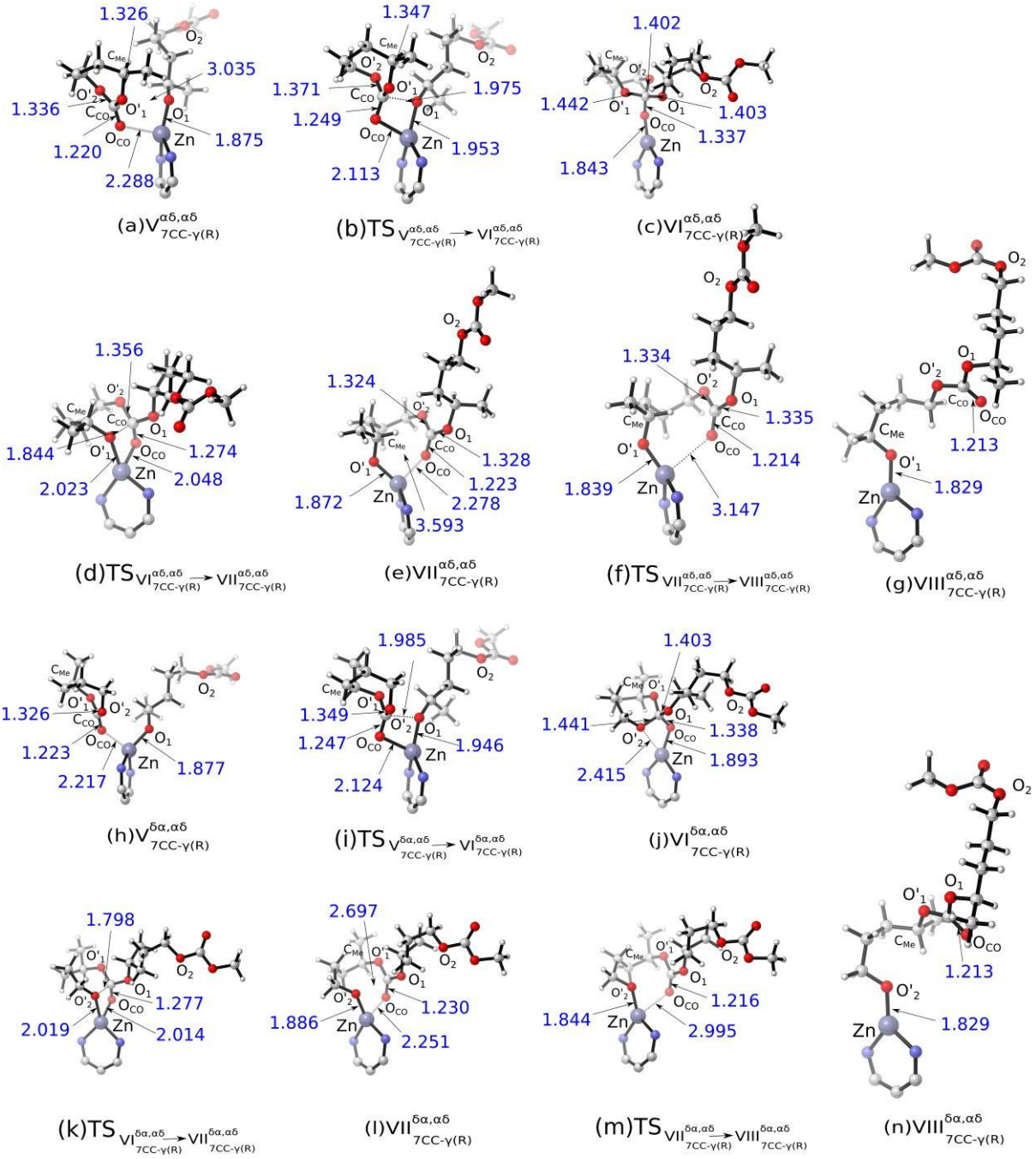

Figure S1. Optimized structures of complexes involved in the propagation step of the ROP of 7CC-γ(*R*) mediated by **IV**$^{\alpha\delta}{}_{\text{7CC-}\gamma(R)}$

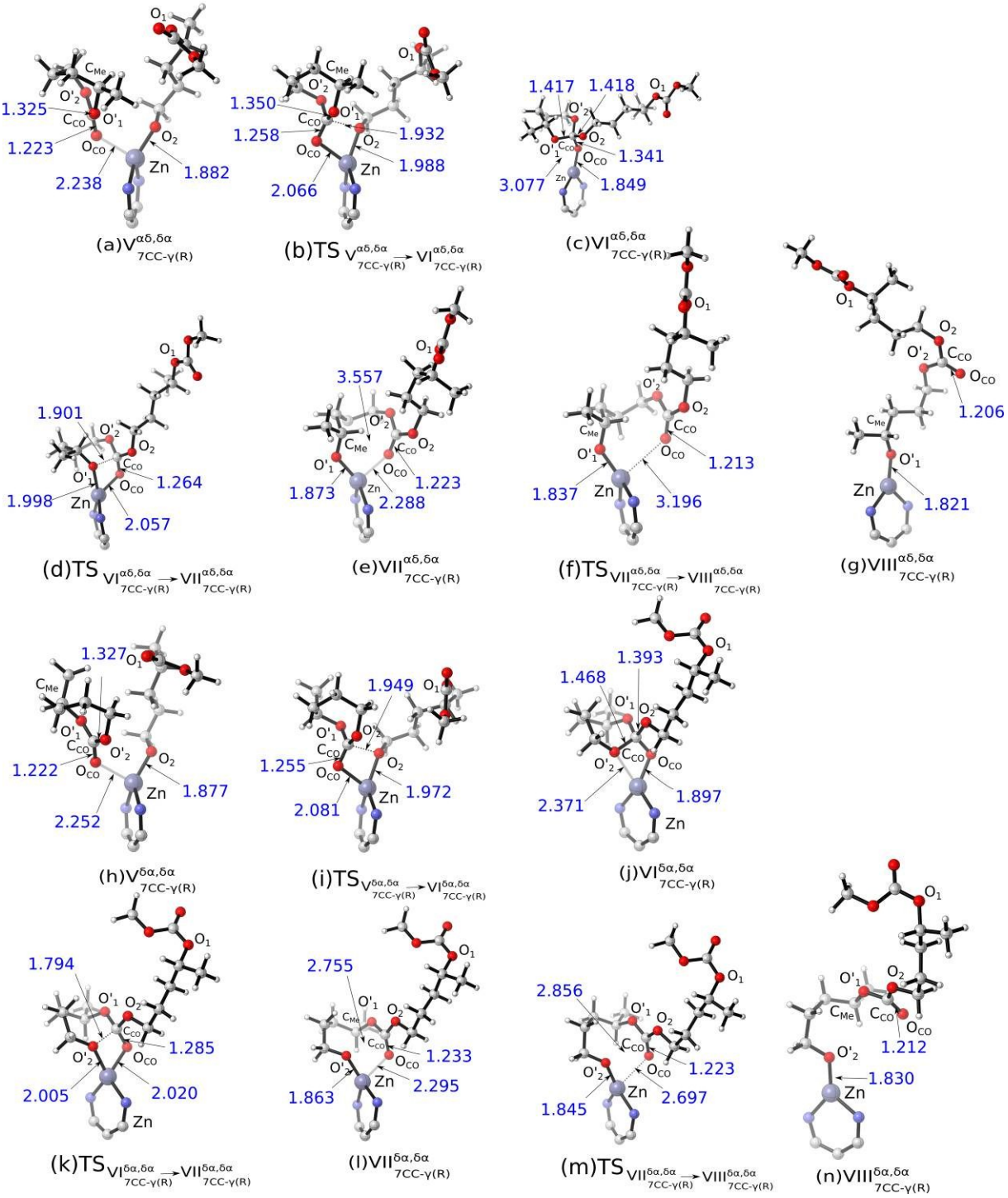

Figure S2. Optimized structures of complexes involved in the propagation step of the ROP of 7CC-γ(*R*) mediated by **IV**$^{\delta\alpha}_{7CC\text{-}\gamma(R)}$

Table S2. Comparison of the relative Gibbs-free energies (kcal.mol^{-1}) of the intermediates and transition states in the initiation reaction of TMC-γ(*R,re*), TMC-γ(*R,si*), TMC-γ(*S,re*) and TMC-γ(*S,si*) ROP. The labels **I** to **IV** refer to the intermediate and transition states shown in Figures 14, 15 and 16.

Monomer	TMC-γ(*R*)	TMC-γ(*S*)		TMC-γ(*R*)	TMC-γ(*S*)
Considered Enantioface	*re*	*re*		*si*	*si*
$\mathbf{I}_{TMC}$	10.3	11.0	$\mathbf{I}_{TMC)}$	11.0	9.9
TS($\mathbf{I}_{TMC}$ →$\mathbf{II}^{\gamma\alpha}_{TMC}$)	17.8	18.5	TS($\mathbf{I}_{TMC}$→$\mathbf{II}^{\alpha\gamma}_{TMC}$)	17.7	18.3
$\mathbf{II}^{\gamma\alpha}_{TMC}$	10.8	9.0	$\mathbf{II}^{\alpha\gamma}_{TMC}$	8.9	11.4
TS($\mathbf{II}^{\gamma\alpha}_{TMC}$ → $\mathbf{III}^{\gamma\alpha}_{TMC}$)	16.4	23.4	TS($\mathbf{II}^{\alpha\gamma}_{TMC}$→ $\mathbf{III}^{\alpha\gamma}_{TMC}$	16.2	15.7
$\mathbf{III}^{\gamma\alpha}_{TMC}$	11.6	12.2	$\mathbf{III}^{\alpha\gamma}_{TMC}$	13.0	9.5
TS($\mathbf{III}^{\gamma\alpha}_{TMC}$ → $\mathbf{IV}^{\gamma\alpha}_{TMC}$)	12.7	16.1	TS($\mathbf{III}^{\alpha\gamma}_{TMC}$ → $\mathbf{IV}^{\alpha\gamma}_{TMC}$)	13.4	10.4
$\mathbf{IV}^{\gamma\alpha}_{TMC}$	2.5	5.0			
TS($\mathbf{II}^{\gamma\alpha}_{TMC}$ → $\mathbf{II}^{\alpha\gamma}_{TMC)}$	14.3	19.5	TS($\mathbf{II}^{\alpha\gamma}_{TMC}$ → $\mathbf{II}^{\gamma\alpha}_{TMC}$)	14.9	12.3
$\mathbf{II}^{\alpha\gamma}_{TMC}$	13.5	15.5	$\mathbf{II}^{\gamma\alpha}_{TMC}$	12.5	10.9
TS($\mathbf{II}^{\alpha\gamma}_{TMC}$ → $\mathbf{III}^{\alpha\gamma}_{TMC}$)	16.6	20.7	TS($\mathbf{II}^{\gamma\alpha}_{TMC}$ → $\mathbf{III}^{\gamma\alpha}_{TMC}$)	14.4	13.7
$\mathbf{III}^{\alpha\gamma}_{TMC}$	9.8	13.9	$\mathbf{III}^{\gamma\alpha}_{TMC}$	9.7	9.0
TS($\mathbf{III}^{\alpha\gamma}_{TMC}$ → $\mathbf{IV}^{\alpha\gamma}_{TMC}$)	12.2	14.8	TS($\mathbf{III}^{\gamma\alpha}_{TMC}$ → $\mathbf{IV}^{\gamma\alpha}_{TMC}$)	9.9	13.4
$\mathbf{IV}^{\alpha\gamma}_{TMC}$	4.4	3.7			

Table S4. Selected bond lengths (Å) of the stationary points calculated for the initiation step of the ROP of TMC-γ(*R,re*) and TMC-γ(*R,si*) mediated by [(BDI^{iPr})Zn(OMe)]. The labels refer to the intermediates and transition states shown in Figures 14, 15 and 16.

	$Zn–O_{OMe}$	$Zn–O_{CO}$	$C_{CO}–O_{CO}$	$C_{CO}–O_1$	$C_{CO}–O_{OMe}$	$C_{CO}–O_2$	$Zn–O_1$	$Zn–O_2$
R-TMC-γMe	–	–	1.199	1.350	–	1.351	–	–
$\mathbf{I}_{TMC\text{-}\gamma(R,re)}$	1.883	2.258	1.224	1.327	2.645	1.330	3.825	3.272
TS($\mathbf{I}_{TMC\text{-}\gamma(R,re)} \rightarrow \mathbf{II}^{\gamma\alpha}_{TMC\text{-}\gamma(R,re)}$)	2.014	2.026	1.266	1.361	1.846	1.358	3.652	3.296
$\mathbf{II}^{\gamma\alpha}_{TMC\text{-}\gamma(R,re)}$	3.450	1.868	1.340	1.408	1.402	1.426	3.913	2.667
TS($\mathbf{II}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,re)} \rightarrow \mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,re)}$)	–	2.039	1.274	1.353	1.344	1.853	3.692	2.021
$\mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,re)}$	–	2.318	1.230	1.322	1.322	2.563	3.748	1.885
TS($\mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,re)} \rightarrow \mathbf{IV}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R)}$)	–	3.093	1.216	1.333	1.331	2.699	4.082	1.846
$\mathbf{IV}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R)}$	–	–	1.213	1.330	1.343	–	–	1.823
TS($\mathbf{II}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,re)} \rightarrow \mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)}$)	4.027	1.839	1.332	1.431	1.408	1.401	3.067	3.470
$\mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)}$	3.755	1.906	1.317	1.503	1.393	1.388	2.310	3.424
TS($\mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)} \rightarrow \mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)}$)	3.708	2.060	1.262	1.889	1.346	1.351	1.983	3.278
$\mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)}$	–	2.259	1.230	2.462	1.323	1.325	1.889	3.228
TS($\mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,re)} \rightarrow \mathbf{IV}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R)}$)	–	4.984	1.209	3.497	1.347	1.329	1.831	3.476
$\mathbf{IV}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R)}$	–	–	1.211	–	1.340	1.334	1.821	–
$\mathbf{I}_{TMC\text{-}\gamma(R,si)}$	1.882	2.259	1.222	1.325	2.877	1.333	3.275	3.994
TS($\mathbf{I}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)}$)	2.011	2.026	1.266	1.358	1.850	1.361	3.310	3.648
$\mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)}$	2.694	1.851	1.341	1.426	1.401	1.403	3.602	3.841
TS($\mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)}$)	3.693	2.069	1.263	1.888	1.348	1.350	1.980	3.380
$\mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)}$	–	2.252	1.230	2.569	1.325	1.323	1.895	3.688
TS($\mathbf{III}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{IV}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R)}$)	–	3.090	1.215	2.739	1.329	1.335	1.849	4.114
TS($\mathbf{II}^{\alpha\gamma}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{II}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)}$)	–	1.832	1.333	1.402	1.411	1.423	3.050	3.662
$\mathbf{II}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)}$	–	1.920	1.316	1.388	1.391	1.515	3.459	2.245
TS($\mathbf{II}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)}$)	–	2.039	1.270	1.352	1.352	1.845	3.363	2.002
$\mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)}$	–	2.285	1.230	1.320	1.325	2.552	3.336	1.878
TS($\mathbf{III}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R,si)} \rightarrow \mathbf{IV}^{\gamma\alpha}_{TMC\text{-}}\gamma_{(R)}$)	–	3.899	1.209	1.332	1.342	2.893	4.211	1.831

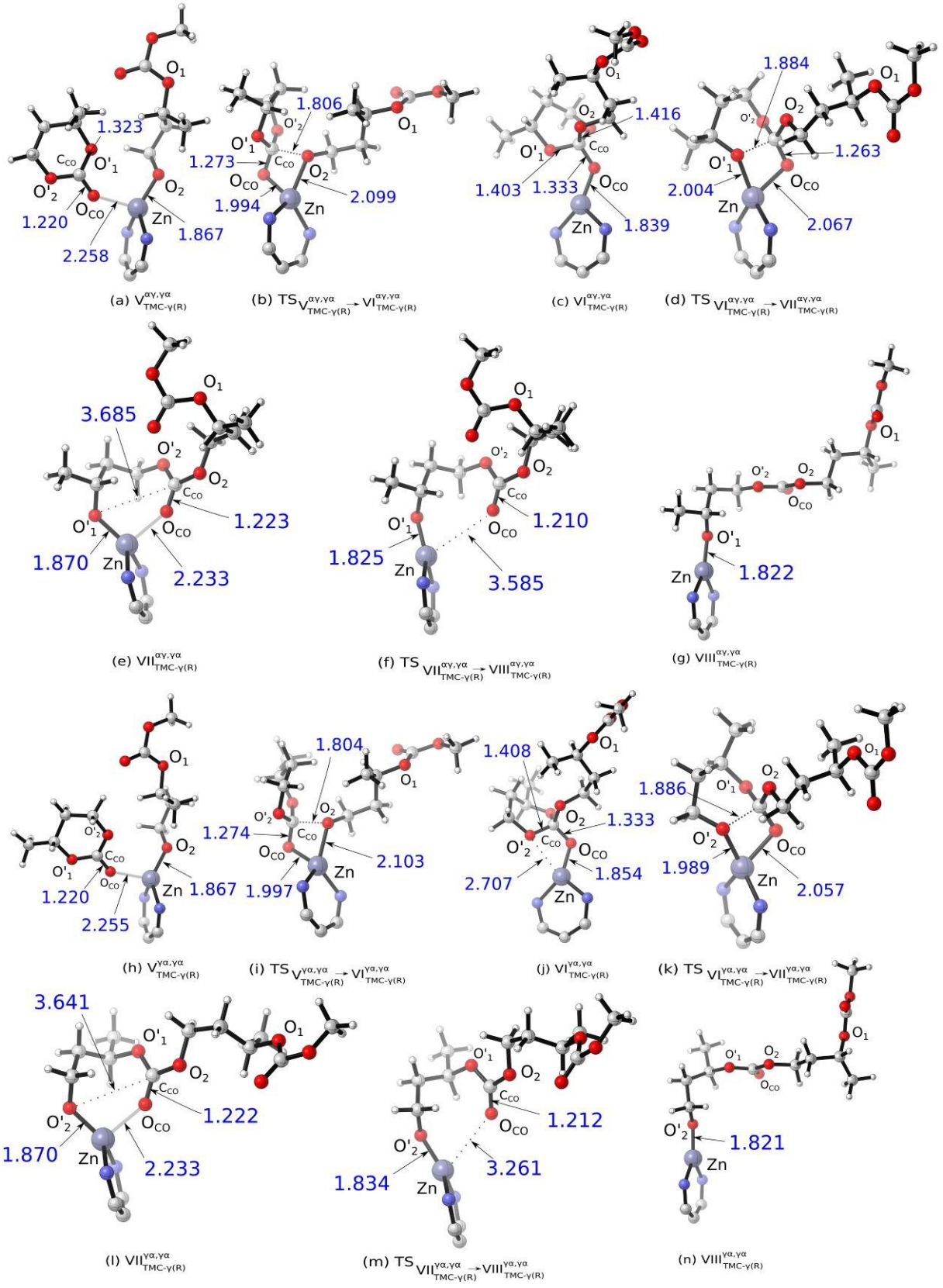

Figure S3. Optimized structures of complexes involved in the propagation step of the ROP of TMC-γ(*R*) mediated by $\mathbf{IV}^{\gamma\alpha}_{TMC\text{-}\gamma(R)}$

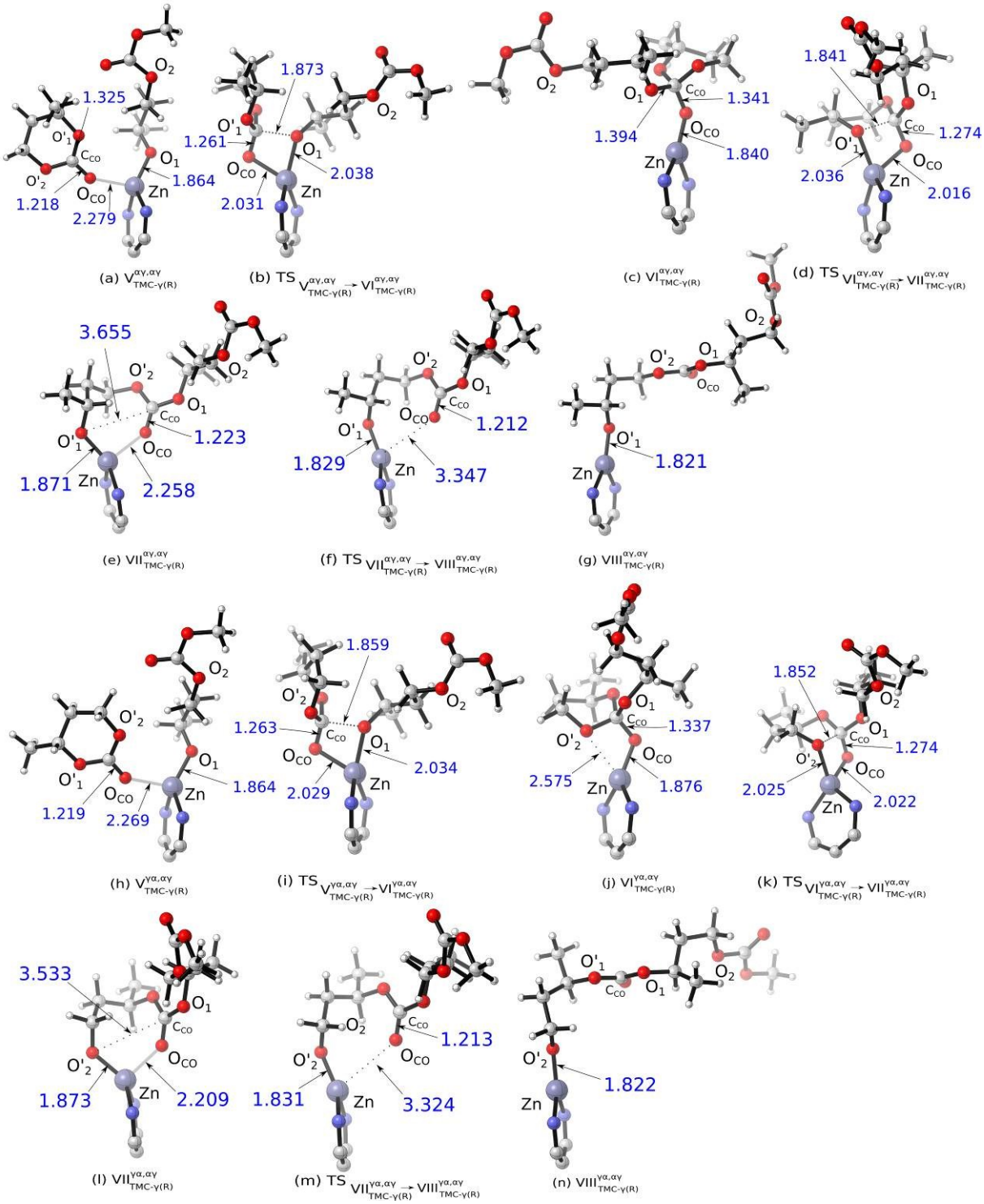

Figure S4. Optimized structures of complexes involved in the propagation step of the ROP of TMC-γ(*R*) mediated by $\mathbf{IV}^{\alpha\gamma}_{TMC\text{-}\gamma(R)}$

Cartesian coordinates :

3. Results and Discussion

[(BDI^{iPr})Zn(N(SiMe$_3$)$_2$)]

G = -2338.489821 kcal.mol^{-1}

C 0.06834 -0.68780 0.10323

C -0.07858 -0.11860 1.38956

C 1.06247 0.19319 2.17315

C 2.32638 -0.11891 1.66137

C 2.48052 -0.70728 0.41256

C 1.35677 -0.97438 -0.35925

N -1.38892 0.10250 1.92756

C -1.89838 1.33695 1.96459

C -1.25283 2.46644 1.18800

C 0.97906 0.90919 3.51802

C 1.66547 0.13979 4.65588

C -1.11905 -0.91294 -0.82058

C -1.12926 -2.30856 -1.45289

Zn -2.46553 -1.42905 2.62889

N -2.33302 -3.28625 2.25371

N -3.82446 -0.36880 3.68250

C -4.69564 -1.02963 4.61264

C -6.07494 -1.19990 4.33528

C -6.86055 -1.89313 5.26415

C -6.32285 -2.41221 6.43258

C -4.97026 -2.23514 6.69717

C -4.13908 -1.54866 5.80910

C -6.76543 -0.65565 3.08919

C -7.43210 -1.76982 2.26805

C -2.68148 -1.31050 6.17565

C -2.05937 -2.44209 6.99975

C -3.84495 0.96143 3.57302

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C -3.03517 1.70593 2.69702

C -7.82594 0.40276 3.43952

C -2.51366 0.03082 6.90734

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C -1.16813 0.17021 -1.91092

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H -5.28318 1.23435 5.19376

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H	-0.07831	1.01158	3.78044
H	-2.11315	-1.23726	5.23975
H	-2.02881	-0.81542	-0.21905
H	-6.00539	-0.18320	2.45760
Si	-3.72736	-4.00172	1.49265
Si	-0.97387	-4.23532	2.78942
C	-1.50728	-5.72770	3.83388
C	0.10824	-4.89486	1.37973
C	0.17207	-3.17642	3.85102
C	-3.30698	-5.46955	0.36683
C	-4.98944	-4.64964	2.74695
C	-4.53821	-2.70698	0.36554
H	-4.23095	-5.84896	-0.08646
H	-2.63256	-5.18481	-0.44680
H	-2.84818	-6.30299	0.90866
H	-5.89474	-5.02430	2.25405
H	-4.55948	-5.47977	3.31841
H	-5.28748	-3.88171	3.46742
H	-5.47685	-3.07778	-0.06179
H	-4.76804	-1.76602	0.87961
H	-3.86785	-2.47352	-0.46782
H	-0.62809	-6.26675	4.20657
H	-2.10182	-5.41537	4.69910
H	-2.10907	-6.44336	3.26346
H	1.00954	-3.77449	4.22881
H	0.59773	-2.36062	3.25736
H	-0.34190	-2.74952	4.71847
H	0.93223	-5.49269	1.78834
H	-0.44273	-5.52965	0.67943
H	0.55057	-4.06976	0.81160

[(BDI^{iPr})Zn(OMe)]

G = -1580.610511 kcal.mol^{-1}

Zn	0.34659	0.00022	0.36938
N	0.35431	-0.00079	2.33191
N	2.26898	0.00085	0.03734
C	1.50186	-0.00091	3.00936
C	3.13992	0.00045	1.05173
C	2.77732	-0.00031	2.40887
C	4.61750	0.00086	0.73861
C	1.46302	-0.00173	4.51947
H	5.21477	0.00090	1.65134
H	4.88792	-0.87605	0.14191
H	4.88754	0.87797	0.14204
H	2.46916	-0.00048	4.94077
H	0.92293	0.87354	4.89337
H	0.92562	-0.87908	4.89242
H	3.60867	-0.00043	3.10330
C	2.72612	0.00167	-1.31992
C	2.90729	-1.22714	-1.99298
C	3.25377	-1.19872	-3.34705
C	3.42433	0.00321	-4.02404
C	3.25269	1.20435	-3.34596
C	2.90617	1.23124	-1.99186
C	2.70203	-2.56204	-1.29157
H	3.38892	-2.13562	-3.88075
H	3.69093	0.00381	-5.07742
H	3.38704	2.14187	-3.87879
C	2.69992	2.56533	-1.28921
C	-0.89635	-0.00158	3.03236
C	-1.52194	1.22671	3.33803
C	-2.76145	1.19860	3.98371
C	-3.37692	-0.00305	4.31314
C	-2.76034	-1.20397	3.98309
C	-1.52080	-1.23061	3.33741
C	-0.91538	2.55850	2.92368
H	-3.25693	2.13537	4.22475
H	-4.34050	-0.00362	4.81548
H	-3.25500	-2.14131	4.22359
C	-0.91314	-2.56161	2.92210
C	-0.87225	-3.58744	4.06161
C	-1.66031	-3.12431	1.70157
C	-0.87527	3.58343	4.06404
C	-1.66304	3.12158	1.70365
C	3.86156	-3.53942	-1.52625
C	1.36476	-3.19681	-1.70276
C	3.85919	3.54339	-1.52230

C	1.36260	3.19996	-1.70046
H	-0.35738	4.49205	3.73810
H	-1.88032	3.88053	4.38206
H	-0.35129	3.19305	4.94270
H	-1.19145	4.04686	1.35317
H	-1.67927	2.40272	0.87799
H	-2.70348	3.35176	1.96001
H	3.72022	4.44528	-0.91660
H	4.82332	3.10015	-1.25271
H	3.92193	3.86209	-2.56834
H	1.20315	4.14672	-1.17239
H	1.34262	3.40700	-2.77629
H	0.51802	2.54098	-1.47494
H	3.72365	-4.44164	-0.92081
H	3.92336	-3.85767	-2.57249
H	4.82577	-3.09584	-1.25748
H	1.20589	-4.14407	-1.17541
H	0.52008	-2.53831	-1.47629
H	1.34442	-3.40295	-2.77876
H	-0.35426	-4.49566	3.73471
H	-0.34798	-3.19766	4.94037
H	-1.87707	-3.88506	4.37985
H	-1.18764	-4.04864	1.35005
H	-2.70044	-3.35601	1.95781
H	-1.67746	-2.40460	0.87668
O	-1.19028	0.00015	-0.59804
C	-1.28472	0.00042	-1.99504
H	-2.34654	0.00229	-2.28427
H	-0.82281	0.88433	-2.46626
H	-0.82599	-0.88513	-2.46626
H	0.11954	2.37130	2.61866
H	2.65108	2.36893	-0.21316
H	0.12163	-2.37337	2.61720
H	2.65362	-2.36680	-0.21529
H	-0.91571	-2.80802	0.31725
H	1.40937	-2.15899	0.76510
H	0.66478	-0.89508	-0.20255
H	1.74730	0.35985	1.50687
H	1.41875	-0.86144	2.75157
H	-0.43341	-4.51455	2.22863
H	0.87099	-3.44440	2.78136
H	-0.42602	-3.90547	3.89478

3.1. Ring-opening polymerization of α-methyl-substituted tetramethylene carbonate

Initiation Step of the ROP of 7CC-γMe.

(*R*)- 7CC-γMe

G = -460.040631 kcal.mol^{-1}

C	-1.02945	-2.45318	2.42401
C	-0.75163	-1.96791	1.00147
C	0.64371	-1.37461	0.78191
C	1.01167	-0.36249	1.86792
O	-0.11715	0.43235	2.25896
C	-1.03318	-0.12057	3.08221
O	-0.79284	-1.41914	3.41533
O	-1.94042	0.52430	3.52842
H	-2.09521	-2.71028	2.49494
C	-0.20098	-3.64897	2.85647
H	-1.50312	-1.21488	0.73622

(*S*)-7CC-γMe

G = -460.042763 kcal.mol^{-1}

H	-1.06812	-2.49199	2.40877
C	-0.89621	-2.12259	1.38991
O	0.49330	-1.69156	1.40435
C	1.28754	-1.86679	0.31445
O	1.75641	-0.95775	-0.31246
C	-1.15932	-3.24544	0.39304
C	-0.33316	-4.51003	0.64165
C	1.13324	-4.17823	0.90571
O	1.60011	-3.14839	0.02457
C	-1.76078	-0.89773	1.13593
H	-0.96705	-2.87046	-0.62031
H	-2.22772	-3.48539	0.42722
H	-0.72344	-5.06410	1.50420
H	-0.42104	-5.17070	-0.22748
H	1.78151	-5.03465	0.70674

H	1.28596	-3.86012	1.94130
H	-1.51690	-0.10770	1.84996
H	-1.59180	-0.51014	0.12656
H	-2.82158	-1.14834	1.24068

$I_{7CC\text{-}\gamma(R,re)}$

G = -2040.63228 kcal.mol^{-1}

C	1.777130	3.238361	-1.651920
C	1.933795	1.884533	-1.266576
C	2.268313	0.896267	-2.218665
C	2.455386	1.286041	-3.549132
C	2.329937	2.614032	-3.937616
C	1.994361	3.575931	-2.990993
N	1.692643	1.512829	0.094018
Zn	-0.090117	0.785138	0.611389
O	-1.242523	-0.092916	-0.586561
C	-2.047173	-1.185691	-0.259530
C	2.421977	-0.570603	-1.845394
C	1.295229	-1.417011	-2.456419
C	1.395622	4.323841	-0.652903
C	0.311152	5.266008	-1.192038
C	2.675771	1.565376	0.989659
C	4.090040	1.882121	0.551084
C	2.522111	1.283702	2.361327
C	1.436145	0.745868	3.072469
C	1.688438	0.491466	4.543423
N	0.258873	0.416062	2.535687
C	-0.703674	-0.307983	3.309076
C	-1.827334	0.366734	3.842022
C	-2.790594	-0.378813	4.529242
C	-2.668129	-1.753537	4.687484
C	-1.554971	-2.403687	4.169043
C	-0.554615	-1.706092	3.485195
C	-1.987739	1.876828	3.738805
C	-3.378477	2.291459	3.243934
C	0.648623	-2.479764	2.958084
C	0.265985	-3.399864	1.790154
C	1.338834	-3.292692	4.064293
C	-1.676250	2.555003	5.082785
O	-1.514017	2.537304	0.420025
C	-2.214566	2.347813	-0.566098
O	-1.711180	2.531342	-1.784618
C	-2.233314	1.752607	-2.879618
C	-3.391401	2.478931	-3.547629
C	-4.261191	3.181545	-2.503769
C	-4.617232	2.338842	-1.284195
O	-3.491165	2.005428	-0.415137
C	3.801673	-1.122055	-2.231383
C	2.614753	5.146509	-0.206013
H	2.106604	-0.509781	4.691632
H	2.411069	1.211427	4.933913
H	0.770559	0.548930	5.130528
H	4.611623	0.943249	0.329146
H	4.125919	2.493571	-0.350515
H	4.642956	2.381898	1.349729
H	3.412524	1.449464	2.957879
H	-3.652312	0.131916	4.950665
H	-3.432167	-2.314699	5.219001
H	-1.456676	-3.478569	4.299461
H	2.712287	0.533647	-4.290824
H	2.492178	2.899464	-4.973911
H	1.892533	4.613035	-3.299385
H	3.914035	-2.152168	-1.875299
H	3.941715	-1.135359	-3.317968
H	4.611972	-0.523906	-1.802009
H	1.405707	-2.467851	-2.163986
H	0.319039	-1.059924	-2.112024
H	1.321401	-1.374044	-3.551927
H	2.268057	-3.734754	3.688241
H	1.582792	-2.676359	4.935062
H	0.705618	-4.115501	4.413978
H	-0.483302	-4.137333	2.099248
H	-0.149326	-2.832476	0.954371
H	1.144195	-3.946733	1.428480
H	-1.772659	3.643079	4.994458
H	-2.368945	2.219081	5.863333
H	-0.659970	2.336978	5.424463
H	-3.413650	3.376986	3.102046

H	-3.614583	1.822531	2.286444
H	-4.163061	2.030897	3.963836
H	2.311802	5.921317	0.507426
H	3.376246	4.530345	0.278046
H	3.083010	5.645399	-1.062776
H	-0.041207	5.924698	-0.390789
H	0.690523	5.909705	-1.994253
H	-0.541428	4.703999	-1.577730
H	-3.058721	-1.067402	-0.688456
H	-1.647260	-2.132197	-0.667361
H	-2.188035	-1.336482	0.822319
H	2.331671	-0.644714	-0.756772
H	1.374794	-1.756049	2.575680
H	0.982108	3.820836	0.226227
H	-1.262454	2.238265	3.005025
H	-2.500643	0.772270	-2.479554
H	-1.381761	1.619835	-3.548567
H	-3.019731	3.225076	-4.257974
H	-3.974206	1.754803	-4.128834
H	-3.759208	4.094057	-2.164324
H	-5.206340	3.505713	-2.954536
H	-5.249788	2.952081	-0.631677
C	-5.354358	1.046979	-1.593094
H	-6.302420	1.273924	-2.091060
H	-4.771748	0.387652	-2.241135
H	-5.570724	0.507802	-0.667830

$TS(\mathbf{I}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)})$

G = -2040.625754 kcal.mol^{-1}

C	1.959966	3.259576	-1.632817
C	2.075318	1.908906	-1.227443
C	2.434058	0.905632	-2.155075
C	2.684760	1.277075	-3.479587
C	2.591722	2.601626	-3.888453
C	2.231069	3.577490	-2.967081
N	1.774110	1.546492	0.125057
Zn	-0.038169	0.898005	0.598858
O	-1.258606	0.024800	-0.641616
C	-2.022258	-1.121604	-0.365407
C	2.536991	-0.560509	-1.762690
C	1.424047	-1.385487	-2.426283
C	1.557750	4.373749	-0.675345
C	0.282039	5.087215	-1.144303
C	2.716500	1.617312	1.063589
C	4.129719	1.995827	0.679987
C	2.512079	1.317068	2.424878
C	1.408395	0.750523	3.085896
C	1.605016	0.478109	4.561622
N	0.255190	0.417516	2.499716
C	-0.731524	-0.324593	3.223552
C	-1.886324	0.334345	3.706745
C	-2.867236	-0.423674	4.353879

C	-2.732521	-1.796494	4.518436
C	-1.592521	-2.432305	4.042283
C	-0.574756	-1.721829	3.398444
C	-2.068265	1.840382	3.585228
C	-3.437496	2.219829	3.008581
C	0.650102	-2.483031	2.904820
C	0.306316	-3.396825	1.719481
C	1.312041	-3.301581	4.023891
C	-1.841950	2.534844	4.937234
O	-1.507132	2.367756	0.173657
C	-2.105437	1.837181	-0.783687
O	-1.695630	2.146055	-2.026778
C	-2.396578	1.517964	-3.108520
C	-3.723184	2.234692	-3.426657
C	-4.204128	3.113407	-2.267979
C	-4.437801	2.356896	-0.955230
O	-3.390023	1.390987	-0.689126
C	3.919700	-1.149907	-2.074585
C	2.690180	5.392190	-0.469906
H	2.014704	-0.525729	4.715182
H	2.313552	1.191712	4.987572
H	0.665056	0.532248	5.113520
H	4.645664	1.115230	0.279222
H	4.156796	2.759039	-0.098609
H	4.691254	2.345100	1.548390
H	3.371551	1.497078	3.060699

H	-3.753088	0.075389	4.737497	H	2.943987	5.899070	-1.407858	C	-0.267890	-0.119646	3.610553
H	-3.509510	-2.367638	5.019533	H	-0.024336	5.836849	-0.405867	C	-1.082944	0.693918	4.426196
H	-1.487099	-3.506331	4.173508	H	0.441193	5.607654	-2.095965	C	-2.010696	0.074567	5.269351
H	2.961847	0.512317	-4.201136	H	-0.534219	4.374112	-1.271084	C	-2.142624	-1.307596	5.307756
H	2.798060	2.872379	-4.920687	H	-3.018195	-1.022466	-0.818482	C	-1.337147	-2.096138	4.493886
H	2.154452	4.612950	-3.289405	H	-1.548418	-2.017980	-0.795930	N	0.646209	0.488978	2.690411
H	3.985345	-2.182202	-1.713179	H	-2.171135	-1.297875	0.709293	Zn	-0.012332	1.092589	0.924007
H	4.117396	-1.167375	-3.152011	H	2.391122	-0.623311	-0.679423	O	-1.858732	1.085578	0.772394
H	4.721817	-0.573772	-1.601945	H	1.382718	-1.752087	2.549524	C	-2.413872	1.080397	-0.453563
H	1.478898	-2.432445	-2.105829	H	1.336582	3.916422	0.293448	O	-1.587086	1.835031	-1.303221
H	0.439014	-0.990019	-2.160445	H	-1.311817	2.211534	2.888271	C	-1.981292	1.970528	-2.671197
H	1.519535	-1.367720	-3.518296	H	-2.546515	0.467764	-2.851465	C	-3.383068	2.554522	-2.855691
H	2.253589	-3.736526	3.671160	H	-1.701421	1.570762	-3.948536	C	-3.742566	3.608888	-1.807392
H	1.528284	-2.691344	4.906110	H	-3.601887	2.874795	-4.307202	C	-3.818497	3.012518	-0.373554
H	0.672940	-4.129811	4.349122	H	-4.481559	1.488397	-3.689369	C	-5.128061	3.343140	0.323309
H	-0.444551	-4.142905	2.002891	H	-3.469108	3.907493	-2.103260	C	-0.995182	2.212252	4.401433
H	-0.092654	-2.826227	0.877642	H	-5.140427	3.612398	-2.544039	C	-0.655237	2.794400	5.780866
H	1.197982	-3.933157	1.375625	H	-4.439957	3.075373	-0.124541	C	0.444664	-2.427203	2.736581
H	-1.951994	3.620157	4.833863	C	-5.728044	1.557106	-0.931614	C	-0.386653	-2.921276	1.542797
H	-2.569686	2.193370	5.682545	H	-6.588096	2.228423	-1.013182	N	1.673124	1.600335	0.094301
H	-0.841695	2.336614	5.334308	H	-5.764223	0.842315	-1.759176	C	2.811645	1.544961	0.801255
H	-3.486791	3.302283	2.848562	H	-5.810673	0.999043	0.004437	C	4.101706	1.958874	0.132381
H	-3.605830	1.728241	2.047724					C	1.720865	2.037158	-1.272248
H	-4.255942	1.951785	3.686694	$\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$				C	1.609345	3.413686	-1.569835
H	2.384717	6.160801	0.248824	G = 2040.641874 kcal.mol^{-1}				C	1.619898	3.807707	-2.911197
H	3.603419	4.924831	-0.089478	C	-0.389941	-1.527757	3.638116	C	1.738208	2.876665	-3.937330

C	1.844471	1.525972	-3.628319
C	1.839242	1.079645	-2.303000
C	1.444234	4.464029	-0.481175
C	2.452199	5.614628	-0.605498
C	1.954966	-0.411208	-2.018865
C	0.709675	-1.170075	-2.501403
C	2.912447	1.127117	2.137131
C	1.930680	0.622576	3.012777
C	2.400657	0.197074	4.383874
C	3.228171	-1.017380	-2.627268
C	0.005921	5.003490	-0.465267
O	-2.504231	-0.204139	-1.020588
C	-3.407327	-1.078179	-0.361803
O	-3.725454	1.589214	-0.419411
C	-2.287828	2.827661	3.845500
C	1.068512	-3.611702	3.487002
H	-0.180267	2.484942	3.722477
H	-2.872350	-1.769869	5.967007
H	3.911812	1.170847	2.552752
H	1.621359	3.974855	0.482017
H	0.222920	-3.539179	0.873723
H	1.267473	-1.828319	2.333415
H	2.376813	-0.893811	4.477256
H	1.747442	-4.162229	2.826876
H	1.638530	-3.283841	4.362413
H	0.309465	-4.321049	3.833874
H	1.743770	0.591837	5.163477
H	3.421194	0.534574	4.571156
H	-1.233227	-3.527837	1.883510
H	-1.447649	-3.176853	4.520849
H	0.280340	2.385321	6.176424
H	-2.644272	0.690747	5.902233
H	-1.443454	2.582622	6.511573
H	-0.547436	3.882995	5.719961
H	-2.193153	3.917383	3.773356
H	-3.139369	2.612107	4.500955
H	-2.513041	2.426803	2.853126
H	-0.206064	-0.787498	-2.041152
H	2.021160	-0.537241	-0.933223
H	0.794754	-2.235699	-2.259498
H	4.285248	1.357964	-0.763120
H	0.598131	-1.087070	-3.588657
H	4.054701	3.000541	-0.198451
H	4.948397	1.845230	0.810431
H	3.213913	-0.971236	-3.721663
H	4.130643	-0.499194	-2.287025
H	3.319472	-2.071967	-2.345260
H	1.934338	0.799481	-4.431966
H	1.747307	3.203298	-4.973805
H	1.532183	4.863364	-3.155198
H	2.290265	6.198661	-1.517884
H	2.350556	6.301090	0.242101
H	3.485887	5.254196	-0.623851
H	-0.717392	4.186915	-0.389173
H	-0.143442	5.688352	0.377164
H	-0.211540	5.555346	-1.387168
H	-5.972194	2.924188	-0.235215
H	-5.264389	4.427930	0.386643
H	-5.143681	2.927918	1.334508
H	-4.711964	4.048182	-2.074595
H	-3.014300	4.428663	-1.828800
H	-4.125705	1.753000	-2.816912
H	-3.437052	2.994629	-3.859692
H	-1.224996	2.643065	-3.085425
H	-1.897216	1.003737	-3.180030
H	-3.250080	-2.068291	-0.796575
H	-4.445776	-0.769973	-0.522226
H	-3.205568	-1.115238	0.714406
H	-0.791385	-2.086691	0.962987
H	-2.986616	3.391207	0.231734

$TS(\mathbf{II}^{\delta\alpha}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{III}^{\delta\alpha}_{7CC\text{-}\gamma(R,re)})$

G = -2040.628419 kcal.mol^{-1}

C	2.423131	1.370135	-2.218333
C	1.853315	2.218589	-1.237732
C	1.446084	3.531912	-1.570232
C	1.547520	3.942943	-2.903676
C	2.048004	3.098722	-3.887176

C	2.494438	1.829161	-3.537172	C	-2.887112	2.494347	3.895234	H	4.504335	-0.172342	-3.452608
N	1.638250	1.718850	0.085810	C	-0.877714	2.344190	5.407331	H	5.081399	0.664546	-2.010000
Zn	-0.115627	0.937923	0.583181	C	0.956396	-3.729866	3.072104	H	2.581799	-2.116972	-2.168581
O	-1.842081	2.032705	0.399468	O	-1.422436	-0.168591	-0.477833	H	1.127791	-1.125582	-1.990402
C	-2.656640	1.105516	0.094913	C	-1.654693	-0.698086	-1.759661	H	2.040502	-1.094280	-3.508398
O	-3.226370	0.460319	1.135649	C	-1.396824	0.263196	-2.929648	H	1.684833	-4.237923	2.430561
C	-4.082719	-0.644949	0.875817	C	-1.750532	1.723045	-2.635347	H	1.490928	-3.325823	3.937769
C	0.955030	4.523856	-0.523032	C	-3.145896	2.013135	-2.084079	H	0.261594	-4.491908	3.441966
C	-0.492645	4.971801	-0.766189	O	-3.498235	1.179459	-0.956236	H	-1.306247	-3.923147	1.426824
C	2.993648	-0.001442	-1.873760	C	-4.265786	1.801855	-3.089485	H	-1.005615	-2.434387	0.507083
C	2.132928	-1.148806	-2.417694	C	1.882433	5.747468	-0.442838	H	0.154249	-3.781946	0.436427
C	2.630534	1.768219	0.982845	C	4.443495	-0.153693	-2.359085	H	-0.851753	3.439283	5.439903
C	3.932358	2.431156	0.594383	H	2.233593	-1.073653	4.183413	H	-1.462185	1.998876	6.268121
C	2.571887	1.230557	2.275735	H	2.731923	0.529412	4.734027	H	0.146995	1.983515	5.535080
C	1.542251	0.525584	2.933501	H	1.061214	-0.034481	4.980335	H	-2.794249	3.584836	3.845933
C	1.907199	-0.032810	4.291885	H	4.447390	1.855582	-0.180859	H	-3.347291	2.144916	2.969370
N	0.332497	0.303230	2.426051	H	3.756112	3.426530	0.178712	H	-3.560256	2.264445	4.729324
C	-0.639303	-0.397398	3.213559	H	4.597857	2.520937	1.454060	H	1.568802	6.408800	0.372246
C	-0.705589	-1.806890	3.159044	H	3.478316	1.349630	2.857310	H	2.924592	5.464497	-0.263708
C	-1.679255	-2.459220	3.922041	H	-3.178252	0.191676	5.397605	H	1.855307	6.330733	-1.369980
C	-2.559843	-1.749208	4.729039	H	-3.301630	-2.274775	5.324890	H	-0.789812	5.710442	-0.013261
C	-2.485598	-0.361367	4.768647	H	-1.743059	-3.543864	3.886082	H	-0.605161	5.440474	-1.750740
C	-1.543020	0.341298	4.012185	H	2.916790	1.182622	-4.302394	H	-1.182935	4.128295	-0.693544
C	0.228760	-2.630776	2.285085	H	2.110523	3.435498	-4.918512	H	-3.527879	-1.442163	0.374061
C	-0.528996	-3.227131	1.090200	H	1.232259	4.948020	-3.172676	H	-4.412357	-0.994042	1.854735
C	-1.503260	1.861812	4.088614	H	4.868606	-1.094462	-1.992876	H	-4.944332	-0.348440	0.271342

H	2.998564	-0.094397	-0.783406
H	0.989738	-1.954174	1.882659
H	0.983558	4.020408	0.448397
H	-0.869847	2.213432	3.268905
H	-2.705507	-1.018722	-1.800075
H	-1.049615	-1.607725	-1.892382
H	-0.336885	0.246448	-3.206350
H	-1.947788	-0.111474	-3.802942
H	-1.018152	2.123328	-1.932962
H	-1.634450	2.315216	-3.551381
H	-3.161877	3.052596	-1.732194
H	-4.132798	2.473295	-3.942852
H	-4.276532	0.772104	-3.459149
H	-5.237324	2.011284	-2.633356

III$^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}$

G = -2040.634709 kcal.mol^{-1}

C	2.437392	1.370421	-2.218901
C	1.852885	2.216984	-1.245102
C	1.450932	3.531247	-1.581262
C	1.569231	3.943003	-2.913219
C	2.080540	3.099033	-3.891402
C	2.524107	1.829777	-3.536623
N	1.620085	1.708501	0.072228
Zn	-0.053369	0.713526	0.460419
O	-1.929394	2.146840	0.459019
C	-2.856160	1.364329	0.256857
O	-3.331645	0.623017	1.245958
C	-4.195501	-0.480280	0.952609
C	0.952675	4.526567	-0.539758
C	-0.481340	5.003586	-0.808004
C	3.010223	0.002154	-1.864700
C	2.153698	-1.152517	-2.401013
C	2.589185	1.788549	0.992368
C	3.877914	2.492236	0.633854
C	2.520655	1.241857	2.280080
C	1.494800	0.511266	2.915554
C	1.857869	-0.051607	4.274062
N	0.301047	0.260919	2.384076
C	-0.674019	-0.442098	3.165671
C	-0.721969	-1.852673	3.137184
C	-1.698756	-2.501655	3.900340
C	-2.596854	-1.787325	4.682537
C	-2.541383	-0.397036	4.695583
C	-1.598830	0.303014	3.937070
C	0.237467	-2.685784	2.299968
C	-0.490074	-3.331535	1.111804
C	-1.576250	1.826935	3.962206
C	-2.974173	2.448452	4.068925
C	-0.686137	2.372852	5.090543
C	0.971974	-3.745378	3.134251
O	-1.186614	-0.428665	-0.503117
C	-1.551797	-0.743968	-1.807412
C	-1.332700	0.329208	-2.885170
C	-1.729216	1.756542	-2.505716
C	-3.155592	2.026055	-2.034513
O	-3.541158	1.237005	-0.868243
C	-4.226719	1.727539	-3.068123
C	1.893196	5.739313	-0.440562
C	4.462945	-0.145716	-2.342580
H	2.272830	-1.058195	4.144973
H	2.622700	0.560573	4.756480
H	0.996235	-0.140260	4.936090
H	4.397724	1.967014	-0.173241
H	3.682456	3.504462	0.271297
H	4.545656	2.551190	1.494423
H	3.413241	1.378050	2.879128
H	-3.251690	0.156910	5.302225
H	-3.339601	-2.310157	5.279791
H	-1.748877	-3.587437	3.883846
H	2.956572	1.183967	-4.296666
H	2.155150	3.436448	-4.921763
H	1.258838	4.948831	-3.185397
H	4.889976	-1.082437	-1.968354
H	4.530147	-0.171193	-3.435631
H	5.095048	0.677444	-1.993958
H	2.616326	-2.115749	-2.157595
H	1.153316	-1.141573	-1.961920

H	2.051439	-1.097648	-3.490952	H	-2.626938	-1.000801	-1.811850	C	2.532052	1.209439	2.283052
H	1.721757	-4.257592	2.521255	H	-1.032806	-1.657494	-2.154843	C	2.607760	1.750112	0.993517
H	1.482399	-3.306050	3.997484	H	-0.270834	0.369690	-3.155404	C	3.897418	2.450368	0.635042
H	0.285229	-4.510335	3.513421	H	-1.863209	0.002642	-3.790940	N	1.640028	1.668715	0.070245
H	-1.273984	-4.016054	1.457401	H	-1.043885	2.124683	-1.741702	Zn	-0.011289	0.660618	0.454484
H	-0.943479	-2.560500	0.481792	H	-1.569281	2.410669	-3.372471	O	-1.295659	-0.312804	-0.449837
H	0.212833	-3.912335	0.502848	H	-3.219326	3.077103	-1.726969	C	-1.593061	-0.651285	-1.769288
H	-0.716253	3.468340	5.101712	H	-4.056941	2.336140	-3.960924	C	-1.377029	0.434946	-2.832163
H	-1.034045	2.018321	6.068003	H	-4.207703	0.674211	-3.361059	C	-1.842327	1.840284	-2.449816
H	0.358317	2.074295	4.975843	H	-5.221191	1.958936	-2.676654	C	-3.300997	2.047380	-2.048228
H	-2.908947	3.529872	3.908379					C	-4.307282	1.709740	-3.134004
H	-3.651405	2.032326	3.319955	TS($\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,re)}\rightarrow\mathbf{IV}^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)				C	1.860849	2.201867	-1.241296
H	-3.417764	2.299532	5.060374	G = -2040.634140 kcal.mol^{-1}				C	2.430396	1.372513	-2.237798
H	1.578387	6.398973	0.375485	C	-1.619291	0.370656	3.917493	C	2.505960	1.857853	-3.546977
H	2.930964	5.446307	-0.253863	C	-0.700325	-0.403253	3.168536	C	2.061446	3.134442	-3.871631
H	1.881440	6.328253	-1.364528	C	-0.771020	-1.812851	3.159712	C	1.563029	3.960062	-2.871373
H	-0.775343	5.749397	-0.060887	C	-1.760993	-2.434388	3.928141	C	1.460254	3.524283	-1.545825
H	-0.568981	5.472998	-1.794661	C	-2.650988	-1.692441	4.693741	C	2.997469	-0.006971	-1.920943
H	-1.190990	4.176411	-0.745678	C	-2.576207	-0.303291	4.681880	C	4.456954	-0.139885	-2.382763
H	-3.667210	-1.190308	0.314257	N	0.296416	0.269140	2.385685	C	0.986879	4.506607	-0.480030
H	-4.410755	-0.932801	1.919880	C	1.490397	0.506653	2.924033	C	1.938485	5.711522	-0.383832
H	-5.116961	-0.142592	0.472511	C	1.829551	-0.041673	4.293710	O	-2.278560	2.339458	0.492244
H	3.014111	-0.082360	-0.773556	C	0.171700	-2.670893	2.328781	C	-3.097806	1.466192	0.261423
H	0.993205	-2.008749	1.888303	C	0.872329	-3.753122	3.162636	O	-3.696132	1.237081	-0.906287
H	0.952739	4.018643	0.429814	C	-1.578450	1.894721	3.909971	O	-3.558159	0.688802	1.237690
H	-1.150878	2.154725	3.008576	C	-0.652822	2.456733	5.001500	C	-4.305207	-0.486346	0.913626

C	-0.448645	4.999383	-0.710628	H	-1.364896	-3.963379	1.475577	H	-1.216375	2.210197	-1.636717
C	2.149378	-1.139986	-2.513723	H	-1.012057	-2.508874	0.512725	H	-1.655126	2.517364	-3.293045
C	-0.568046	-3.291917	1.134578	H	0.122183	-3.880829	0.518913	H	-3.420003	3.094438	-1.743317
C	-2.965704	2.534884	4.037524	H	-0.683659	3.552172	4.995753	H	-4.119152	2.325624	-4.018338
H	2.210588	-1.064076	4.185280	H	-0.970456	2.118511	5.994896	H	-4.235195	0.658253	-3.425915
H	2.611672	0.553996	4.768729	H	0.388431	2.158209	4.859853	H	-5.327611	1.901645	-2.790533
H	0.962042	-0.089585	4.952240	H	-2.890560	3.610572	3.847364				
H	4.406220	1.935441	-0.185396	H	-3.665075	2.110040	3.314808	**IV**$^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$			
H	3.704481	3.469489	0.290912	H	-3.383991	2.416329	5.044150	G = -2040.652800 kcal.mol^{-1}			
H	4.572736	2.491950	1.490607	H	1.650449	6.356481	0.453445	C	-0.802614	-1.316034	3.010141
H	3.424942	1.338270	2.883135	H	2.979683	5.409747	-0.233083	C	-0.555111	0.069729	3.129616
H	-3.284387	0.271071	5.271180	H	1.903879	6.318862	-1.295133	C	-1.428875	0.902955	3.861425
H	-3.405151	-2.193329	5.295413	H	-0.712399	5.747831	0.045053	C	-2.543306	0.322077	4.474001
H	-1.829486	-3.519248	3.927922	H	-0.553804	5.473290	-1.693435	C	-2.796565	-1.040186	4.371646
H	2.928479	1.225780	-4.324018	H	-1.172362	4.185856	-0.631554	C	-1.930694	-1.846516	3.642539
H	2.124875	3.491909	-4.895913	H	-3.693183	-1.149975	0.300521	N	0.555875	0.651730	2.434361
H	1.251869	4.971479	-3.120515	H	-4.520431	-0.957123	1.872625	Zn	0.271715	1.401768	0.650613
H	4.875833	-1.093266	-2.042950	H	-5.233950	-0.234778	0.395170	O	-1.334658	1.550465	-0.198381
H	4.539322	-0.117683	-3.474780	H	2.985333	-0.129119	-0.833228	C	-1.526066	2.047441	-1.498129
H	5.086189	0.665186	-1.990033	H	0.949477	-2.014562	1.924085	C	-2.812358	2.870460	-1.586366
H	2.599676	-2.113443	-2.289084	H	1.005106	3.986532	0.482937	C	-4.092052	2.162798	-1.127103
H	1.136717	-1.137033	-2.103306	H	-1.177382	2.198198	2.937797	C	-4.436248	0.900179	-1.927766
H	2.073137	-1.050636	-3.603302	H	-2.654941	-0.948596	-1.804367	C	-3.931087	-0.379386	-1.285931
H	1.610237	-4.284404	2.551510	H	-1.025984	-1.544658	-2.090856	C	-1.214602	2.405420	3.964833
H	1.390937	-3.330047	4.029087	H	-0.308053	0.516516	-3.064434	C	-1.212838	2.902287	5.416880
H	0.163070	-4.499646	3.536604	H	-1.862693	0.097229	-3.758585	C	0.087684	-2.225176	2.175185

C	-0.607101	-2.593085	0.855032	H	-0.692859	2.683168	-1.840626	H	1.418488	-0.250659	-3.731427
N	2.099607	1.947238	0.224607	H	-0.228610	2.630779	3.544627	H	5.189884	2.005507	1.539635
C	3.086406	1.773359	1.108927	H	-3.669818	-1.471567	4.853230	H	4.819994	1.698295	-0.169964
C	4.482398	2.212065	0.735573	H	3.818503	1.148958	2.980969	H	4.047897	-0.179277	-3.751798
C	2.355547	2.552421	-1.048230	H	2.086456	4.269629	0.913547	H	4.907320	0.148875	-2.243446
C	2.250651	3.955346	-1.185208	H	0.052721	-3.199086	0.223879	H	4.098566	-1.408331	-2.486922
C	2.403592	4.511720	-2.458571	H	0.994677	-1.666032	1.923504	H	2.965934	1.719472	-4.288527
C	2.657396	3.715749	-3.569824	H	1.725997	-0.939422	4.416841	H	2.769670	4.168022	-4.551383
C	2.767822	2.338996	-3.417701	H	1.230551	-4.066645	2.323419	H	2.317874	5.587950	-2.582575
C	2.623349	1.731909	-2.166343	H	1.011990	-3.247495	3.878848	H	2.725580	6.762841	-0.748538
C	1.940617	4.857130	0.001401	H	-0.324637	-4.144314	3.151237	H	2.686757	6.629170	1.008673
C	2.876432	6.070089	0.086187	H	1.217092	0.599126	5.085754	H	3.929680	5.771234	0.082397
C	2.727187	0.218545	-2.047732	H	2.941778	0.304155	4.769891	H	-0.210808	4.450005	-0.014905
C	1.496046	-0.466604	-2.660025	H	-1.518417	-3.171980	1.041947	H	0.242022	5.931446	0.846046
C	2.917199	1.204577	2.382765	H	-2.138770	-2.909550	3.554885	H	0.257740	5.891006	-0.925346
C	1.762717	0.686787	3.001982	H	-0.469630	2.375977	6.024842	H	-2.686210	3.775426	-0.978308
C	1.930352	0.135702	4.397875	H	-3.228506	0.951726	5.035463	H	-2.937055	3.204294	-2.626581
C	4.019369	-0.330910	-2.667419	H	-2.188688	2.765671	5.895599	H	-4.009506	1.907046	-0.065410
C	0.471448	5.305967	-0.023864	H	-0.980511	3.972260	5.451395	H	-4.922355	2.870148	-1.223613
O	-5.881613	0.726875	-2.007394	H	-2.074155	4.239167	3.160362	H	-4.056395	0.994311	-2.950669
C	-6.616213	1.407453	-2.883816	H	-3.269588	2.981160	3.509709	H	-5.912356	3.548570	-5.188625
O	-7.816045	1.296025	-2.958712	H	-2.236622	2.836215	2.080483	H	-7.365718	3.596395	-4.138460
O	-5.875173	2.218444	-3.672147	H	0.570254	-0.124361	-2.187073	H	-7.167130	2.271933	-5.305414
C	-6.635960	2.950769	-4.633511	H	2.744824	-0.030034	-0.981480	H	-0.895622	-1.698992	0.294028
C	-2.258654	3.159290	3.126015	H	1.557604	-1.553904	-2.540129	H	-1.582800	1.215267	-2.224201
C	0.523967	-3.488672	2.928872	H	4.507149	3.283338	0.512942	H	-2.866763	-0.287597	-1.058001

H	-4.458034	-0.548610	-0.341853
H	-4.099184	-1.242838	-1.936092

TS($\mathbf{II}^{6\alpha}{}_{7CC\text{-}\gamma(R,re)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$)

G = -2040.625301 kcal.mol^{-1}

C	-0.431752	-1.598125	3.282670
C	-0.459787	-0.185679	3.360325
C	-1.398637	0.473255	4.184666
C	-2.298383	-0.302110	4.923160
C	-2.286314	-1.689310	4.853077
C	-1.358850	-2.324784	4.036118
N	0.439305	0.578020	2.543959
Zn	-0.019070	0.951295	0.673327
O	-1.290103	0.007911	-0.287052
C	-2.440517	0.562766	-0.678782
O	-2.390701	0.836120	-2.041490
C	-3.621163	1.035057	-2.741438
C	-4.642725	1.896242	-2.008151
C	-4.077898	3.189199	-1.422672
C	-2.753867	3.024372	-0.652844
C	-2.594120	4.145984	0.361800
C	-1.474324	1.989217	4.287161
C	-1.242337	2.486323	5.722028
C	0.554888	-2.350379	2.399614
C	-0.156409	-3.012704	1.209327
N	1.632862	1.822143	0.053535
C	2.690561	1.850024	0.870206
C	4.056187	2.212916	0.327501
C	1.788865	2.199703	-1.323284
C	1.590846	3.551238	-1.696430
C	1.765806	3.898907	-3.039180
C	2.098762	2.947989	-3.997035
C	2.250499	1.620787	-3.620822
C	2.102020	1.218749	-2.289362
C	1.198239	4.620518	-0.683067
C	2.413788	5.348718	-0.086597
C	2.267368	-0.254124	-1.944781
C	1.154960	-1.098534	-2.585604
C	2.664939	1.489170	2.230951
C	1.658327	0.880987	2.999559
C	2.025361	0.510608	4.417281
C	3.653567	-0.785092	-2.338439
C	0.226915	5.656018	-1.264529
O	-3.531424	-0.287631	-0.464274
C	-3.733297	-0.693642	0.876390
O	-2.657260	1.796617	0.078758
C	-2.814448	2.511298	3.749761
C	1.368296	-3.385368	3.190320
H	-0.679862	2.404756	3.658522
H	-2.996808	-2.273303	5.431854
H	3.605711	1.631448	2.749663
H	0.688594	4.107503	0.141300
H	0.569185	-3.532804	0.573519
H	1.264694	-1.621777	1.994394
H	2.063659	-0.577593	4.531845
H	2.122046	-3.848138	2.544168
H	1.886447	-2.934936	4.043347
H	0.732988	-4.189230	3.577713
H	1.274650	0.870875	5.125043
H	2.997755	0.921633	4.691805
H	-0.886053	-3.755151	1.552830
H	-1.352575	-3.410220	3.979576
H	-0.286844	2.140365	6.128987
H	-3.025262	0.194286	5.561117
H	-2.032127	2.140480	6.397933
H	-1.241586	3.581501	5.750577
H	-2.842284	3.606081	3.790759
H	-3.652747	2.137339	4.348466
H	-2.972329	2.202255	2.713109
H	0.165260	-0.762469	-2.265123
H	2.176467	-0.357552	-0.858097
H	1.268587	-2.151488	-2.304000
H	4.559130	1.297822	-0.006473
H	1.201086	-1.041587	-3.679146
H	4.008305	2.886741	-0.527550
H	4.676169	2.660195	1.107598
H	3.795239	-0.768810	-3.424576
H	4.460079	-0.194002	-1.892635

H	3.771251	-1.823192	-2.009078
H	2.489882	0.875630	-4.374813
H	2.226913	3.241212	-5.035495
H	1.630259	4.932202	-3.344309
H	3.013105	5.813431	-0.877809
H	2.085082	6.141502	0.594766
H	3.063055	4.677865	0.479470
H	-0.612903	5.182645	-1.780632
H	-0.173265	6.284765	-0.462722
H	0.724597	6.324481	-1.975587
H	-3.386463	4.090249	1.114304
H	-2.663511	5.118788	-0.134544
H	-1.629652	4.090868	0.874957
H	-4.833732	3.624062	-0.755503
H	-3.903058	3.929485	-2.215295
H	-5.075818	1.300911	-1.201976
H	-5.456628	2.129283	-2.706594
H	-3.314635	1.509353	-3.680619
H	-4.066824	0.061743	-2.980792
H	-4.535128	-1.435561	0.853227
H	-4.039863	0.148169	1.507917
H	-2.831759	-1.148736	1.297001
H	-0.683713	-2.276142	0.595828
H	-1.926712	3.058756	-1.373082

$\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$

G = -2040.628134 kcal.mol^{-1}

C	-1.603931	0.357502	4.040870
C	-0.552030	-0.184178	3.266709
C	-0.373871	-1.586245	3.179087
C	-1.265597	-2.418849	3.861428
C	-2.301724	-1.898264	4.627354
C	-2.459121	-0.521317	4.715131
N	0.314506	0.677279	2.517623
Zn	-0.096664	1.128269	0.641411
O	-2.106965	1.959390	0.351559
C	-2.222551	3.308676	-0.133438
C	-1.651754	4.225070	0.937859
C	0.740066	-2.218938	2.355023
C	0.180790	-2.892576	1.092760
C	-1.832734	1.855213	4.183791
C	-1.578188	2.333284	5.622214
N	1.642837	1.909108	0.050785
C	2.637844	1.973023	0.935350
C	4.043277	2.338012	0.502631
C	1.895053	2.162260	-1.341786
C	2.102765	1.068341	-2.214345
C	2.330444	1.326264	-3.569300
C	2.356783	2.621397	-4.068491
C	2.146566	3.687132	-3.203849
C	1.908245	3.488072	-1.839964
C	2.137763	-0.375185	-1.733858

C	1.170492	-1.272041	-2.517104
C	1.699233	4.712252	-0.957443
C	2.984769	5.541894	-0.806458
C	2.521510	1.667781	2.307881
C	1.503835	1.018811	3.023982
C	1.839531	0.633587	4.447054
C	0.576282	5.615420	-1.488752
C	3.569095	-0.932963	-1.782848
O	-1.177293	0.105257	-0.585786
C	-2.287047	0.800398	-0.686916
O	-2.449063	1.384234	-1.925798
C	-3.742615	1.876358	-2.294137
C	-4.484196	2.638313	-1.200569
C	-3.662142	3.711314	-0.482583
O	-3.452450	0.129374	-0.356570
C	-3.347262	-0.851834	0.662235
C	1.574977	-3.214835	3.173072
C	-3.244662	2.255751	3.733982
H	-1.115908	2.360999	3.529026
H	-2.980859	-2.562598	5.154924
H	3.425140	1.852223	2.878731
H	1.408209	4.359794	0.037272
H	0.990563	-3.343238	0.507892
H	1.413512	-1.419924	2.029491
H	2.080086	-0.433503	4.504910
H	2.428621	-3.566609	2.583737

H	1.961481	-2.765292	4.093461
H	0.991170	-4.096854	3.457853
H	0.996328	0.801707	5.119812
H	2.703169	1.194625	4.808151
H	-0.522362	-3.691333	1.355638
H	-1.143310	-3.496642	3.792218
H	-0.565481	2.096279	5.962165
H	-3.265078	-0.114197	5.320523
H	-2.279021	1.868152	6.324505
H	-1.708372	3.418881	5.693838
H	-3.385844	3.337432	3.842264
H	-4.013895	1.768070	4.342685
H	-3.413460	1.989766	2.687534
H	0.146183	-0.903451	-2.427335
H	1.818750	-0.388949	-0.686629
H	1.203296	-2.293107	-2.121378
H	4.096119	2.679415	-0.529757
H	1.437792	-1.326473	-3.578300
H	4.449600	3.112779	1.159439
H	4.690270	1.460286	0.606016
H	3.943746	-0.967329	-2.812173
H	4.263863	-0.320489	-1.199604
H	3.598105	-1.953203	-1.384310
H	2.497590	0.490689	-4.243568
H	2.540483	2.799428	-5.124569
H	2.169405	4.701737	-3.593155
H	3.316601	5.926345	-1.777424
H	2.809632	6.402455	-0.150964
H	3.806480	4.959840	-0.383242
H	-0.347422	5.056884	-1.658139
H	0.367122	6.421432	-0.777056
H	0.856570	6.084832	-2.437886
H	-2.221028	4.129627	1.866223
H	-1.703604	5.268009	0.610565
H	-0.603453	3.991573	1.149199
H	-4.192176	3.998918	0.434507
H	-3.593294	4.618908	-1.097627
H	-4.844482	1.917072	-0.465537
H	-5.370133	3.098054	-1.656833
H	-3.538249	2.524504	-3.153243
H	-4.362615	1.039675	-2.638269
H	-4.361097	-1.228880	0.814118
H	-2.978914	-0.428773	1.602299
H	-2.692238	-1.670936	0.355388
H	-0.342720	-2.175107	0.454262
H	-1.614047	3.384070	-1.042971

TS($\mathbf{II}^{\alpha\delta}_{7CC\text{-}\gamma(R,re)}$→$\mathbf{III}^{\alpha\delta}_{7CC\text{-}\gamma(R,re}$

G = -2040.626102 kcal.mol^{-1}

C	-1.613789	0.357213	4.038528
C	-0.561504	-0.185375	3.264780
C	-0.391111	-1.588259	3.169536
C	-1.292944	-2.419868	3.840008
C	-2.332411	-1.898225	4.600976
C	-2.480636	-0.520771	4.698872
N	0.305688	0.676937	2.520799
Zn	-0.159051	1.231321	0.677292
O	-2.052525	1.990838	0.416947
C	-2.155962	3.317841	-0.091893
C	-1.609422	4.287598	0.950061
C	0.726528	-2.222941	2.351854
C	0.175394	-2.897128	1.086548
C	-1.825851	1.855617	4.199027
C	-1.576489	2.308146	5.646539
N	1.608306	1.932081	0.050183
C	2.614747	1.972976	0.923129
C	4.018666	2.334170	0.480176
C	1.853831	2.176829	-1.345218
C	2.060996	1.077079	-2.211657
C	2.287914	1.326555	-3.568331
C	2.312250	2.618368	-4.076379
C	2.102058	3.689396	-3.218578
C	1.866378	3.499155	-1.852847
C	2.101783	-0.362673	-1.719655
C	1.184893	-1.285063	-2.532624
C	1.666174	4.729492	-0.977149
C	2.963192	5.539443	-0.816916
C	2.514248	1.655351	2.294239

C	1.502885	1.001980	3.015780
C	1.853831	0.598381	4.430274
C	0.563147	5.649568	-1.520952
C	3.543315	-0.896128	-1.712839
O	-1.138298	0.049623	-0.585244
C	-2.248894	0.669888	-0.760533
O	-2.394363	1.329789	-1.935535
C	-3.683231	1.862324	-2.283959
C	-4.403884	2.611940	-1.169802
C	-3.594078	3.705043	-0.469787
O	-3.408085	0.056593	-0.401183
C	-3.322004	-0.877960	0.668779
C	1.553727	-3.220428	3.176054
C	-3.226870	2.282235	3.740206
H	-1.096980	2.361075	3.557645
H	-3.019831	-2.562052	5.118471
H	3.426665	1.828149	2.854847
H	1.360766	4.384039	0.015559
H	0.988235	-3.353916	0.510655
H	1.402150	-1.424973	2.028803
H	2.093340	-0.469465	4.474156
H	2.411736	-3.572974	2.593520
H	1.933108	-2.772679	4.100227
H	0.966173	-4.101797	3.455361
H	1.017837	0.761383	5.113543
H	2.722359	1.153788	4.788509
H	-0.534362	-3.691798	1.344622
H	-1.176057	-3.497984	3.765168
H	-0.571165	2.047801	5.991722
H	-3.287326	-0.112530	5.302658
H	-2.291734	1.845439	6.335849
H	-1.688094	3.394717	5.732822
H	-3.356762	3.362714	3.871909
H	-4.010285	1.788924	4.326130
H	-3.379018	2.044999	2.684270
H	0.153536	-0.928188	-2.500275
H	1.740938	-0.374035	-0.686630
H	1.209010	-2.297747	-2.115668
H	4.069481	2.650903	-0.560236
H	1.503604	-1.358031	-3.578414
H	4.417372	3.129527	1.117211
H	4.673685	1.466113	0.608148
H	3.956483	-0.924685	-2.727605
H	4.205276	-0.271861	-1.105131
H	3.574895	-1.915267	-1.311504
H	2.456525	0.487245	-4.237423
H	2.495256	2.789535	-5.133763
H	2.124775	4.701456	-3.614362
H	3.309902	5.914455	-1.786437
H	2.795385	6.405259	-0.166406
H	3.771549	4.946238	-0.383925
H	-0.367667	5.105925	-1.700121
H	0.358999	6.458324	-0.810984
H	0.861337	6.115893	-2.466235
H	-2.196398	4.224344	1.870604
H	-1.657058	5.317892	0.582988
H	-0.564918	4.067733	1.193909
H	-4.138913	4.005178	0.434782
H	-3.530394	4.600242	-1.103553
H	-4.740774	1.887385	-0.427407
H	-5.306732	3.052839	-1.612198
H	-3.464053	2.524909	-3.127075
H	-4.316814	1.043971	-2.645734
H	-4.343654	-1.221444	0.839719
H	-2.937787	-0.407639	1.577685
H	-2.684909	-1.722519	0.398063
H	-0.335549	-2.176407	0.441993
H	-1.540046	3.385397	-1.001531

III$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$

G = -2040.640785 kcal.mol^{-1}

C	1.806497	3.482545	-1.907401
C	1.785999	2.167815	-1.380574
C	1.964682	1.054545	-2.237026
C	2.193576	1.282904	-3.597369
C	2.239307	2.568339	-4.120399
C	2.041136	3.652584	-3.275952
N	1.566947	1.949697	0.021563

Zn	-0.253483	1.580927	0.777754	C	-1.430229	2.360179	5.568652	H	-1.273437	-3.424383	3.736199
O	-1.918215	2.454801	0.782259	C	4.011598	2.217874	0.371758	H	-3.169010	-2.453792	4.991775
C	-2.185777	3.611668	0.046449	C	1.918429	0.518356	4.359856	H	-3.402014	0.001174	5.157259
C	-3.681018	3.697595	-0.325308	C	3.374449	-0.960009	-1.664839	H	2.073298	4.658660	-3.685558
C	-4.327859	2.404354	-0.823562	C	1.511730	-3.139411	3.327308	H	1.241958	4.384262	-0.068123
C	-3.687364	1.727805	-2.025842	C	0.584112	5.689887	-1.636616	H	-0.357985	5.187100	-1.869418
O	-2.375731	1.177929	-1.736797	C	-3.245373	2.429685	3.813298	H	0.373152	6.497436	-0.928202
C	-2.257119	0.198713	-0.865121	C	-1.800376	4.870477	0.830587	H	0.953808	6.154880	-2.557181
O	-1.173929	-0.099528	-0.368769	O	-3.383158	-0.464823	-0.633662	H	3.358528	5.816722	-1.757771
C	1.953201	-0.379358	-1.727096	C	-3.317510	-1.498428	0.362613	H	3.687724	4.842377	-0.321492
C	1.049327	-1.288341	-2.570260	H	3.473575	1.722001	2.763271	H	2.771535	6.347826	-0.174425
C	1.614821	4.720214	-1.041372	H	2.425442	2.724375	-5.179677	H	-1.153482	2.433978	3.441293
C	2.937009	5.468941	-0.807678	H	2.344968	0.433224	-4.257775	H	-3.485331	2.205690	2.771892
C	2.605959	1.921967	0.859892	H	4.030990	-0.361518	-1.027725	H	-4.002665	1.983147	4.468014
C	2.536487	1.600845	2.229195	H	3.357484	-1.981449	-1.268205	H	-3.304696	3.515931	3.944546
C	1.519781	0.972493	2.971821	H	3.825834	-0.996265	-2.663038	H	-2.082825	1.894105	6.316008
N	0.295028	0.729291	2.512221	H	2.401727	-3.509069	2.806221	H	-1.511084	3.446728	5.685293
C	-0.597713	-0.122618	3.230302	H	1.836788	-2.644075	4.247206	H	-0.400347	2.074191	5.803945
C	-0.440409	-1.529678	3.156746	H	1.451158	-1.442086	-3.578043	H	4.633426	1.322667	0.472597
C	-1.383474	-2.344095	3.792446	H	0.964672	-2.274397	-2.101381	H	2.427639	-0.450196	4.312937
C	-2.450498	-1.803282	4.499844	H	1.071222	-3.420047	0.653637	H	1.055630	0.406514	5.018124
C	-2.580494	-0.422350	4.585341	H	0.918644	-4.013292	3.618993	H	2.617551	1.232757	4.801734
C	-1.672548	0.439513	3.961075	H	1.548891	-0.364772	-0.711104	H	1.392752	-1.408249	2.073821
C	0.713391	-2.194311	2.415963	H	0.045568	-0.868235	-2.664006	H	4.464444	2.988945	1.002642
C	0.227420	-2.947208	1.169330	H	-0.479939	-3.740455	1.439312	H	4.045283	2.544268	-0.666630
C	-1.830652	1.942039	4.144830	H	-0.264335	-2.266274	0.470895	H	-1.619886	3.614725	-0.904618

H	-2.028554	5.789272	0.277059
H	-2.350254	4.891873	1.777733
H	-0.731253	4.870908	1.065299
H	-3.806156	4.492652	-1.074416
H	-4.245365	4.019082	0.560663
H	-4.375939	1.684742	-0.002784
H	-5.368164	2.614005	-1.108111
H	-3.487118	2.435459	-2.833995
H	-4.323472	0.924840	-2.409610
H	-2.685201	-2.317055	0.014624
H	-4.344969	-1.838468	0.487947
H	-2.924105	-1.102878	1.300341

TS(**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,re)}$→**IV**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)

G = -2040.636299 kcal.mol^{-1}

C	1.924385	3.554262	-1.801661
C	1.964109	2.258825	-1.234839
C	2.214635	1.127547	-2.049309
C	2.422759	1.322491	-3.417976
C	2.388183	2.589100	-3.985373
C	2.140937	3.690153	-3.176905
N	1.741078	2.065279	0.174457
Zn	-0.061517	1.733960	0.926294
O	-1.842958	2.107946	0.670908
C	-2.322052	3.225815	-0.029475
C	-3.859759	3.226768	-0.020796
C	-4.555372	1.965049	-0.527122
C	-4.311619	1.614864	-1.989895
O	-3.049981	0.944144	-2.197072
C	-2.925135	-0.336819	-1.863133
O	-1.864672	-0.917704	-1.879051
C	2.315907	-0.285730	-1.491547
C	1.453968	-1.286994	-2.270842
C	1.700267	4.811089	-0.974333
C	2.998150	5.617002	-0.803476
C	2.788250	2.005676	1.006677
C	2.731357	1.609692	2.354250
C	1.695008	1.000721	3.084336
N	0.449420	0.853708	2.633459
C	-0.497038	0.090661	3.392430
C	-0.559436	-1.312052	3.222219
C	-1.521661	-2.030434	3.938615
C	-2.399902	-1.397281	4.808953
C	-2.326088	-0.019553	4.968677
C	-1.388308	0.747486	4.270514
C	0.370286	-2.066381	2.281816
C	-0.398025	-2.644886	1.085018
C	-1.368610	2.253801	4.481246
C	-1.030381	2.629406	5.931454
C	4.178156	2.380087	0.531130
C	2.069559	0.452535	4.442133
C	3.778043	-0.760471	-1.456845
C	1.147430	-3.177895	3.002929
C	0.611211	5.710759	-1.575687
C	-2.700111	2.882243	4.049574
C	-1.838408	4.535683	0.599920
O	-4.099798	-0.913061	-1.544102
C	-4.010925	-2.295576	-1.193054
H	3.678092	1.677979	2.879064
H	2.555036	2.717733	-5.051392
H	2.619956	0.460956	-4.049674
H	4.417230	-0.088929	-0.877233
H	3.845942	-1.759815	-1.012669
H	4.192003	-0.817852	-2.470098
H	1.869536	-3.640834	2.321541
H	1.696876	-2.797638	3.869867
H	1.810177	-1.409381	-3.299940
H	1.508283	-2.272597	-1.795520
H	0.281621	-3.182344	0.414738
H	0.480616	-3.970308	3.360251
H	1.949341	-0.264791	-0.460038
H	0.405574	-0.983797	-2.302158
H	-1.162406	-3.356117	1.419853
H	-0.893066	-1.865716	0.499180
H	-1.580782	-3.108521	3.811459
H	-3.137908	-1.974530	5.359557
H	-3.014043	0.476689	5.648614
H	2.120589	4.682161	-3.619844

H	1.372713	4.495863	0.022572	H	-4.190020	3.402675	1.011650	C	4.395177	1.993026	0.428575
H	-0.306159	5.152980	-1.779973	H	-4.270386	1.111667	0.095150	N	1.946565	1.988688	0.284408
H	0.369176	6.527791	-0.887884	H	-5.638841	2.091827	-0.400680	Zn	0.161978	1.620573	0.973756
H	0.942804	6.165815	-2.515315	H	-4.233005	2.513583	-2.608742	O	-1.619704	1.685971	0.603655
H	3.372566	5.960244	-1.774496	H	-5.114693	0.988778	-2.386571	C	-2.305974	1.856142	-0.610933
H	3.789397	5.027592	-0.334043	H	-3.543112	-2.868439	-1.997006	C	-1.820521	3.064570	-1.407711
H	2.821379	6.501935	-0.181802	H	-5.038541	-2.624002	-1.035454	C	2.088363	2.565649	-1.020309
H	-0.584669	2.668676	3.839449	H	-3.427367	-2.422201	-0.278317	C	2.156685	3.971508	-1.156909
H	-2.910817	2.635095	3.005979					C	2.194562	4.512565	-2.445428
H	-3.530175	2.523446	4.668714	**IV**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$				C	2.173072	3.700198	-3.573090
H	-2.660499	3.972950	4.151967	G = -2040.654217 kcal.mol^{-1}				C	2.121999	2.319890	-3.423061
H	-1.788658	2.256210	6.628817	C	-1.053363	1.530069	4.463679	C	2.082466	1.726847	-2.157215
H	-0.987033	3.718525	6.042983	C	-0.401978	0.561242	3.670573	C	2.166330	4.904370	0.046487
H	-0.064111	2.221927	6.245332	C	-0.812715	-0.790142	3.692301	C	0.832454	5.653782	0.179555
H	4.883343	1.573754	0.750847	C	-1.868950	-1.151049	4.533524	C	2.026121	0.210463	-2.043124
H	2.196066	-0.634010	4.389575	C	-2.511244	-0.210514	5.330627	C	3.193884	-0.469008	-2.772460
H	1.289576	0.643208	5.182252	C	-2.105080	1.117512	5.287348	C	-3.804390	1.992342	-0.305133
H	3.009336	0.884967	4.790046	N	0.642316	0.966055	2.777283	C	-4.397028	0.834892	0.500203
H	1.102590	-1.353436	1.889803	C	1.914889	0.882567	3.157158	C	-4.486231	-0.481116	-0.247111
H	4.519858	3.260966	1.085197	C	2.240800	0.390163	4.547489	O	-5.383826	-0.295342	-1.364101
H	4.218430	2.601413	-0.534267	C	-0.179518	-1.835135	2.785369	C	-5.628509	-1.298580	-2.205438
H	-1.986490	3.198533	-1.082616	C	0.202782	-3.123359	3.525158	O	-4.967803	-2.426161	-1.864968
H	-2.185403	5.413699	0.042638	C	-0.675168	3.002163	4.407809	C	-5.204239	-3.528378	-2.741964
H	-2.205841	4.613783	1.628419	C	-1.756899	3.804710	3.667535	O	-6.362473	-1.192956	-3.157333
H	-0.744623	4.572233	0.631024	C	3.007361	1.223795	2.333453	C	0.681960	-0.336404	-2.545376
H	-4.205461	4.091574	-0.606101	C	3.032888	1.727049	1.024436	C	3.338062	5.895748	0.009479

C	-1.108070	-2.140502	1.599474
C	-0.398697	3.597215	5.794798
H	3.981285	1.080989	2.785568
H	2.198309	4.141827	-4.565468
H	2.110392	1.686716	-4.306456
H	4.161884	-0.097306	-2.421447
H	3.167693	-1.551505	-2.606796
H	3.148257	-0.301771	-3.854021
H	0.735788	-3.803342	2.851823
H	0.851703	-2.921788	4.383738
H	0.534788	-0.111370	-3.607471
H	0.637254	-1.424389	-2.424201
H	-0.631110	-2.835166	0.898520
H	-0.678004	-3.658925	3.895250
H	2.110001	-0.045755	-0.981842
H	-0.157919	0.101065	-1.996942
H	-2.040582	-2.600390	1.946028
H	-1.370743	-1.225009	1.060195
H	-2.198549	-2.186321	4.559482
H	-3.330860	-0.510861	5.977797
H	-2.618819	1.853299	5.900486
H	2.236305	5.591845	-2.566714
H	2.285402	4.289776	0.944368
H	-0.008075	4.960499	0.272754
H	0.840497	6.301603	1.063155
H	0.645447	6.283958	-0.697087
H	3.244395	6.605797	-0.819265
H	4.300948	5.386671	-0.101145
H	3.369413	6.479406	0.935778
H	0.250921	3.083909	3.828958
H	-1.943957	3.389325	2.672297
H	-2.702956	3.784456	4.220675
H	-1.455420	4.853098	3.560610
H	-1.297565	3.605660	6.420969
H	-0.058257	4.634298	5.701657
H	0.373310	3.035652	6.331154
H	4.510809	1.472277	-0.526531
H	1.901750	-0.641579	4.683451
H	1.720282	0.988830	5.300965
H	3.313482	0.433252	4.740873
H	0.742046	-1.408421	2.376439
H	5.188831	1.670323	1.103624
H	4.528730	3.058851	0.219748
H	-2.168499	0.964063	-1.252613
H	-2.361716	3.159747	-2.356168
H	-1.978707	3.983627	-0.832035
H	-0.753040	2.982417	-1.639649
H	-4.358220	2.110267	-1.244506
H	-3.941806	2.919337	0.266513
H	-3.778193	0.670286	1.388964
H	-5.402520	1.102263	0.846820
H	-3.510871	-0.805035	-0.622743
H	-4.878888	-1.274892	0.396822
H	-6.265342	-3.789538	-2.757118
H	-4.613698	-4.354045	-2.343730
H	-4.887280	-3.287475	-3.759792

$I_{7CC\text{-}\gamma(R,si)}$

G = -2040.634648 kcal.mol^{-1}

C	1.905230	3.248021	-1.661308
C	2.080968	1.898485	-1.270994
C	2.507374	0.926462	-2.204160
C	2.764977	1.328764	-3.518952
C	2.619740	2.654284	-3.910338
C	2.193904	3.599221	-2.983750
N	1.776411	1.510173	0.071525
Zn	-0.026785	0.784864	0.504240
O	-1.116628	-0.062305	-0.782950
C	-1.788955	-1.263411	-0.557240
C	2.683221	-0.536419	-1.824629
C	1.600130	-1.407341	-2.478480
C	1.442106	4.319731	-0.682766
C	0.325848	5.200507	-1.259162
C	2.721065	1.546915	1.009925
C	4.145582	1.900225	0.638412
C	2.513408	1.221217	2.362489
C	1.389050	0.698989	3.026266
C	1.569704	0.525511	4.521388

N	0.233209	0.380298	2.439999	H	4.679558	0.986211	0.352220	H	-3.401256	2.177193	2.254474
C	-0.802840	-0.274110	3.183330	H	4.201270	2.583580	-0.209280	H	-4.006260	2.324095	3.918672
C	-1.828507	0.483825	3.794140	H	4.673068	2.336153	1.489568	H	2.255420	5.962285	0.491847
C	-2.842721	-0.194201	4.478790	H	3.377667	1.371804	3.000646	H	3.388727	4.621518	0.290243
C	-2.859951	-1.579939	4.566170	H	-3.630824	0.380500	4.958405	H	3.074438	5.720046	-1.059372
C	-1.848619	-2.314824	3.959165	H	-3.655768	-2.085856	5.106483	H	-0.060564	5.867619	-0.480720
C	-0.812282	-1.689921	3.258963	H	-1.861207	-3.399011	4.031786	H	0.686653	5.834746	-2.077393
C	-1.844812	2.005526	3.771350	H	3.093049	0.589199	-4.245445	H	-0.501805	4.594485	-1.632259
C	-3.173338	2.566381	3.248354	H	2.836499	2.950047	-4.933582	H	-2.663992	-1.348149	-1.228413
C	0.287926	-2.544086	2.641108	H	2.079669	4.634725	-3.293283	H	-1.160048	-2.147046	-0.767901
C	-0.255462	-3.746521	1.857551	H	4.208817	-2.084758	-1.792235	H	-2.173742	-1.373768	0.469930
C	1.281659	-3.032867	3.707682	H	4.266185	-1.076048	-3.239072	H	2.552428	-0.612568	-0.740304
C	-1.540215	2.582399	5.163393	H	4.869534	-0.442168	-1.704527	H	0.839516	-1.910495	1.938545
O	-1.440438	2.506351	0.307107	H	1.715359	-2.454828	-2.175905	H	1.030924	3.804682	0.190126
C	-2.232414	2.257171	-0.595599	H	0.603097	-1.065077	-2.183178	H	-1.059493	2.335877	3.085354
O	-1.922782	2.545989	-1.855030	H	1.673113	-1.368531	-3.571921	H	-2.554292	0.719682	-2.537230
C	-2.423250	1.724060	-2.949412	H	2.079802	-3.625853	3.246757	C	-1.325218	1.690019	-3.990204
C	-3.737872	2.308055	-3.448751	H	1.746757	-2.204018	4.246326	H	-3.546592	3.176127	-4.090024
C	-4.644662	2.709071	-2.283023	H	0.776344	-3.666858	4.445419	H	-4.229310	1.552810	-4.074577
C	-4.601452	1.720698	-1.130562	H	-0.716425	-4.488993	2.518338	H	-4.372395	3.701017	-1.906039
O	-3.443783	1.811592	-0.271659	H	-1.000909	-3.444097	1.118692	H	-5.684988	2.783785	-2.619730
C	4.087293	-1.059250	-2.158348	H	0.562002	-4.250173	1.330129	H	-5.431681	1.896951	-0.442484
C	2.610206	5.201243	-0.212407	H	-1.491579	3.676443	5.123448	H	-4.672188	0.685711	-1.483302
H	2.537593	0.065627	4.738445	H	-2.323155	2.310406	5.880944	H	-0.419115	1.250159	-3.570589
H	1.570165	1.511334	4.999384	H	-0.589552	2.215923	5.560785	H	-1.648099	1.087335	-4.845441
H	0.780683	-0.072080	4.977129	H	-3.116283	3.658334	3.179581	H	-1.094745	2.699001	-4.344704

TS($\mathbf{I}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$)

G = -2040.626620 kcal.mol^{-1}

C	1.983317	3.252523	-1.643292
C	2.103036	1.907368	-1.221921
C	2.485373	0.897340	-2.133156
C	2.755265	1.257096	-3.457273
C	2.660414	2.577298	-3.880715
C	2.276408	3.559413	-2.975676
N	1.786764	1.556566	0.129920
Zn	-0.033700	0.923960	0.594926
O	-1.262298	0.063016	-0.651828
C	-2.016806	-1.092610	-0.386384
C	2.592195	-0.563437	-1.722139
C	1.474959	-1.397117	-2.367588
C	1.554056	4.372042	-0.704170
C	0.292059	5.082471	-1.213092
C	2.723660	1.625863	1.074539
C	4.139160	2.003711	0.698867
C	2.511026	1.324328	2.433796
C	1.404465	0.752832	3.086265
C	1.597223	0.469970	4.560619
N	0.254072	0.423674	2.493119
C	-0.735330	-0.323565	3.208328
C	-1.890244	0.333116	3.694340
C	-2.873112	-0.428555	4.334052
C	-2.740181	-1.802729	4.488685
C	-1.600077	-2.436241	4.009914
C	-0.580370	-1.722135	3.373093
C	-2.069695	1.840217	3.583432
C	-3.442424	2.226129	3.019755
C	0.645091	-2.481275	2.877844
C	0.302113	-3.394967	1.692141
C	1.308129	-3.300025	3.996187
C	-1.830850	2.526135	4.937666
O	-1.483451	2.395556	0.166009
C	-2.117294	1.857302	-0.766136
O	-1.772398	2.178370	-2.025125
C	-2.508437	1.545608	-3.095704
C	-3.823111	2.310963	-3.359245
C	-4.273892	3.145216	-2.158702
C	-4.454407	2.339196	-0.878227
O	-3.395493	1.402011	-0.610185
C	3.972244	-1.158566	-2.034386
C	2.680113	5.391891	-0.472772
H	2.030857	-0.525042	4.705904
H	2.286462	1.195727	4.997816
H	0.653304	0.496376	5.107442
H	4.653398	1.127108	0.287359
H	4.170146	2.776962	-0.069790
H	4.699825	2.340173	1.572832
H	3.366611	1.502847	3.075299
H	-3.759265	0.068486	4.719399
H	-3.518764	-2.376668	4.984064
H	-1.495810	-3.511269	4.133680
H	3.051305	0.487533	-4.166045
H	2.883333	2.839292	-4.911716
H	2.198273	4.591121	-3.309271
H	4.040568	-2.183744	-1.653875
H	4.161848	-1.197324	-3.112679
H	4.778082	-0.573814	-1.579045
H	1.530816	-2.439914	-2.034106
H	0.490934	-0.998536	-2.101927
H	1.564523	-1.393509	-3.460326
H	2.249535	-3.734786	3.642786
H	1.524710	-2.689976	4.878386
H	0.669142	-4.128311	4.321517
H	-0.446352	-4.143372	1.975743
H	-0.099519	-2.825017	0.851116
H	1.194724	-3.928819	1.346866
H	-1.940609	3.612182	4.841813
H	-2.552717	2.180797	5.686932
H	-0.827496	2.324503	5.325007
H	-3.487052	3.308630	2.858465
H	-3.623479	1.732537	2.062271
H	-4.255670	1.964253	3.706461
H	2.352351	6.167693	0.228182
H	3.580433	4.928235	-0.058597

H	2.963782	5.889159	-1.407393
H	-0.038773	5.831302	-0.484523
H	0.479481	5.603934	-2.159088
H	-0.518506	4.367880	-1.365450
H	-3.014845	-0.996693	-0.835194
H	-1.536493	-1.979865	-0.828050
H	-2.161505	-1.280582	0.686697
H	2.452721	-0.611773	-0.637394
H	1.376667	-1.748958	2.523171
H	1.305554	3.919366	0.260166
H	-1.317926	2.213736	2.882653
H	-2.722736	0.524562	-2.771208
C	-1.583037	1.519829	-4.295992
H	-3.691513	2.982887	-4.215850
H	-4.601106	1.591493	-3.642567
H	-3.547997	3.947082	-1.990176
H	-5.230146	3.634766	-2.379693
H	-4.562561	3.008417	-0.015725
H	-5.346816	1.709299	-0.937207
H	-0.674354	0.957753	-4.070276
H	-2.088706	1.050108	-5.146080
H	-1.297657	2.536771	-4.582897

II$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$

G = -2040.637096 kcal.mol^{-1}

C	1.944498	1.481077	-2.336698
C	1.674127	2.341861	-1.249564
C	1.378360	3.706622	-1.456430
C	1.319899	4.180587	-2.770646
C	1.558694	3.341467	-3.852376
C	1.875896	2.006316	-3.630407
N	1.631422	1.804696	0.079321
C	2.754282	1.701593	0.797381
C	2.830053	1.134011	2.080716
C	1.830997	0.536322	2.870524
C	2.266516	-0.023358	4.203812
C	1.122955	4.661253	-0.298945
C	-0.359028	5.054963	-0.214087
C	2.283248	0.010365	-2.136432
C	3.567610	-0.401770	-2.869214
Zn	-0.081961	1.251100	0.841471
O	-1.826869	1.771075	0.494247
C	-2.657099	1.067679	-0.297486
O	-3.925793	1.659926	-0.365784
C	-3.973490	3.005691	-0.823256
H	-5.044107	3.237048	-0.840946
N	0.547039	0.441659	2.516777
C	-0.388668	-0.212010	3.384166
C	-0.592227	-1.605412	3.265005
C	-1.556985	-2.207139	4.078555
C	-2.305358	-1.464662	4.984492
C	-2.094457	-0.094865	5.089116
C	-1.140365	0.556780	4.301226
C	0.182463	-2.458080	2.269511
C	0.895666	-3.639265	2.943261
C	-0.955717	2.061151	4.441060
C	-2.174704	2.821555	3.895968
O	-2.086333	0.934052	-1.582566
C	-3.042044	0.684866	-2.624153
C	-3.628388	2.020524	-3.153091
C	-3.363792	3.196860	-2.212418
O	-2.879326	-0.254224	0.141050
C	-3.661842	-0.379402	1.319981
C	-0.652739	2.477718	5.887304
C	-0.730925	-2.954157	1.137928
C	4.043399	2.226082	0.211115
C	2.015149	5.908896	-0.367931
C	1.111413	-0.889025	-2.553038
H	-0.090893	2.346733	3.833148
H	-3.051713	-1.951808	5.606171
H	3.818179	1.140514	2.524214
H	1.375754	4.132733	0.626470
H	-0.151202	-3.513393	0.394909
H	0.952529	-1.824484	1.817921
H	2.083966	-1.100974	4.250707
H	1.499386	-4.185816	2.210608
H	1.560648	-3.312266	3.749304
H	0.182236	-4.350250	3.373781

H	1.690073	0.424501	5.018758
H	3.327314	0.158936	4.380599
H	-1.503384	-3.627091	1.528211
H	-1.727111	-3.277534	3.995676
H	0.215696	1.947076	6.291226
H	-2.683469	0.484424	5.795639
H	-1.500153	2.278558	6.552205
H	-0.444875	3.552065	5.936719
H	-2.015445	3.903453	3.971448
H	-3.076067	2.578492	4.470312
H	-2.362617	2.573816	2.846768
H	0.189770	-0.613805	-2.033179
H	2.451305	-0.150628	-1.066974
H	1.335366	-1.939748	-2.336432
H	4.313205	1.674008	-0.694179
H	0.918441	-0.802900	-3.628150
H	3.935151	3.273897	-0.084679
H	4.863110	2.143421	0.926046
H	3.451898	-0.339471	-3.956586
H	4.418661	0.229132	-2.592098
H	3.824198	-1.439210	-2.628787
H	2.070833	1.355300	-4.478762
H	1.504842	3.728752	-4.866273
H	1.084720	5.226850	-2.947875
H	1.776880	6.530647	-1.237640
H	1.870198	6.527322	0.524432
H	3.076679	5.647535	-0.429558
H	-0.998182	4.174844	-0.094919
H	-0.530660	5.722884	0.637947
H	-0.675159	5.583299	-1.120771
H	-3.770041	4.120393	-2.644656
H	-2.282776	3.333652	-2.125151
H	-4.705569	1.897586	-3.323065
H	-3.184177	2.255584	-4.128758
C	-2.342298	-0.103159	-3.716691
H	-3.845706	0.074768	-2.199921
H	-3.619259	-1.432509	1.604677
H	-4.701019	-0.088752	1.136649
H	-3.255546	0.223434	2.138819
H	-1.236062	-2.126347	0.631420
H	-3.492891	3.671359	-0.095153
H	-3.030810	-0.281573	-4.549792
H	-1.480448	0.454384	-4.097479
H	-1.995349	-1.069583	-3.341566

TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$)

G = -2040.628493 kcal.mol^{-1}

C	1.927237	1.402758	-2.366260
C	1.618335	2.247983	-1.278565
C	1.281101	3.608432	-1.480868
C	1.305166	4.105387	-2.787576
C	1.628018	3.289880	-3.867011
C	1.924243	1.950291	-3.653230
N	1.591712	1.717609	0.053946
C	2.714670	1.698269	0.785999
C	2.800210	1.253393	2.115731
C	1.822731	0.681993	2.954042
C	2.250724	0.325349	4.357381
C	0.899396	4.520760	-0.319426
C	-0.106678	5.609841	-0.712255
C	2.227807	-0.077810	-2.184794
C	3.551076	-0.493899	-2.842785
Zn	0.001422	0.825859	0.733472
O	-1.512147	-0.026307	0.135850
C	-2.539849	0.469637	-0.566556
O	-2.993046	1.713860	0.014229
C	-2.720911	2.894623	-0.723329
H	-2.757689	3.709149	0.008076
N	0.572902	0.427954	2.571190
C	-0.354933	-0.191778	3.470495
C	-0.462439	-1.600162	3.497499
C	-1.421301	-2.176202	4.336023
C	-2.254779	-1.394681	5.127586
C	-2.143036	-0.010381	5.082525
C	-1.203447	0.616529	4.258545
C	0.399107	-2.497492	2.620682
C	1.135382	-3.575211	3.429140
C	-1.148750	2.136593	4.208434

C	-2.406575	2.706699	3.534100
O	-2.156591	0.658156	-1.894924
C	-3.178084	0.846404	-2.890166
C	-4.258840	1.840589	-2.453615
C	-3.732775	3.145963	-1.853120
O	-3.619961	-0.417539	-0.562808
C	-4.139876	-0.724941	0.719120
C	-0.943518	2.761554	5.595162
C	-0.438053	-3.133098	1.499080
C	4.018422	2.126415	0.149835
C	2.122200	5.178873	0.341142
C	1.068131	-0.940499	-2.707277
H	-0.287971	2.417397	3.592651
H	-2.993039	-1.863170	5.772852
H	3.783453	1.345665	2.561477
H	0.422635	3.887874	0.439900
H	0.196514	-3.744520	0.846990
H	1.160297	-1.868860	2.146761
H	2.184329	-0.755332	4.517925
H	1.807008	-4.144820	2.777747
H	1.734939	-3.142741	4.237021
H	0.438535	-4.289021	3.881933
H	1.588471	0.789359	5.094007
H	3.275204	0.645441	4.552005
H	-1.212835	-3.787172	1.915552
H	-1.519016	-3.258325	4.363247
H	-0.045076	2.374915	6.087119
H	-2.803450	0.599671	5.693516
H	-1.793590	2.563978	6.257038
H	-0.840326	3.848983	5.511333
H	-2.337970	3.798133	3.456313
H	-3.303297	2.473019	4.119389
H	-2.551595	2.295773	2.530043
H	0.118118	-0.674590	-2.235482
H	2.323936	-0.269028	-1.110670
H	1.265947	-2.001592	-2.517646
H	4.433096	1.287061	-0.420387
H	0.950324	-0.813031	-3.789623
H	3.890338	2.953658	-0.549452
H	4.749752	2.406787	0.910055
H	3.503824	-0.408180	-3.933738
H	4.390529	0.119888	-2.500422
H	3.777367	-1.539820	-2.609190
H	2.156593	1.311928	-4.501604
H	1.638073	3.698085	-4.874030
H	1.058805	5.147378	-2.966815
H	2.697375	5.752262	-0.394717
H	1.801030	5.870364	1.128122
H	2.789692	4.446945	0.800381
H	-0.958638	5.203320	-1.263618
H	-0.487768	6.104640	0.187126
H	0.355278	6.387197	-1.331221
H	-4.589433	3.712480	-1.468624
H	-3.261635	3.777248	-2.617370
H	-4.885341	1.348033	-1.706007
H	-4.899863	2.055350	-3.317747
C	-2.437932	1.265905	-4.150928
H	-3.663741	-0.123077	-3.062440
H	-4.912698	-1.481008	0.560575
H	-4.587430	0.158435	1.188885
H	-3.363210	-1.128343	1.375975
H	-0.931532	-2.371493	0.888016
H	-1.704327	2.858122	-1.133886
H	-3.135319	1.344531	-4.991126
H	-1.940337	2.231245	-4.018283
H	-1.672524	0.527646	-4.404038

II$^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$

G = -2040.631792 kcal.mol^{-1}

C	1.613356	3.643978	-1.578702
C	1.800710	2.265593	-1.304513
C	2.087942	1.354293	-2.344897
C	2.203334	1.847457	-3.648771
C	2.047609	3.197748	-3.929870
C	1.753133	4.082839	-2.898794
N	1.655737	1.795018	0.043030
C	2.715105	1.773498	0.855430
C	2.686546	1.379865	2.207519

C	1.657086	0.813236	2.977171	C	-3.575939	1.397527	-2.478623	H	-2.714218	3.785624	3.526132
C	2.001546	0.459344	4.405383	O	-2.316449	0.900368	-1.981563	H	-3.632200	2.382189	4.082973
C	2.287215	-0.134984	-2.104045	H	-1.590653	3.749189	0.216168	H	-2.871826	2.359279	2.480280
C	3.696080	-0.590489	-2.514934	C	-0.135662	-3.078043	1.366417	H	0.213606	-0.700417	-2.484851
C	1.279564	4.649358	-0.481146	C	-1.258061	2.649594	5.552469	H	2.182147	-0.316919	-1.029377
C	0.306118	5.741417	-0.946630	C	4.088867	2.125614	0.324029	H	1.370917	-2.036181	-2.615782
Zn	-0.029123	0.927813	0.640542	C	1.217084	-0.970801	-2.821718	H	4.053898	2.788844	-0.539871
O	-1.136172	-0.230325	-0.439262	C	2.533974	5.315920	0.107475	H	1.272190	-0.833690	-3.907836
C	-2.212027	0.489794	-0.670609	H	-0.621394	2.456535	3.519063	H	4.702338	2.580428	1.105184
O	-3.415633	-0.073476	-0.289471	H	-3.225697	-2.029787	5.385502	H	4.591911	1.203462	0.010656
C	-3.421252	-0.780818	0.939983	H	3.633593	1.483391	2.724350	H	3.847223	-0.492416	-3.595750
N	0.432664	0.544503	2.519506	H	0.797489	4.090472	0.329395	H	4.477887	-0.005735	-2.020017
C	-0.509640	-0.145276	3.347347	H	0.619529	-3.654034	0.819386	H	3.845363	-1.644789	-2.257514
C	-1.460249	0.589953	4.091462	H	1.265192	-1.703284	2.206498	H	2.422706	1.154651	-4.457018
C	-2.426018	-0.113091	4.819478	H	2.020558	-0.626932	4.539992	H	2.148798	3.560785	-4.949109
C	-2.463440	-1.502230	4.818406	H	1.999565	-3.921615	2.921192	H	1.622885	5.136970	-3.125238
C	-1.514546	-2.212639	4.091929	H	1.653774	-2.951637	4.362878	H	3.107413	5.821644	-0.677628
C	-0.521997	-1.560270	3.354467	H	0.512670	-4.190114	3.831382	H	2.250431	6.067134	0.853261
C	-1.463167	2.111679	4.128297	H	1.248968	0.845696	5.097711	H	3.193251	4.597121	0.597549
C	-2.746802	2.689895	3.514960	H	2.977636	0.858355	4.684732	H	-0.559255	5.326511	-1.470512
C	0.498355	-2.387476	2.583419	H	-0.920489	-3.777087	1.678947	H	-0.055901	6.312297	-0.084797
C	1.203853	-3.416488	3.479420	H	-1.542949	-3.299238	4.096825	H	0.790966	6.456804	-1.619902
O	-1.998679	1.773738	0.204545	H	-0.341085	2.263110	6.008537	H	-3.924263	3.950303	-0.112273
C	-2.005770	3.024304	-0.491194	H	-3.163457	0.440613	5.395160	H	-3.232688	4.283573	-1.691262
C	-3.388320	3.488582	-0.950043	H	-2.092491	2.376722	6.207969	H	-4.667304	1.789682	-0.684811
C	-4.268381	2.370676	-1.517678	H	-1.192423	3.743201	5.541564	H	-5.128349	2.807713	-2.040353

C	-3.251033	2.003346	-3.835308
H	-4.242399	0.536173	-2.617025
H	-4.448857	-1.123232	1.079890
H	-3.141047	-0.137509	1.780230
H	-2.749330	-1.640935	0.905751
H	-0.575366	-2.351622	0.676740
H	-1.326823	2.961181	-1.348618
H	-4.170701	2.308983	-4.344021
H	-2.602218	2.878858	-3.734964
H	-2.733910	1.271843	-4.461940

TS(**II**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$→**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$)

G = -2040.631591 kcal.mol^{-1}

C	1.283285	3.497613	-1.491912
C	1.851311	2.218425	-1.269732
C	2.559599	1.556590	-2.300525
C	2.639710	2.170780	-3.555361
C	2.068843	3.414479	-3.791938
C	1.410114	4.073125	-2.759593
C	3.270671	0.225421	-2.090733
C	4.767784	0.324160	-2.426401
N	1.664419	1.589890	0.003304
Zn	-0.004028	0.550649	0.402747
O	-1.850604	2.010260	0.396171
C	-2.830870	1.293325	0.221052
O	-3.359282	0.613733	1.225183
C	-4.368821	-0.370177	0.971913
C	0.596312	4.266479	-0.370827
C	1.589899	5.186100	0.357945
C	-0.614210	5.080041	-0.840997
C	2.629532	-0.907315	-2.901531
C	2.643975	1.635143	0.912465
C	2.589067	1.058808	2.190625
C	1.542959	0.400255	2.862000
N	0.330756	0.185926	2.351924
C	-0.686586	-0.360782	3.201547
C	-1.536229	0.528648	3.904212
C	-2.527323	-0.011914	4.728093
C	-2.699336	-1.386916	4.849936
C	-1.866628	-2.245901	4.144679
C	-0.846338	-1.758229	3.320426
C	-1.376610	2.040333	3.797437
C	-2.715234	2.788180	3.799474
C	0.042352	-2.747636	2.581305
C	0.687616	-3.771935	3.525806
C	-0.471942	2.600513	4.907106
C	-0.739924	-3.453348	1.465522
C	3.957989	2.316740	0.586490
C	1.884690	-0.113473	4.245099
O	-1.081130	-0.662466	-0.532965
C	-1.612236	-0.970200	-1.785649
C	-1.153884	-2.355952	-2.252347
C	-1.353538	0.061825	-2.899303
C	-1.634527	1.521417	-2.549320
C	-3.037285	1.871999	-2.084307
O	-3.506875	1.163090	-0.910199
H	-3.197889	2.765583	4.783523
H	-3.180533	0.656295	5.281940
H	-0.060403	-4.438655	3.968753
H	3.862395	3.053733	-0.211216
H	-3.785357	1.610328	-2.837478
H	2.149436	-1.174991	4.180207
H	2.742191	0.420119	4.659294
H	1.045380	-0.036797	4.937415
H	4.691737	1.570358	0.263039
H	4.361513	2.803963	1.477155
H	3.502116	1.161157	2.766356
H	-3.477574	-1.785683	5.495808
H	-2.002286	-3.320341	4.240546
H	3.171472	1.666461	-4.358438
H	2.148295	3.875907	-4.772698
H	0.984267	5.055505	-2.942695
H	5.281118	-0.603706	-2.151091
H	4.926720	0.478360	-3.499299
H	5.253720	1.151807	-1.901688
H	3.162620	-1.849904	-2.733801
H	1.586800	-1.054692	-2.614414
H	2.658954	-0.693864	-3.976029

H	1.397267	-4.400218	2.976224	H	-0.916163	1.876943	-1.809987	C	-2.190175	0.364330	-0.726680
H	1.226679	-3.291915	4.349044	H	-1.458334	2.138774	-3.440361	O	-3.377917	-0.138554	-0.303213
H	-1.581639	-4.023005	1.877404	H	-3.112794	2.943799	-1.874094	C	-3.365989	-0.862465	0.921930
H	-1.120955	-2.718189	0.751693	H	-1.613883	-2.626004	-3.210767	N	0.404449	0.569535	2.519457
H	-0.092425	-4.155833	0.927751	H	-0.066411	-2.388087	-2.372955	C	-0.530642	-0.135545	3.340615
H	-0.397693	3.690894	4.824007	H	-1.429897	-3.115118	-1.515944	C	-1.497065	0.584112	4.080270
H	-0.879465	2.367124	5.897837					C	-2.463988	-0.133720	4.792400
H	0.542256	2.197226	4.856254	TS($\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}\rightarrow\mathbf{III}^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$)				C	-2.485602	-1.523195	4.784125
H	-2.551103	3.841720	3.549047	G = -2040.631373 kcal.mol^{-1}				C	-1.517200	-2.218671	4.068673
H	-3.406303	2.365067	3.067386	C	1.630564	3.659317	-1.597473	C	-0.523888	-1.551313	3.345660
H	1.084860	5.734720	1.160873	C	1.784173	2.278401	-1.314511	C	-1.509654	2.105096	4.136442
H	2.413012	4.624108	0.806141	C	2.050399	1.355227	-2.350646	C	-2.788974	2.686439	3.517677
H	2.020505	5.920043	-0.333186	C	2.181945	1.839362	-3.656523	C	0.520570	-2.365187	2.592113
H	-1.153662	5.475823	0.025430	C	2.058473	3.191338	-3.945397	C	1.229300	-3.377874	3.504376
H	-0.322357	5.937034	-1.458599	C	1.782308	4.088051	-2.919476	O	-1.945417	1.836512	0.267698
H	-1.310896	4.466444	-1.417673	N	1.630966	1.820402	0.036451	C	-1.956513	3.053918	-0.460595
H	-3.969993	-1.150372	0.321541	C	2.693205	1.773455	0.842530	C	-3.351499	3.494271	-0.907548
H	-4.606762	-0.783735	1.951035	C	2.664911	1.381535	2.195752	C	-4.224887	2.356252	-1.444433
H	-5.254451	0.083319	0.520624	C	1.635396	0.820616	2.968587	C	-3.565220	1.397636	-2.441384
H	3.179515	-0.040524	-1.033147	C	1.987640	0.455870	4.392643	O	-2.299408	0.864409	-1.980013
H	0.847061	-2.178799	2.103943	C	2.217613	-0.137276	-2.103706	H	-1.527819	3.829164	0.187353
H	0.232876	3.532425	0.354042	C	3.635786	-0.611011	-2.458798	C	-0.081810	-3.075622	1.370822
H	-0.894383	2.242643	2.836459	C	1.324042	4.679790	-0.506539	C	-1.319058	2.621578	5.570700
H	-2.713083	-1.030964	-1.683050	C	0.357832	5.778434	-0.971318	C	4.073538	2.098589	0.309565
H	-0.304230	0.000343	-3.215014	Zn	-0.100788	1.058230	0.669814	C	1.170437	-0.959463	-2.868545
H	-1.954298	-0.232356	-3.772209	O	-1.103467	-0.260921	-0.449759	C	2.596216	5.334796	0.056295

H	-0.663312	2.462432	3.540907
H	-3.248415	-2.062534	5.339353
H	3.615915	1.473442	2.707726
H	0.846250	4.136526	0.316701
H	0.689912	-3.650340	0.845901
H	1.279630	-1.670136	2.220171
H	2.019853	-0.630950	4.518670
H	2.045244	-3.868781	2.962879
H	1.652580	-2.903045	4.395533
H	0.546385	-4.163883	3.845033
H	1.233288	0.829031	5.090413
H	2.960579	0.862518	4.672302
H	-0.866393	-3.778988	1.674507
H	-1.530292	-3.305685	4.071585
H	-0.404567	2.230917	6.028434
H	-3.213052	0.409124	5.363409
H	-2.158076	2.335860	6.214881
H	-1.257216	3.715438	5.576941
H	-2.766300	3.781780	3.557748
H	-3.680384	2.356522	4.063679
H	-2.889203	2.382686	2.471854
H	0.157884	-0.670364	-2.580086
H	2.062665	-0.319085	-1.035361
H	1.295899	-2.025775	-2.649257
H	4.050923	2.736783	-0.573230
H	1.278443	-0.831284	-3.951747
H	4.684023	2.571909	1.082295
H	4.573144	1.164142	0.029738
H	3.831669	-0.507194	-3.531962
H	4.404944	-0.040876	-1.928903
H	3.760038	-1.669009	-2.202806
H	2.388812	1.137857	-4.460613
H	2.171461	3.546635	-4.966172
H	1.678009	5.144073	-3.151016
H	3.161011	5.831201	-0.741007
H	2.334985	6.091794	0.804376
H	3.256417	4.609747	0.536001
H	-0.521059	5.366541	-1.474529
H	0.016941	6.365583	-0.111767
H	0.840881	6.477996	-1.662302
H	-3.884326	3.955506	-0.067141
H	-3.223984	4.282908	-1.661140
H	-4.585858	1.768503	-0.599244
H	-5.112650	2.774642	-1.935709
C	-3.252376	2.027767	-3.788815
H	-4.242825	0.546363	-2.585489
H	-4.394752	-1.191960	1.076521
H	-3.058323	-0.224091	1.754175
H	-2.702546	-1.726403	0.859273
H	-0.511102	-2.359562	0.664665
H	-1.304162	2.967741	-1.340770
H	-4.175233	2.370397	-4.266815
H	-2.579062	2.883036	-3.680231
H	-2.770210	1.299837	-4.446652

III$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$

G = -2040.638264 kcal.mol^{-1}

C	1.384652	3.574452	-1.417407
C	1.861850	2.264284	-1.160243
C	2.453881	1.496051	-2.188806
C	2.530708	2.046451	-3.472964
C	2.060211	3.325323	-3.741886
C	1.502585	4.080948	-2.715498
C	3.020573	0.104374	-1.941698
C	4.489238	0.003505	-2.380680
N	1.683890	1.702158	0.142012
Zn	0.067833	0.578345	0.497444
O	-1.491825	2.114136	-0.073558
C	-2.677681	2.063318	-0.366643
O	-3.609091	2.037215	0.580377
C	-4.990587	1.958026	0.205662
C	0.801876	4.448888	-0.313204
C	1.851411	5.424696	0.245860
C	-0.435607	5.239893	-0.753865
C	2.174566	-0.985234	-2.616455
C	2.640700	1.823805	1.062825
C	2.541950	1.354340	2.383467
C	1.534201	0.603474	3.016663

N	0.388939	0.229093	2.445429
C	-0.498688	-0.641639	3.153230
C	-1.659003	-0.100247	3.758150
C	-2.532328	-0.971514	4.416007
C	-2.289180	-2.339736	4.467375
C	-1.155268	-2.857918	3.856901
C	-0.238768	-2.031298	3.198179
C	-1.949523	1.395658	3.713495
C	-3.439207	1.726984	3.851584
C	0.983467	-2.661159	2.542880
C	1.749434	-3.585321	3.501131
C	-1.157061	2.174490	4.776091
C	0.600159	-3.411251	1.258661
C	3.971548	2.443768	0.693042
C	1.851110	0.171059	4.433787
O	-0.624462	-0.777115	-0.597771
C	-1.912758	-0.902127	-1.111158
C	-2.396894	-2.347359	-0.970407
C	-1.968292	-0.480100	-2.599050
C	-1.370193	0.897686	-2.887961
C	-2.296253	2.093813	-2.738320
O	-3.186204	2.068923	-1.586549
H	-3.802351	1.558024	4.872064
H	-3.423162	-0.575490	4.893331
H	1.171486	-4.482796	3.747451
H	3.882895	3.185226	-0.101627
H	-3.009167	2.147523	-3.564676
H	2.357541	-0.800295	4.422380
H	2.523305	0.887838	4.910628
H	0.953593	0.060042	5.043809
H	4.644284	1.658481	0.328329
H	4.443367	2.902733	1.564567
H	3.410112	1.556098	3.000930
H	-2.985110	-2.998878	4.979716
H	-0.972987	-3.928818	3.890953
H	2.976575	1.461678	-4.273660
H	2.136933	3.737579	-4.744670
H	1.155129	5.088707	-2.926675
H	4.904734	-0.967471	-2.089810
H	4.592491	0.088629	-3.468056
H	5.105836	0.787409	-1.929188
H	2.628750	-1.969979	-2.455939
H	1.162335	-1.008674	-2.201331
H	2.113049	-0.820936	-3.698868
H	2.682677	-3.920799	3.035760
H	1.999378	-3.087365	4.443806
H	-0.103410	-4.223601	1.476928
H	0.137766	-2.734009	0.534634
H	1.490523	-3.857264	0.799435
H	-1.420323	3.237896	4.742708
H	-1.386704	1.803052	5.781560
H	-0.078982	2.098618	4.621439
H	-3.605474	2.783887	3.620613
H	-4.049882	1.129765	3.168998
H	1.412628	6.046343	1.034547
H	2.711212	4.904928	0.674594
H	2.221195	6.092334	-0.541066
H	-0.875339	5.753401	0.107973
H	-0.191928	6.008985	-1.495353
H	-1.199857	4.585814	-1.179505
H	-5.185991	1.040851	-0.354482
H	-5.539293	1.949188	1.146773
H	-5.281169	2.823449	-0.393984
H	2.985344	-0.080433	-0.863204
H	1.663825	-1.855142	2.251023
H	0.494400	3.782663	0.497986
H	-1.623386	1.758982	2.731887
H	-2.638342	-0.282754	-0.548243
H	-1.389029	-1.224921	-3.159161
H	-3.001841	-0.546466	-2.968137
H	-0.481424	1.028390	-2.268110
H	-1.020392	0.946234	-3.927211
H	-1.722592	3.024299	-2.705411
H	-3.404173	-2.478956	-1.384635
H	-1.714306	-3.021656	-1.499361
H	-2.413675	-2.639722	0.082966

III$^{6\alpha}{}_{7CC\text{-}\gamma(R,sl)}$

G = -2040.643743 kcal.mol^{-1}

C	1.747793	3.688495	-1.658188
C	1.838600	2.311808	-1.330972
C	2.080836	1.347997	-2.335810
C	2.267543	1.785987	-3.651372
C	2.212893	3.133060	-3.980673
C	1.948084	4.070108	-2.988018
N	1.649821	1.904202	0.029839
C	2.706652	1.790700	0.835734
C	2.651026	1.414768	2.191813
C	1.599459	0.871991	2.950187
C	1.962059	0.445327	4.356275
C	2.142784	-0.144572	-2.044780
C	3.533613	-0.729187	-2.335256
C	1.454830	4.747865	-0.601792
C	0.612904	5.912023	-1.139835
Zn	-0.172818	1.484563	0.744409
O	-1.154236	-0.262198	-0.304202
C	-2.244256	0.018033	-0.798233
O	-3.395252	-0.518843	-0.411164
C	-3.348443	-1.362080	0.750812
N	0.359108	0.689167	2.499393
C	-0.582615	-0.068959	3.258932
C	-1.619789	0.597828	3.954608
C	-2.591866	-0.170213	4.604767
C	-2.552878	-1.559278	4.584732
C	-1.514454	-2.202843	3.920701
C	-0.513898	-1.485378	3.257170
C	-1.672727	2.114515	4.073929
C	-3.004990	2.697826	3.587764
C	0.603946	-2.258638	2.566767
C	1.315715	-3.219578	3.532096
O	-1.796303	2.405085	0.538311
C	-1.945229	3.392298	-0.437409
C	-3.416080	3.596398	-0.825749
C	-4.195890	2.313997	-1.129397
C	-3.651325	1.383670	-2.213586
O	-2.350727	0.829704	-1.829054
H	-1.569436	4.370687	-0.086535
C	0.096625	-3.027815	1.338646
C	-1.374446	2.555576	5.516155
C	4.106695	2.026859	0.305629
C	1.072219	-0.912476	-2.833555
C	2.737249	5.306175	0.036970
H	-0.887844	2.524073	3.431008
H	-3.318508	-2.137340	5.095629
H	3.601338	1.466022	2.711959
H	0.879912	4.258620	0.193328
H	0.920229	-3.571767	0.861856
H	1.342478	-1.535666	2.208560
H	2.299544	-0.596214	4.369508
H	2.191749	-3.665045	3.047992
H	1.650267	-2.715828	4.444186
H	0.659632	-4.042544	3.836690
H	1.109525	0.520396	5.033818
H	2.779233	1.060845	4.738905
H	-0.663109	-3.765750	1.623672
H	-1.474941	-3.289459	3.919730
H	-0.406260	2.183209	5.866209
H	-3.388090	0.334834	5.145644
H	-2.139990	2.189972	6.210120
H	-1.358516	3.648965	5.584988
H	-3.002848	3.786617	3.713179
H	-3.855260	2.305138	4.157624
H	-3.143088	2.484880	2.524997
H	0.076786	-0.508578	-2.639742
H	1.932496	-0.285542	-0.980120
H	1.074523	-1.970130	-2.547484
H	4.125767	2.655367	-0.584437
H	1.259400	-0.861912	-3.912310
H	4.735812	2.477193	1.077423
H	4.558713	1.064047	0.042831
H	3.778817	-0.658608	-3.401007
H	4.321369	-0.208561	-1.783141
H	3.569298	-1.788780	-2.058442
H	2.460632	1.052943	-4.430552
H	2.367590	3.453690	-5.007518
H	1.892528	5.121505	-3.254037

H	3.386556	5.751987	-0.725450
H	2.489294	6.086677	0.765110
H	3.307987	4.536211	0.559538
H	-0.262597	5.560748	-1.692164
H	0.264552	6.534479	-0.308912
H	1.194170	6.562624	-1.803166
H	-3.936290	4.094249	0.002662
H	-3.459117	4.291515	-1.675965
H	-4.295122	1.737731	-0.206495
H	-5.217729	2.576507	-1.435645
C	-3.415168	2.036498	-3.562262
H	-4.338497	0.538278	-2.326929
H	-4.384748	-1.638040	0.943315
H	-2.930834	-0.820634	1.600735
H	-2.748379	-2.250482	0.549497
H	-0.336302	-2.346331	0.603256
H	-1.374923	3.161168	-1.354946
H	-4.351798	2.464809	-3.931470
H	-2.673316	2.835465	-3.489789
H	-3.059400	1.302720	-4.290536

TS(**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R,si)}$→**IV**$^{\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)

G = -2040.631024 kcal.mol^{-1}

C	1.250712	3.435209	-1.512600
C	1.868827	2.176351	-1.305028
C	2.620311	1.563799	-2.335575
C	2.710157	2.213990	-3.571726
C	2.099437	3.441046	-3.791970
C	1.385324	4.045086	-2.763078
N	1.694521	1.523694	-0.039769
Zn	0.075012	0.434766	0.355313
O	-1.157364	-0.641157	-0.511969
C	-1.502658	-1.011516	-1.817072
C	-0.867477	-2.348698	-2.206277
C	3.372335	0.251671	-2.148883
C	2.850980	-0.853528	-3.076592
C	0.497806	4.147148	-0.395605
C	-0.698315	4.968148	-0.889274
C	2.650542	1.620586	0.892378
C	3.942918	2.353261	0.592753
C	2.588480	1.059357	2.176558
C	1.543959	0.395202	2.844570
C	1.865523	-0.077258	4.246633
N	0.346227	0.144939	2.315164
C	-0.675114	-0.409409	3.157397
C	-0.791898	-1.807578	3.310489
C	-1.806606	-2.306704	4.134370
C	-2.676961	-1.456121	4.803013
C	-2.550795	-0.080356	4.642193
C	-1.565370	0.471497	3.818669
C	0.129062	-2.786412	2.597299
C	-0.624317	-3.506194	1.470357
C	-1.458340	1.984122	3.666555
C	-2.818738	2.689972	3.695258
C	-0.534389	2.605096	4.727143
C	0.772609	-3.798006	3.555784
O	-2.149859	2.107983	0.306794
C	-2.992429	1.248122	0.116079
O	-3.487024	0.535645	1.122186
C	-4.279477	-0.623575	0.849383
O	-3.574014	0.969010	-1.050178
C	-3.113351	1.694885	-2.211227
C	-1.654779	1.471382	-2.575269
C	-1.222341	0.043287	-2.900908
C	4.883863	0.431646	-2.368385
C	1.439752	5.045975	0.422768
H	-1.019754	2.175994	2.682465
H	3.217079	-0.081826	-1.117702
H	1.786180	-1.038169	-2.922070
H	-3.262181	2.688839	4.698101
H	-3.238311	0.579711	5.162553
H	0.028002	-4.476064	3.986789
H	3.853669	3.039053	-0.249567
H	-3.783323	1.348683	-3.003393
H	2.131395	-1.140092	4.217958
H	2.716014	0.469706	4.657534
H	1.015349	0.020063	4.923048
H	4.729317	1.628674	0.355838

H	4.272314	2.910242	1.473160
H	3.487485	1.196671	2.766888
H	-3.451999	-1.862074	5.448162
H	-1.909867	-3.381906	4.257057
H	3.281345	1.751098	-4.372549
H	2.186905	3.930783	-4.758171
H	0.921296	5.011666	-2.935020
H	5.417842	-0.493030	-2.123119
H	5.104878	0.669746	-3.414601
H	5.297525	1.237277	-1.756060
H	3.387653	-1.791345	-2.894765
H	2.994458	-0.589353	-4.130219
H	1.502275	-4.415962	3.020922
H	1.288580	-3.306759	4.387115
H	-1.453495	-4.099702	1.873460
H	-1.026235	-2.778099	0.760652
H	0.044424	-4.187655	0.931569
H	-0.506097	3.694857	4.614021
H	-0.897089	2.383332	5.737809
H	0.492761	2.240744	4.649156
H	-2.695254	3.737721	3.402021
H	-3.521162	2.222362	3.002563
H	0.884573	5.554200	1.218946
H	2.245817	4.476635	0.891598
H	1.894714	5.813558	-0.214109
H	-1.289104	5.307403	-0.033048
H	-0.385741	5.861273	-1.442396
H	-1.355483	4.377573	-1.532142
H	-3.688648	-1.346034	0.283658
H	-4.529715	-1.030683	1.828663
H	-5.188183	-0.361620	0.301615
H	0.935484	-2.208291	2.133808
H	0.104126	3.380601	0.278635
H	-2.596480	-1.169330	-1.821744
H	-0.145578	0.070391	-3.115162
H	-1.710111	-0.292441	-3.827327
H	-1.034581	1.876529	-1.774938
H	-1.457896	2.107570	-3.448234
H	-3.297403	2.760404	-2.037035
H	-1.162146	-2.652571	-3.218033
H	0.225142	-2.283991	-2.172666
H	-1.174957	-3.135052	-1.512119

TS(**III**$^{\delta\alpha}{}_{7CC\text{-}\gamma(R,si)}$→**IV**$^{\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)

G = -2040.641636 kcal.mol^{-1}

C	1.787490	3.842953	-1.375509
C	1.950997	2.441432	-1.237993
C	2.214006	1.627800	-2.361058
C	2.338126	2.242546	-3.612290
C	2.210854	3.616585	-3.759287
C	1.934194	4.404384	-2.646627
N	1.786869	1.855402	0.059479
C	2.851040	1.639904	0.834675
C	2.787427	1.162090	2.156720
C	1.697921	0.691492	2.909028
C	2.014941	0.260566	4.323469
C	2.355855	0.115418	-2.265636
C	3.698747	-0.371965	-2.831146
C	1.463730	4.730320	-0.178279
C	0.642928	5.973249	-0.544273
Zn	-0.023356	1.408054	0.720095
O	-1.665802	2.000830	0.143107
C	-1.759115	2.748926	-1.044689
C	-3.205323	3.179621	-1.304270
C	-4.236545	2.048216	-1.284343
C	-4.080771	0.932155	-2.318306
O	-2.837204	0.198694	-2.126550
C	-2.653840	-0.574619	-1.062233
O	-3.788607	-0.818096	-0.391626
C	-3.643175	-1.613304	0.788254
N	0.445469	0.595242	2.453655
C	-0.565030	-0.036142	3.248009
C	-1.536029	0.764208	3.894120
C	-2.569936	0.130054	4.590431
C	-2.649338	-1.254920	4.665961
C	-1.676316	-2.029950	4.045535
C	-0.621896	-1.449662	3.332302
C	-1.471452	2.284923	3.894572

C	-2.707795	2.914316	3.238596
C	0.407991	-2.364304	2.679230
C	1.041502	-3.331188	3.692401
C	-4.038792	1.401428	-3.761755
C	-0.192615	-3.156024	1.508446
C	-1.259530	2.830661	5.315296
C	4.241703	1.890039	0.294378
C	1.191272	-0.600849	-2.966101
C	2.725797	5.164135	0.585432
O	-1.569485	-1.043833	-0.785801
H	-1.148853	3.666348	-1.000294
H	-0.598706	2.580156	3.302530
H	-3.459955	-1.728497	5.213502
H	3.741058	1.124306	2.670615
H	0.857229	4.129511	0.511691
H	0.576404	-3.782612	1.041943
H	1.205075	-1.737225	2.268242
H	2.196513	-0.817469	4.371244
H	1.860619	-3.887368	3.223861
H	1.439605	-2.814306	4.571163
H	0.313414	-4.066888	4.051117
H	1.187903	0.479298	5.002372
H	2.914264	0.765397	4.681437
H	-0.989623	-3.823341	1.858626
H	-1.734304	-3.113376	4.113574
H	-0.363661	2.409442	5.783032
H	-3.321908	0.736645	5.088735
H	-2.111763	2.600262	5.964219
H	-1.147391	3.920268	5.291852
H	-2.631414	4.007566	3.263449
H	-3.626308	2.637106	3.768618
H	-2.789726	2.602643	2.193439
H	0.228014	-0.356158	-2.512334
H	2.320590	-0.159681	-1.206281
H	1.319903	-1.686979	-2.899359
H	4.271146	2.722505	-0.410153
H	1.150468	-0.334783	-4.028632
H	4.945557	2.080692	1.107040
H	4.587641	0.998891	-0.241252
H	3.760478	-0.211015	-3.913093
H	4.549445	0.144069	-2.375002
H	3.817349	-1.446539	-2.654601
H	2.538475	1.627233	-4.485714
H	2.317365	4.074725	-4.738954
H	1.820472	5.476605	-2.772520
H	3.409876	5.707866	-0.076093
H	2.458954	5.830354	1.413492
H	3.265458	4.314408	1.008476
H	-0.230010	5.725278	-1.155175
H	0.288732	6.464173	0.367961
H	1.241541	6.709930	-1.091924
H	-3.497790	3.899248	-0.528687
H	-3.240107	3.724640	-2.257776
H	-4.238383	1.594134	-0.290330
H	-5.239223	2.471974	-1.432537
H	-4.905385	0.222598	-2.188296
H	-4.650927	-1.725571	1.188648
H	-3.001185	-1.111192	1.514215
H	-3.219419	-2.589476	0.542785
H	-0.608454	-2.496502	0.743444
H	-1.392056	2.177903	-1.911183
H	-4.950342	1.958348	-3.998948
H	-3.178954	2.052315	-3.940359
H	-3.967375	0.547879	-4.441400

$I_{7CC\text{-}\gamma(S,re)}$

G = -2040.631963 kcal.mol^{-1}

C	1.663582	3.204238	-1.634147
C	1.925501	1.874604	-1.221248
C	2.373748	0.905302	-2.145571
C	2.566121	1.291263	-3.476702
C	2.338681	2.597121	-3.890818
C	1.891814	3.540523	-2.971521
N	1.677474	1.509733	0.140010
Zn	-0.073403	0.700922	0.642392
O	-1.080288	-0.430794	-0.471009
C	-2.276906	-1.013495	-0.037907
C	2.647788	-0.537020	-1.744535

C	1.600970	-1.490137	-2.341338
C	1.152475	4.257278	-0.658492
C	0.150327	5.226917	-1.298209
C	2.656017	1.595700	1.041080
C	4.056771	1.968171	0.601578
C	2.516213	1.298693	2.410382
C	1.450490	0.711509	3.115881
C	1.718735	0.400732	4.572629
N	0.277649	0.377742	2.577787
C	-0.651154	-0.414420	3.323358
C	-1.777327	0.194071	3.922861
C	-2.702945	-0.620147	4.584149
C	-2.541628	-1.998231	4.646163
C	-1.429650	-2.584726	4.052407
C	-0.464957	-1.817209	3.393753
C	-1.990603	1.701012	3.900409
C	-3.385316	2.085152	3.390399
C	0.733687	-2.511712	2.758014
C	0.352056	-3.192467	1.434775
C	1.402067	-3.515831	3.708111
C	-1.741825	2.320572	5.284752
O	-1.609213	2.331075	0.499876
C	-2.291357	2.396016	-0.511798
O	-1.752201	2.415257	-1.727372
C	-2.134006	1.419435	-2.722122
C	-3.637113	1.358948	-2.955663
C	-4.245528	2.752407	-2.832473
C	-4.473402	3.164294	-1.372333
O	-3.613630	2.498328	-0.397630
C	4.068779	-0.979386	-2.123224
C	2.294704	5.059653	-0.014284
H	2.030640	-0.642970	4.690489
H	2.519016	1.034125	4.960613
H	0.824942	0.535703	5.184720
H	4.591978	1.057838	0.306560
H	4.065156	2.639033	-0.257973
H	4.613909	2.425522	1.422117
H	3.404679	1.481121	3.004299
H	-3.567286	-0.162197	5.058269
H	-3.276733	-2.613581	5.158194
H	-1.306148	-3.663311	4.102730
H	2.907374	0.553113	-4.198362
H	2.505942	2.880332	-4.926891
H	1.708001	4.558512	-3.303324
H	4.270887	-1.982240	-1.731347
H	4.202827	-1.021639	-3.209790
H	4.828169	-0.298953	-1.724486
H	1.825751	-2.525279	-2.058867
H	0.597226	-1.249427	-1.977122
H	1.603894	-1.437309	-3.436680
H	2.328459	-3.895704	3.263663
H	1.649613	-3.062623	4.673763
H	0.760943	-4.381940	3.905107
H	-0.425138	-3.948792	1.594552
H	-0.019781	-2.467407	0.704632
H	1.223639	-3.696365	1.000701
H	-1.875849	3.407676	5.248206
H	-2.442201	1.922239	6.027969
H	-0.728022	2.121807	5.645009
H	-3.470924	3.174924	3.318017
H	-3.574707	1.670130	2.398255
H	-4.175060	1.739141	4.067016
H	1.889815	5.830486	0.651356
H	2.958450	4.428321	0.580075
H	2.898713	5.560768	-0.779809
H	-0.327340	5.833274	-0.520698
H	0.637850	5.923636	-1.989924
H	-0.626650	4.689666	-1.847792
H	-3.055933	-0.273804	0.224841
H	-2.698350	-1.646524	-0.837897
H	-2.157282	-1.661858	0.845014
H	2.562968	-0.600456	-0.654787
H	1.478862	-1.746667	2.519903
H	0.629793	3.722472	0.141060
H	-1.259952	2.126084	3.206210
H	-1.706658	0.472494	-2.377778
H	-1.613443	1.769067	-3.615546
H	-3.807050	0.947384	-3.956679

H	-4.113303	0.671641	-2.248217
H	-3.597660	3.481856	-3.333106
H	-5.217841	2.799328	-3.335069
C	-4.398402	4.663981	-1.148524
H	-5.453167	2.793893	-1.056889
H	-5.128229	5.170300	-1.788568
H	-4.615405	4.916048	-0.107612
H	-3.403891	5.044016	-1.403205

TS($\mathbf{I}_{7CC\text{-}\gamma(S,re)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(S,re)}$)

G = -2040.624509 kcal.mol^{-1}

C	1.899509	3.301508	-1.585708
C	2.037715	1.951522	-1.186530
C	2.405596	0.956332	-2.119694
C	2.639935	1.335616	-3.444998
C	2.526190	2.660699	-3.847627
C	2.159118	3.628448	-2.920185
N	1.751600	1.581261	0.166844
Zn	-0.073349	0.987118	0.670483
O	-1.352371	0.162767	-0.559735
C	-2.165731	-0.954653	-0.308930
C	2.529187	-0.509378	-1.730522
C	1.378977	-1.332477	-2.330070
C	1.493000	4.403586	-0.616652
C	0.264875	5.177169	-1.115154
C	2.715238	1.606607	1.085700
C	4.128603	1.963342	0.681932
C	2.534389	1.272058	2.442326
C	1.436855	0.699114	3.107874
C	1.667751	0.355391	4.563776
N	0.261925	0.415699	2.539175
C	-0.718420	-0.343152	3.254069
C	-1.846664	0.312032	3.800582
C	-2.822343	-0.458894	4.440260
C	-2.708454	-1.840129	4.535615
C	-1.595243	-2.472409	3.995503
C	-0.583044	-1.749582	3.356690
C	-2.003323	1.824846	3.753573
C	-3.383194	2.255693	3.243406
C	0.611031	-2.506873	2.787328
C	0.214596	-3.339145	1.559032
C	1.282869	-3.404292	3.837608
C	-1.715686	2.452246	5.126826
O	-1.501621	2.478005	0.289727
C	-2.135924	1.980664	-0.667163
O	-1.731984	2.303362	-1.911415
C	-2.152186	1.506610	-3.030233
C	-3.669244	1.496314	-3.264823
C	-4.329467	2.702675	-2.605586
C	-4.456288	2.513841	-1.086108
O	-3.443222	1.630381	-0.534918
C	3.890117	-1.105442	-2.115394
C	2.652075	5.372628	-0.335253
H	2.065745	-0.660426	4.658951
H	2.398862	1.037775	5.002657
H	0.744097	0.397196	5.143369
H	4.629713	1.072338	0.285299
H	4.156548	2.719469	-0.103520
H	4.703704	2.312846	1.541538
H	3.411700	1.414679	3.063165
H	-3.687231	0.036152	4.873426
H	-3.481194	-2.420993	5.032075
H	-1.506763	-3.553217	4.071610
H	2.921598	0.578120	-4.172301
H	2.721901	2.938123	-4.880170
H	2.068094	4.664071	-3.237761
H	3.974976	-2.132849	-1.744375
H	4.025684	-1.139490	-3.201918
H	4.719114	-0.524807	-1.697865
H	1.452163	-2.381253	-2.019763
H	0.410752	-0.940089	-2.003844
H	1.408233	-1.306372	-3.425688
H	2.203869	-3.838764	3.433693
H	1.538290	-2.851148	4.746708
H	0.633748	-4.235854	4.132956
H	-0.546687	-4.083808	1.817681
H	-0.191623	-2.708998	0.764238
H	1.083815	-3.873726	1.159527

H	-1.805279	3.543198	5.076234	H	-5.366562	1.939220	-0.885673	C	1.720084	0.562078	3.075978
H	-2.425055	2.092150	5.881079	H	-5.328784	4.444969	-0.711624	C	1.963720	0.061551	4.480606
H	-0.707211	2.215904	5.479672	H	-4.667229	3.661342	0.739587	N	0.511886	0.370579	2.525265
H	-3.417854	3.346230	3.147208	H	-3.575588	4.388305	-0.452581	C	-0.501407	-0.300645	3.289251
H	-3.590557	1.823421	2.261881					C	-1.381239	0.456174	4.094795
H	-4.184403	1.962919	3.931647	$\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(S,re)}$				C	-2.372421	-0.219401	4.813665
H	2.340849	6.141672	0.380588	G = -2040.637528 kcal.mol^{-1}				C	-2.502730	-1.601887	4.742660
H	3.524865	4.862776	0.083043	C	1.760105	3.860916	-1.084543	C	-1.637513	-2.330739	3.935502
H	2.972848	5.882054	-1.251297	C	2.069396	2.488041	-0.962916	C	-0.627709	-1.704452	3.197989
H	-0.061557	5.894645	-0.353988	C	2.470970	1.731202	-2.085204	C	-1.302354	1.973644	4.179427
H	0.488082	5.745284	-2.025858	C	2.548035	2.372395	-3.325362	C	-2.504187	2.622613	3.475202
H	-0.561334	4.495958	-1.325440	C	2.242754	3.721265	-3.462113	C	0.283881	-2.549420	2.319039
H	-3.176526	-0.770197	-0.698364	C	1.854429	4.454172	-2.346738	C	-0.487944	-3.152517	1.135615
H	-1.768791	-1.848728	-0.815308	N	1.898250	1.839318	0.301803	C	1.000465	-3.652186	3.112471
H	-2.265646	-1.184516	0.760714	Zn	0.147024	1.021274	0.730328	C	-1.181533	2.479301	5.623895
H	2.441286	-0.570477	-0.641105	O	-1.065455	1.214781	-0.663545	O	-1.979169	-0.802597	-1.139388
H	1.351561	-1.772862	2.455813	C	-2.198930	0.506496	-0.588511	C	-2.933436	-1.302485	-2.065050
H	1.215460	3.926295	0.327717	O	-2.513256	0.357830	0.779479	C	-2.716715	-0.739193	-3.472268
H	-1.263775	2.213711	3.047854	C	-3.641001	-0.440167	1.097085	C	-2.338017	0.743754	-3.440673
H	-1.746395	0.502253	-2.887992	C	2.798108	0.248282	-1.983386	C	-3.220445	1.600995	-2.535777
H	-1.638415	1.980713	-3.869315	C	1.706918	-0.607961	-2.643969	C	-2.806791	3.066932	-2.548387
H	-3.855356	1.501946	-4.344644	C	1.298616	4.689957	0.105331	O	-3.304618	1.116257	-1.180778
H	-4.113312	0.575538	-2.872057	C	-0.206537	4.984000	0.016328	C	4.178553	-0.086323	-2.565743
H	-3.754604	3.609242	-2.827996	C	2.897985	1.798659	1.178443	C	2.098224	5.990123	0.266787
H	-5.336640	2.861539	-3.007687	C	4.222885	2.427785	0.818953	H	-4.260335	1.524154	-2.883953
C	-4.507892	3.829669	-0.327553	C	2.801074	1.203515	2.451662	H	1.784084	-1.014948	4.550069

H	2.986545	0.268128	4.798063
H	1.275072	0.535703	5.186261
H	4.606839	2.015916	-0.118953
H	4.107704	3.504816	0.660716
H	4.963161	2.268137	1.604119
H	3.703327	1.257475	3.048459
H	-3.055751	0.350265	5.438241
H	-3.277755	-2.108396	5.311755
H	-1.745715	-3.410628	3.874666
H	2.850898	1.802694	-4.200182
H	2.307095	4.200340	-4.435390
H	1.614811	5.508517	-2.458198
H	4.415766	-1.142387	-2.397065
H	4.215705	0.086990	-3.646658
H	4.970950	0.514764	-2.107620
H	1.940097	-1.673864	-2.538880
H	0.725749	-0.426136	-2.196222
H	1.634497	-0.387585	-3.715346
H	1.703021	-4.188576	2.465457
H	1.565055	-3.248344	3.959090
H	0.293689	-4.389148	3.509404
H	-1.269985	-3.835615	1.487518
H	-0.962643	-2.380275	0.523195
H	0.189038	-3.728603	0.494169
H	-1.052197	3.567035	5.634895
H	-2.079190	2.252392	6.209540
H	-0.326891	2.034364	6.143904
H	-2.403603	3.713883	3.469305
H	-2.595370	2.272342	2.443249
H	-3.438221	2.378853	3.994775
H	1.798310	6.508217	1.184193
H	3.175385	5.801325	0.322416
H	1.926654	6.680159	-0.566405
H	-0.547584	5.530324	0.903160
H	-0.432419	5.598587	-0.862404
H	-0.788713	4.061758	-0.067288
H	-3.502162	-1.473344	0.760019
H	-3.723660	-0.430396	2.184849
H	-4.552259	-0.024340	0.653285
H	2.821665	-0.013460	-0.920441
H	1.054436	-1.889326	1.907894
H	1.461520	4.093979	1.009137
H	-0.399029	2.288498	3.647189
H	-3.950204	-1.079099	-1.724202
H	-2.809209	-2.390756	-2.057718
H	-1.918403	-1.293565	-3.979711
H	-3.632609	-0.897403	-4.057547
H	-1.301820	0.850312	-3.106385
H	-2.389175	1.161679	-4.453442
H	-1.762542	3.169663	-2.246261
H	-2.929500	3.489598	-3.551997
H	-3.429795	3.639152	-1.855206

TS($\mathbf{II}^{6\alpha}_{7CC\text{-}\gamma(S,re)} \rightarrow \mathbf{III}^{6\alpha}_{7CC\text{-}\gamma(S,re)}$)

G = -2040.626648 kcal.mol^{-1}

C	1.545839	3.553788	-1.530742
C	1.907713	2.223852	-1.213540
C	2.447395	1.368141	-2.204247
C	2.509333	1.831010	-3.522454
C	2.083547	3.110617	-3.861108
C	1.629108	3.966244	-2.864883
N	1.680097	1.717969	0.106031
Zn	-0.095654	0.965809	0.590316
O	-1.832362	2.050971	0.376541
C	-2.638026	1.104150	0.099856
O	-3.155656	0.454366	1.165146
C	-4.004339	-0.664513	0.939676
C	3.005971	-0.011012	-1.870559
C	2.141156	-1.149181	-2.425911
C	1.133709	4.559921	-0.463191
C	-0.328134	5.002956	-0.600568
C	2.668826	1.750743	1.007374
C	3.977489	2.405602	0.628849
C	2.597828	1.209151	2.298051
C	1.553079	0.521738	2.949087
C	1.892248	-0.038891	4.312422
N	0.342000	0.319364	2.435194
C	-0.640334	-0.368638	3.221613

C	-1.511552	0.374890	4.051180
C	-2.480618	-0.316356	4.784406
C	-2.604216	-1.698646	4.703719
C	-1.743168	-2.415001	3.880955
C	-0.748875	-1.774377	3.134824
C	-1.418546	1.888945	4.190760
C	-2.740780	2.584095	3.838510
C	0.169436	-2.608604	2.253070
C	-0.594922	-3.184830	1.052814
C	0.875029	-3.726679	3.034240
C	-0.962008	2.299003	5.600014
O	-1.389484	-0.146462	-0.486856
C	-1.597780	-0.618783	-1.793803
C	-1.324928	0.394521	-2.910661
C	-1.841864	1.809021	-2.629076
C	-3.276590	1.902429	-2.122974
C	-3.758861	3.331623	-1.919742
O	-3.524556	1.138504	-0.914784
C	4.456098	-0.165243	-2.355074
C	2.063922	5.784025	-0.465271
H	-3.937488	1.402376	-2.842420
H	2.068419	-1.117579	4.234416
H	2.797044	0.422672	4.711319
H	1.076290	0.094432	5.024501
H	4.465035	1.866842	-0.188993
H	3.811814	3.426923	0.275089
H	4.661470	2.435592	1.478061
H	3.503429	1.312961	2.883358
H	-3.152483	0.242943	5.430746
H	-3.364845	-2.215436	5.283271
H	-1.838732	-3.496201	3.819307
H	2.906739	1.178630	-4.296125
H	2.132745	3.448395	-4.892816
H	1.339997	4.981737	-3.123849
H	4.874979	-1.113323	-2.000686
H	4.518393	-0.169021	-3.448663
H	5.098269	0.644335	-1.993853
H	2.588138	-2.121350	-2.189474
H	1.138100	-1.127837	-1.994490
H	2.044793	-1.081831	-3.515523
H	1.594410	-4.244401	2.390195
H	1.416442	-3.339896	3.903575
H	0.164582	-4.477132	3.397947
H	-1.385990	-3.868316	1.382916
H	-1.052612	-2.380051	0.471183
H	0.080810	-3.749681	0.399792
H	-0.869570	3.388692	5.668805
H	-1.685410	1.979470	6.358834
H	0.007323	1.865075	5.863282
H	-2.618614	3.671815	3.893104
H	-3.061550	2.321144	2.829548
H	-3.537861	2.308863	4.538925
H	1.827274	6.440163	0.379312
H	3.118614	5.500685	-0.388315
H	1.948727	6.373858	-1.381204
H	-0.569726	5.755167	0.158981
H	-0.516606	5.450641	-1.583188
H	-1.007043	4.158607	-0.463303
H	-3.474396	-1.431461	0.368639
H	-4.245460	-1.050217	1.930495
H	-4.917627	-0.371028	0.414709
H	3.008787	-0.113000	-0.780933
H	0.943657	-1.943141	1.857343
H	1.234804	4.067887	0.509397
H	-0.665382	2.241654	3.479811
H	-2.646580	-0.943473	-1.866622
H	-0.987083	-1.519160	-1.959381
H	-0.248810	0.468679	-3.102008
H	-1.777386	-0.000467	-3.831651
H	-1.183026	2.309061	-1.917087
H	-1.790496	2.396930	-3.553571
H	-3.142320	3.845947	-1.179869
H	-3.710269	3.884644	-2.863415
H	-4.795614	3.335810	-1.571730

III$^{6\alpha}{}_{7CC\text{-}\gamma(S,re)}$

G = -2040.633247 kcal.mol^{-1}

C	1.568197	3.553925	-1.520471

C	1.923215	2.221869	-1.203606	C	-0.743797	-1.837070	3.134178	H	-1.791063	-3.562807	3.873903
C	2.478277	1.370066	-2.189394	C	-1.567903	1.849744	3.955519	H	2.972028	1.189068	-4.273855
C	2.563406	1.838882	-3.504021	C	-2.959409	2.482420	4.078062	H	2.214897	3.464355	-4.872373
C	2.146690	3.121315	-3.843448	C	0.209457	-2.678506	2.297954	H	1.394711	4.990408	-3.110023
C	1.676461	3.972752	-2.850966	C	-0.518917	-3.305867	1.100411	H	4.891622	-1.122196	-1.967096
N	1.674157	1.704067	0.107262	C	0.922573	-3.754965	3.129374	H	4.549676	-0.180448	-3.419742
Zn	-0.023342	0.737396	0.470432	C	-0.658742	2.393944	5.069435	H	5.122978	0.634593	-1.962073
O	-1.935070	2.174957	0.424787	O	-1.155391	-0.391311	-0.505703	H	2.607159	-2.119233	-2.175059
C	-2.854584	1.376138	0.256834	C	-1.508565	-0.654170	-1.825034	H	1.157788	-1.129138	-1.959662
O	-3.285288	0.640639	1.272328	C	-1.284827	0.457661	-2.857933	H	2.051042	-1.073713	-3.491000
C	-4.129201	-0.488391	1.022158	C	-1.828572	1.847957	-2.514581	H	1.670617	-4.271725	2.518125
C	3.027890	-0.011362	-1.850371	C	-3.285351	1.932043	-2.074688	H	1.431436	-3.330455	4.000908
C	2.156209	-1.146597	-2.402444	C	-3.808552	3.354824	-1.945831	H	0.222612	-4.514126	3.495685
C	1.140649	4.558789	-0.457076	O	-3.577354	1.206766	-0.838795	H	-1.317200	-3.978493	1.436293
C	-0.305323	5.037921	-0.636772	C	4.479785	-0.172955	-2.326599	H	-0.952913	-2.524392	0.469604
C	2.636968	1.760171	1.035535	C	2.092303	5.766373	-0.422258	H	0.179261	-3.895918	0.494888
C	3.938587	2.447699	0.692959	H	-3.908358	1.382225	-2.789464	H	-0.686713	3.489481	5.080509
C	2.547310	1.207019	2.319020	H	2.218909	-1.104778	4.170852	H	-0.991788	2.040676	6.052480
C	1.501570	0.492779	2.940077	H	2.623618	0.500512	4.785006	H	0.383319	2.094075	4.937899
C	1.839819	-0.084131	4.299031	H	0.973242	-0.143201	4.957982	H	-2.887867	3.562638	3.912312
N	0.308119	0.267834	2.395788	H	4.437274	1.948665	-0.143331	H	-3.649504	2.068785	3.339431
C	-0.681392	-0.427158	3.166517	H	3.761561	3.479951	0.379493	H	-3.391064	2.340967	5.075855
C	-1.602676	0.325921	3.934279	H	4.616581	2.454117	1.547481	H	1.844090	6.420410	0.420743
C	-2.554739	-0.365873	4.688389	H	3.436914	1.322544	2.926662	H	3.139820	5.465819	-0.319627
C	-2.623050	-1.755801	4.673692	H	-3.262561	0.193777	5.292565	H	2.012510	6.364285	-1.336815
C	-1.729929	-2.477653	3.892678	H	-3.372519	-2.272243	5.268112	H	-0.549861	5.794841	0.117177

H	-0.454313	5.491976	-1.623222
H	-1.009180	4.211844	-0.519845
H	-3.612870	-1.184288	0.358808
H	-4.283028	-0.944579	1.999430
H	-5.082352	-0.178611	0.586897
H	3.028055	-0.108729	-0.760199
H	0.977720	-2.009895	1.895852
H	1.199055	4.056725	0.513805
H	-1.152592	2.170851	2.994987
H	-2.582295	-0.916949	-1.850277
H	-0.982216	-1.550015	-2.205577
H	-0.211393	0.572217	-3.049911
H	-1.730183	0.109640	-3.802214
H	-1.201878	2.325866	-1.761440
H	-1.746179	2.478551	-3.408969
H	-3.220799	3.924514	-1.222532
H	-3.749262	3.861281	-2.913983
H	-4.854311	3.351444	-1.625250

TS(**III**$^{\delta\alpha}{}_{7CC\text{-}\gamma(S,re)}$→**IV**$^{\delta\alpha}{}_{7CC\text{-}\gamma(S)}$)

G = -2040.632858 kcal.mol^{-1}

C	-0.754346	-1.799681	3.172421
C	-0.662070	-0.391245	3.178846
C	-1.572869	0.397958	3.921509
C	-2.543350	-0.259160	4.683318
C	-2.638772	-1.647129	4.698565
C	-1.756900	-2.404281	3.938245
N	0.349751	0.264737	2.401769
C	1.545116	0.475636	2.948451
C	1.862184	-0.083780	4.318846
C	-1.509909	1.921097	3.907914
C	-0.583661	2.474673	5.003164
C	0.178820	-2.673805	2.347208
C	0.849940	-3.772806	3.183516
C	2.605192	1.158661	2.316963
C	2.695411	1.713311	1.034195
C	3.991886	2.411976	0.697132
N	1.730417	1.659819	0.106468
Zn	0.056026	0.676537	0.469928
O	-1.213681	-0.301576	-0.452498
C	-1.502999	-0.598408	-1.782999
C	-1.287350	0.518055	-2.810449
C	-1.880835	1.887866	-2.470487
C	-3.357627	1.929126	-2.091501
O	-3.670513	1.187157	-0.875503
C	-3.023420	1.438860	0.260256
O	-3.449792	0.674556	1.262937
C	-4.200516	-0.509195	0.981840
C	1.960732	2.211699	-1.195467
C	1.591021	3.548322	-1.474017
C	1.686524	4.002402	-2.793951
C	2.157330	3.182352	-3.812086
C	2.583051	1.893685	-3.510949
C	2.508326	1.388404	-2.209237
C	1.162584	4.524939	-0.384721
C	2.122167	5.725199	-0.315721
C	3.059575	-0.003044	-1.917808
C	4.523346	-0.135096	-2.366636
O	-2.192857	2.310897	0.459121
C	2.210655	-1.115406	-2.546699
C	-0.279156	5.021141	-0.556640
C	-2.888851	2.581395	4.021634
C	-0.561985	-3.276623	1.144271
C	-3.919529	3.339543	-1.982837
H	-3.935265	1.368610	-2.835931
H	2.194915	-1.123127	4.213955
H	2.670890	0.477440	4.791101
H	0.994289	-0.090209	4.978767
H	4.433222	2.010680	-0.218970
H	3.817902	3.477305	0.519694
H	4.714192	2.311871	1.508354
H	3.497702	1.264658	2.921893
H	-3.245462	0.327304	5.267981
H	-3.402474	-2.135179	5.298786
H	-1.841656	-3.487988	3.940585
H	2.988996	1.266861	-4.301036
H	2.216524	3.554007	-4.831547
H	1.394014	5.023870	-3.023994

H	4.930159	-1.101681	-2.050162	H	-5.155394	-0.268602	0.507391	C	-0.990049	1.975682	-1.961578
H	4.617895	-0.081161	-3.456559	H	3.034418	-0.149923	-0.833415	C	-2.194218	2.832842	-2.358276
H	5.154989	0.652062	-1.942922	H	0.972822	-2.031753	1.951322	C	-3.544406	2.321049	-1.845903
H	2.653351	-2.096802	-2.342488	H	1.215341	3.997789	0.573127	C	-3.903104	0.912402	-2.312095
H	1.194804	-1.116309	-2.144888	H	-1.096774	2.213686	2.937396	C	-4.079531	0.739862	-3.813017
H	2.144330	-0.998613	-3.634295	H	-2.563137	-0.901645	-1.835404	C	2.638123	4.431296	-0.283582
H	1.585085	-4.314207	2.578010	H	-0.929619	-1.477587	-2.131596	C	1.253639	5.047736	-0.537644
H	1.365987	-3.364256	4.058459	H	-0.212668	0.665027	-2.974780	C	3.112554	-0.411383	-1.913569
H	0.122918	-4.508356	3.544747	H	-1.697082	0.159959	-3.766983	C	1.884811	-0.996558	-2.627767
H	-1.377675	-3.929759	1.476247	H	-1.302965	2.361896	-1.676715	C	3.284207	1.276713	1.138598
H	-0.979997	-2.483135	0.517553	H	-1.769496	2.537126	-3.348111	C	4.763366	1.458507	0.895307
H	0.121371	-3.881144	0.536062	H	-3.371075	3.920094	-1.237951	C	2.899281	0.822441	2.411963
H	-0.598376	3.570434	4.992564	H	-3.839942	3.847507	-2.948894	C	1.617993	0.563734	2.936824
H	-0.912717	2.145532	5.995876	H	-4.975481	3.309795	-1.698684	C	1.553661	0.078776	4.365659
H	0.454050	2.160244	4.869517					N	0.480704	0.724445	2.258069
H	-2.797862	3.654892	3.825783	**IV**$^{\delta\alpha}{}_{7CC\cdot\gamma(S)}$				C	-0.778586	0.427458	2.875530
H	-3.588798	2.161159	3.296698	G = -2040.650674 kcal.mol^{-1}				C	-1.321223	-0.871167	2.757110
H	-3.316239	2.474813	5.025778	C	3.207532	1.090621	-2.139754	C	-2.575224	-1.121676	3.321596
H	1.878267	6.356986	0.545254	C	2.906094	2.020825	-1.120259	C	-3.282575	-0.123656	3.981487
H	3.168104	5.416011	-0.223374	C	2.981568	3.411515	-1.359965	C	-2.742387	1.153218	4.076085
H	2.045310	6.348609	-1.213358	C	3.351381	3.846452	-2.636175	C	-1.491730	1.455671	3.529322
H	-0.515262	5.764060	0.213650	C	3.644052	2.942974	-3.651225	C	-0.604965	-1.972639	1.989705
H	-0.420227	5.500653	-1.532127	C	3.572948	1.578416	-3.398143	C	-1.269817	-2.187332	0.620585
H	-0.997993	4.205390	-0.459346	N	2.431149	1.553165	0.147914	C	-0.961317	2.879464	3.604537
H	-3.613541	-1.170873	0.342503	Zn	0.504370	1.377741	0.414405	C	-1.723778	3.786381	2.624949
H	-4.363718	-0.976133	1.952899	O	-0.976405	1.761891	-0.574245	C	-0.998118	3.455094	5.026133

C	-0.522813	-3.291562	2.768770	H	0.960124	-0.514897	-2.294891	H	0.087182	2.859816	3.289212
O	-5.069784	0.417880	-1.584897	H	1.957587	-0.855685	-3.711880	H	-1.035826	1.012592	-2.504382
C	-6.256715	1.011008	-1.761861	H	0.077069	-4.021891	2.215097	H	-0.078445	2.479639	-2.324855
O	-6.518483	1.925957	-2.504799	H	-0.062847	-3.153526	3.752655	H	-2.048024	3.842629	-1.954844
O	-7.204450	0.454056	-0.987686	H	-1.511492	-3.736314	2.924653	H	-2.206342	2.937733	-3.451887
C	-6.852760	-0.608849	-0.102858	H	-2.300042	-2.541307	0.740022	H	-3.511781	2.306052	-0.751749
C	3.704199	5.525703	-0.142673	H	-1.307470	-1.256430	0.045879	H	-4.338907	3.008270	-2.150531
C	4.388481	-1.152102	-2.336487	H	-0.722851	-2.935156	0.035259	H	-4.818360	1.439560	-4.207243
H	-3.131954	0.221657	-1.958788	H	-0.528204	4.444304	5.045837	H	-3.123277	0.910564	-4.316886
H	1.041669	-0.886340	4.425959	H	-2.023641	3.576272	5.390912	H	-4.399815	-0.281029	-4.043582
H	2.551663	-0.024790	4.793398	H	-0.466963	2.814576	5.737883				
H	0.976809	0.774597	4.983148	H	-1.312270	4.802081	2.638589	TS($\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(S,re)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$)			
H	5.106611	0.802294	0.089266	H	-1.671197	3.404698	1.600359	G = -2040.619389 kcal.mol^{-1}			
H	4.981487	2.482436	0.576589	H	-2.782581	3.850759	2.900233	C	-0.59528	-1.45726	3.52925
H	5.341646	1.238794	1.793645	H	3.467500	6.175492	0.706565	C	-0.51416	-0.07034	3.27344
H	3.717609	0.644294	3.098944	H	4.700250	5.102305	0.022415	C	-1.43387	0.83329	3.85921
H	-3.305076	1.934459	4.580200	H	3.757272	6.162037	-1.032465	C	-2.41882	0.32013	4.70756
H	-4.255379	-0.338730	4.415414	H	0.998906	5.764563	0.250930	C	-2.50575	-1.04166	4.97519
H	-3.006934	-2.115574	3.237634	H	1.233027	5.580123	-1.495095	C	-1.60118	-1.91578	4.38658
H	3.800879	0.875323	-4.195070	H	0.470314	4.283229	-0.565428	N	0.54281	0.43748	2.45055
H	3.926996	3.301888	-4.636990	H	-6.092247	-0.292653	0.616046	C	0.27586	0.80095	1.19024
H	3.407409	4.912569	-2.839168	H	-7.775441	-0.866788	0.419342	C	1.18511	1.43457	0.32768
H	4.317164	-2.212696	-2.072324	H	-6.482507	-1.478113	-0.653461	C	2.50929	1.85333	0.55222
H	4.551960	-1.096317	-3.418026	H	2.977036	-0.577868	-0.839997	C	3.17861	2.61506	-0.56712
H	5.277354	-0.741273	-1.846923	H	0.421278	-1.637730	1.807261	C	-1.35869	2.33746	3.62374
H	1.797961	-2.071325	-2.433297	H	2.589572	3.899998	0.672624	C	-0.70862	3.05372	4.81671

C	0.34126	-2.46504	2.87755	C	5.82826	-1.26834	1.75680	H	1.08152	-1.90446	2.29709
C	-0.41876	-3.36856	1.89365	C	-1.10269	0.54315	0.62454	H	1.78011	-3.99970	3.39948
Zn	2.38250	0.54089	3.13101	C	-2.72647	2.95881	3.30839	H	-1.08906	0.61019	-0.46455
O	3.48077	-0.52716	4.19101	C	1.10441	-3.30484	3.91046	H	0.41982	-3.90432	4.52145
C	3.57262	-0.26912	5.49700	H	2.72667	3.85046	2.41929	H	-1.47342	-0.44178	0.91790
O	2.78978	0.93576	5.74542	H	8.20279	3.23552	2.34420	H	-1.82308	1.27759	0.99909
C	2.00769	1.05854	6.94755	H	0.79424	1.66469	-0.65609	H	-1.17116	-3.97380	2.41156
H	1.68473	2.10614	6.89773	H	-0.71268	2.51307	2.75830	H	-0.93408	-2.78974	1.12030
N	3.18983	1.61398	1.67319	H	5.63011	-2.24941	1.30987	H	0.27363	-4.05561	1.39495
C	4.54032	2.07403	1.79848	H	4.29644	-0.26930	0.64970	H	-1.67643	-2.98052	4.59148
C	5.60422	1.22542	1.41537	H	4.09272	2.10933	-0.89114	H	-3.27846	-1.41928	5.63936
C	6.91395	1.67026	1.62219	H	5.80378	-1.26310	-1.01062	H	-3.12740	1.00023	5.17252
C	7.17716	2.91166	2.18902	H	5.74440	0.48859	-1.26331	H	-3.39404	2.94095	4.17653
C	6.12017	3.73743	2.55439	H	7.14564	-0.24721	-0.47880	H	-2.60608	4.00756	3.01645
C	4.79182	3.34380	2.36574	H	3.47898	3.61105	-0.22764	H	-3.23531	2.43615	2.49188
C	5.37374	-0.15043	0.80547	H	2.51294	2.72381	-1.42440	H	0.30620	2.68705	4.99495
C	6.05449	-0.29492	-0.56401	H	6.90561	-1.20510	1.94912	H	-0.65214	4.13294	4.63488
C	3.66533	4.27827	2.78588	H	7.74226	1.02621	1.33829	H	-1.28841	2.89536	5.73277
C	3.56077	4.37397	4.31557	H	3.89412	5.63227	1.07659	H	3.38505	1.84097	8.40776
O	3.07081	-1.33312	6.23808	H	6.32919	4.70846	2.99606	H	2.04710	0.92042	9.05820
C	3.46161	-1.52310	7.59968	H	4.68851	6.20181	2.54793	H	4.76664	0.05551	8.18678
C	3.75587	-0.27182	8.42596	H	2.93156	6.28918	2.41073	H	3.76633	-0.58272	9.47870
C	2.79997	0.92623	8.26015	H	2.73525	5.03466	4.60396	H	2.62514	-2.08223	8.03526
O	4.89606	-0.07839	5.91703	H	4.48145	4.78519	4.74523	H	4.34420	-2.17480	7.62880
C	5.60286	0.97218	5.28797	H	3.38830	3.39363	4.76996	H	6.63512	0.89847	5.63831
C	3.80619	5.67627	2.16697	H	1.70480	-2.67805	4.57403	H	5.19848	1.95170	5.56765

H	5.58691	0.87186	4.19944
H	5.30261	-1.21529	2.71448
C	0.73614	0.20930	6.92585
H	0.23141	0.30300	5.96211
H	0.92730	-0.84923	7.09842
H	0.04955	0.57062	7.70010

II$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$

G = -2040.632188 kcal.mol^{-1}

C	-0.587005	-1.363873	3.634096
C	-0.292360	0.014467	3.524815
C	-1.002592	0.971234	4.284710
C	-2.017605	0.525847	5.136788
C	-2.324277	-0.825261	5.249718
C	-1.608795	-1.755671	4.505326
N	0.689846	0.458459	2.582700
Zn	0.157158	0.811773	0.700938
O	-1.242914	-0.224653	0.032134
C	-2.294751	0.416314	-0.476776
O	-2.390982	0.179187	-1.854394
C	-3.677308	0.155111	-2.469323
C	-4.244016	1.551559	-2.701248
C	-4.166435	2.461006	-1.472257
C	-2.751062	2.831314	-0.997958
C	-1.848451	3.305490	-2.130689
C	-0.705082	2.461093	4.186408
C	-0.460934	3.100382	5.560700
C	0.155854	-2.424740	2.833776
C	-0.763720	-3.090476	1.798792
N	1.814867	1.642780	0.065593
C	2.931832	1.534071	0.796284
C	4.242989	2.017217	0.217576
C	1.856973	2.341810	-1.184366
C	1.855224	3.757917	-1.190233
C	1.835740	4.415700	-2.423577
C	1.824036	3.709260	-3.621100
C	1.837921	2.320503	-3.598225
C	1.855631	1.610595	-2.393168
C	1.851703	4.581170	0.093140
C	2.902066	5.701221	0.077940
C	1.926136	0.090091	-2.426215
C	0.776089	-0.536164	-3.225355
C	2.993343	1.019528	2.101302
C	1.963552	0.578472	2.953404
C	2.356600	0.234912	4.370781
C	3.284184	-0.384415	-2.968473
C	0.460749	5.164521	0.383767
O	-3.512927	0.013046	0.088257
C	-3.592204	0.081233	1.498257
O	-2.072560	1.824404	-0.216554
C	-1.821542	3.202911	3.436247
C	0.806281	-3.480102	3.740611
H	-2.873570	3.654587	-0.281834
H	0.214272	2.577215	3.603446
H	-3.117059	-1.152123	5.917233
H	3.984456	1.009155	2.538732
H	2.097857	3.913926	0.924508
H	-0.205563	-3.834979	1.219281
H	0.958833	-1.923135	2.283933
H	2.036845	-0.777046	4.633811
H	1.399477	-4.179454	3.141620
H	1.469030	-3.030980	4.487721
H	0.053870	-4.067434	4.278288
H	1.863941	0.910103	5.077959
H	3.435578	0.312982	4.511304
H	-1.595527	-3.609862	2.288970
H	-1.850361	-2.811502	4.596485
H	0.323659	2.578304	6.117852
H	-2.577645	1.251075	5.721578
H	-1.364772	3.093700	6.179614
H	-0.154211	4.145604	5.444432
H	-1.589842	4.271006	3.356862
H	-2.777559	3.106794	3.963505
H	-1.957209	2.807781	2.424673
H	-0.198218	-0.256907	-2.817091
H	1.843867	-0.268747	-1.394911
H	0.852952	-1.628670	-3.193482
H	4.337777	3.103130	0.322220

H	0.812317	-0.238201	-4.279691	H	-0.909969	3.699336	-1.737214	C	1.65453	0.88984	2.96408
H	5.083401	1.557228	0.740596	H	-1.603407	2.482596	-2.804255	C	1.91223	0.60904	4.42855
H	4.316998	1.792212	-0.848357					C	2.78082	1.23706	2.20255
H	3.429214	-0.061740	-4.005645	TS(**II**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$→**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$				C	2.89882	1.58173	0.84533
H	4.120759	0.006029	-2.380094	G = -2040.616066 kcal.mol^{-1}				C	4.31846	1.82116	0.37396
H	3.341462	-1.478241	-2.949045	C	-1.54702	1.07306	3.92058	N	1.87745	1.72781	-0.00258
H	1.840616	1.770113	-4.535425	C	-0.60009	0.21596	3.31480	C	2.13868	2.25350	-1.30916
H	1.808809	4.240940	-4.568670	C	-0.67972	-1.18830	3.48881	C	2.38656	3.64035	-1.47137
H	1.827132	5.502167	-2.446463	C	-1.74294	-1.70423	4.23608	C	2.55547	4.13800	-2.76711
H	2.654620	6.482288	-0.648958	C	-2.69345	-0.87306	4.81927	C	2.49781	3.30519	-3.87771
H	2.957644	6.180962	1.061066	C	-2.58348	0.50372	4.66830	C	2.27876	1.94480	-3.70186
H	3.899013	5.324617	-0.172397	N	0.41918	0.76439	2.47581	C	2.09610	1.39191	-2.43049
H	-0.290480	4.376622	0.487101	Zn	0.02252	1.18144	0.55256	C	2.46525	4.61435	-0.29911
H	0.473562	5.744280	1.313699	O	-1.80881	1.93691	0.02715	C	3.74935	5.45820	-0.33660
H	0.138580	5.832468	-0.423094	C	-2.08595	3.15962	-0.65714	C	1.92862	-0.11469	-2.29050
H	-4.721631	2.021895	-0.638216	C	-3.58094	3.33474	-0.98517	C	3.28123	-0.82529	-2.46433
H	-4.658933	3.411258	-1.716745	C	-4.33506	2.11279	-1.53543	C	0.88820	-0.69563	-3.25479
H	-5.292007	1.452477	-3.013764	C	-3.59738	1.16798	-2.48125	C	1.24176	5.54064	-0.23222
H	-3.719398	2.027000	-3.538120	O	-2.30832	0.69192	-2.05505	O	-1.01114	-0.22115	-0.45542
H	-3.517733	-0.353656	-3.425420	C	-2.11537	0.35065	-0.75750	C	0.89406	-3.12421	3.95473
H	-4.362444	-0.450650	-1.871453	O	-3.27854	-0.10617	-0.22758	C	-1.19211	3.23873	5.17304
H	-4.547337	-0.373776	1.771290	C	-3.23118	-0.71095	1.05737	C	-1.21331	3.40371	-1.89081
H	-3.577314	1.119028	1.851181	C	0.34761	-2.14981	2.89936	H	3.71798	1.22904	2.74755
H	-2.778825	-0.473080	1.973331	C	-0.20523	-2.93143	1.69789	H	4.02270	-0.47729	-1.73839
H	-1.175385	-2.352170	1.105082	C	-1.45859	2.58804	3.80720	H	5.00913	1.18891	0.93633
H	-2.337472	4.100693	-2.705809	C	-2.71333	3.18560	3.15677	H	0.12972	-3.83778	4.28095

H	-1.83861	3.95123	0.06777
H	-0.60740	2.81825	3.15810
H	-3.50954	-1.29728	5.39811
H	2.47550	4.03287	0.62724
H	0.55574	-3.62018	1.31304
H	1.19030	-1.55712	2.53133
H	1.93147	-0.46798	4.62300
H	1.72297	-3.70595	3.53757
H	1.25898	-2.60528	4.84710
H	1.12429	1.02896	5.05795
H	2.87320	1.02462	4.73662
H	-1.07612	-3.53202	1.98693
H	-1.82529	-2.78003	4.36765
H	-0.27900	2.85290	5.63707
H	-3.31601	1.15395	5.14028
H	-2.01903	3.05660	5.86858
H	-1.08191	4.32358	5.06574
H	-2.60692	4.27143	3.05149
H	-3.60716	3.00210	3.76382
H	-2.87368	2.75529	2.16475
H	-0.08273	-0.21281	-3.12779
H	1.57621	-0.32019	-1.27578
H	0.75747	-1.76457	-3.05596
H	4.61368	2.86149	0.54441
H	1.19930	-0.59610	-4.30118
H	4.43571	1.61878	-0.69139
H	3.68980	-0.65177	-3.46658
H	3.16496	-1.90686	-2.33255
H	2.25348	1.29224	-4.57004
H	2.63157	3.71409	-4.87565
H	2.73386	5.20100	-2.90794
H	3.73742	6.17152	-1.16775
H	3.84905	6.03886	0.58692
H	4.64579	4.84100	-0.44984
H	0.31599	4.97741	-0.09304
H	1.33910	6.24150	0.60471
H	1.14060	6.12808	-1.15147
H	-4.11157	3.65812	-0.08207
H	-3.65151	4.17108	-1.69211
H	-4.71074	1.52557	-0.69824
H	-5.21787	2.46217	-2.08727
H	-3.38338	1.65711	-3.43686
H	-4.23676	0.29996	-2.68148
H	-4.24832	-1.05338	1.25546
H	-2.93444	0.01022	1.82214
H	-2.54573	-1.55843	1.06456
H	-0.49820	-2.26352	0.88347
H	-1.32381	4.44457	-2.21545
H	-0.15850	3.24214	-1.66400
H	-1.46823	2.75226	-2.72652
III$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$			

G = -2040.634075 kcal.mol^{-1}

C	-0.547346	-1.307044	3.451614
C	-0.650214	0.095614	3.261923
C	-1.736832	0.818818	3.814701
C	-2.704576	0.117438	4.540952
C	-2.617686	-1.257730	4.730473
C	-1.545023	-1.955042	4.189245
N	0.322331	0.778600	2.471382
Zn	-0.138222	1.517714	0.637703
O	-1.224726	-0.401893	-0.183447
C	-2.360212	-0.227183	-0.608799
O	-2.613927	0.555241	-1.640809
C	-3.953660	1.078585	-1.827645
C	-4.382670	2.014679	-0.707119
C	-3.716917	3.391232	-0.611060
C	-2.174326	3.421525	-0.458622
C	-1.478745	3.424774	-1.823924
C	-1.821630	2.333111	3.688281
C	-1.000302	3.019625	4.791064
C	0.591758	-2.146825	2.880064
C	0.126479	-3.016443	1.703014
N	1.728071	1.823784	-0.014454
C	2.770379	1.639188	0.801244
C	4.176991	1.854446	0.282563
C	1.961195	2.357322	-1.321114
C	2.230892	3.740482	-1.477235

C	2.375492	4.246497	-2.772554	H	2.155959	-3.502101	3.544012	H	2.568762	5.307282	-2.908960
C	2.275153	3.424980	-3.889142	H	1.548793	-2.448600	4.834534	H	3.531507	6.308982	-1.197049
C	2.030982	2.068064	-3.720290	H	0.591539	-3.826296	4.288256	H	3.732902	6.146173	0.546171
C	1.867496	1.509786	-2.448663	H	1.014884	0.498712	5.001785	H	4.511862	4.991495	-0.550778
C	2.350120	4.697090	-0.294577	H	2.568133	1.332478	4.770796	H	0.207543	4.971870	0.045040
C	3.604154	5.580040	-0.382659	H	-0.652208	-3.721472	2.018526	H	1.219522	6.266929	0.700638
C	1.648506	0.009797	-2.312231	H	-1.477291	-3.029520	4.339978	H	0.921508	6.170653	-1.043404
C	0.536288	-0.513954	-3.228633	H	0.053170	2.729638	4.752188	H	-4.160658	3.880137	0.265156
C	2.677198	1.278538	2.153442	H	-3.539165	0.660684	4.973046	H	-3.999536	4.005939	-1.476904
C	1.568937	0.889722	2.928057	H	-1.384930	2.761613	5.784955	H	-4.259517	1.490115	0.244153
C	1.901879	0.562431	4.371295	H	-1.050267	4.109124	4.683344	H	-5.463990	2.163989	-0.833426
C	2.955899	-0.758975	-2.562728	H	-3.245104	3.937683	3.441251	H	-3.893343	1.592505	-2.790028
C	1.099435	5.575051	-0.140933	H	-3.747846	2.767663	4.657876	H	-4.645496	0.236787	-1.920101
O	-3.444767	-0.838619	-0.141448	H	-3.866635	2.363687	2.931235	H	-4.276637	-1.987383	1.291159
C	-3.270407	-1.682113	1.005446	H	-0.401614	0.020525	-3.061081	H	-2.789945	-1.135259	1.816584
O	-1.763935	2.408430	0.411429	H	1.341235	-0.188185	-1.281038	H	-2.670052	-2.554590	0.742492
C	-3.255460	2.870111	3.683444	H	0.359977	-1.576938	-3.031372	H	-0.268319	-2.399398	0.892926
C	1.257918	-3.024646	3.950986	H	4.447394	2.914711	0.310810	H	-1.812233	4.280956	-2.423356
H	-1.954020	4.411564	-0.009863	H	0.800721	-0.420180	-4.288036	H	-0.396217	3.513911	-1.706767
H	-1.394632	2.607386	2.718698	H	4.896408	1.310635	0.897768	H	-1.669765	2.509467	-2.386961
H	-3.379863	-1.781069	5.301929	H	4.275606	1.528467	-0.754787				
H	3.623470	1.259169	2.683682	H	3.323012	-0.588283	-3.581326	TS(**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,re)}$→**IV**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S)}$)			
H	2.431447	4.100590	0.618868	H	3.745822	-0.454407	-1.869377	G = -2040.631665 kcal.mol^{-1}			
H	0.964085	-3.604786	1.311077	H	2.798809	-1.836420	-2.438776	C	-2.579990	0.229207	4.624948
H	1.352988	-1.468647	2.485366	H	1.968342	1.424665	-4.593821	C	-1.582730	0.903612	3.913008
H	2.435955	-0.390560	4.438765	H	2.392368	3.840892	-4.886265	C	-0.588447	0.143354	3.254466

C	-0.583051	-1.272183	3.349076	C	2.388097	4.799304	-0.306022	H	1.511847	-2.551359	4.609363
C	-1.604340	-1.893292	4.076323	C	3.644637	5.679128	-0.381204	H	1.112739	0.541656	4.989072
C	-2.602629	-1.157602	4.704725	C	1.577668	0.105992	-2.258324	H	2.770027	1.133478	4.725224
C	-1.558492	2.424963	3.938108	C	2.872758	-0.720098	-2.311476	H	-0.844839	-3.662180	1.869209
C	-2.878247	3.041126	3.461838	C	2.831992	1.706670	0.802501	H	-1.613493	-2.977780	4.152562
N	0.400151	0.806559	2.460640	C	4.230182	1.934225	0.269034	H	-0.217440	2.545692	5.670194
C	1.653154	0.884224	2.911121	C	2.755360	1.297001	2.142431	H	-3.344956	0.806260	5.137668
C	1.982805	0.484212	4.333879	C	1.134351	5.679856	-0.197199	H	-1.933925	2.649966	6.080876
C	0.486609	-2.148613	2.704802	C	0.564812	-0.421219	-3.280709	H	-1.118474	4.033553	5.337582
C	-0.067408	-2.966832	1.529588	C	-1.182909	2.939720	5.337053	H	-2.808763	4.134740	3.476196
Zn	-0.066854	1.655072	0.702400	C	1.150029	-3.086488	3.726168	H	-3.717983	2.759201	4.107169
O	-1.754404	2.325789	0.370876	C	-1.489624	3.337140	-1.862231	H	-3.087401	2.726554	2.437111
C	-2.130596	3.381740	-0.473217	O	-3.711039	-0.782106	-0.192520	H	-0.354556	0.168841	-3.270913
C	-3.675838	3.454768	-0.553635	C	-3.491037	-1.711401	0.872287	H	1.134443	-0.041428	-1.268655
C	-4.443706	2.131256	-0.613441	H	3.707891	1.250833	2.658802	H	0.299051	-1.454100	-3.035420
C	-4.192988	1.199356	-1.790794	H	3.573061	-0.432030	-1.521847	H	4.494175	2.995696	0.312919
O	-2.895278	0.563432	-1.752819	H	4.960016	1.383238	0.865033	H	0.968397	-0.421042	-4.299742
C	-2.611522	-0.295096	-0.781178	H	0.452831	-3.856128	4.075256	H	4.316988	1.627795	-0.775349
O	-1.473404	-0.627177	-0.515122	H	-1.824575	4.348000	-0.025776	H	3.380631	-0.589491	-3.274198
N	1.776382	1.930274	0.013159	H	-0.778094	2.755354	3.245654	H	2.652568	-1.786412	-2.188829
C	1.994692	2.451440	-1.302837	H	-3.385224	-1.662363	5.265059	H	1.965882	1.479365	-4.561887
C	2.281841	3.827429	-1.475893	H	2.450049	4.215000	0.617095	H	2.464124	3.876098	-4.883799
C	2.441003	4.313661	-2.777132	H	0.731459	-3.565643	1.076935	H	2.652014	5.369120	-2.927542
C	2.332653	3.477450	-3.881431	H	1.262657	-1.494196	2.297458	H	3.592374	6.391359	-1.211657
C	2.051155	2.129523	-3.696107	H	2.359926	-0.542629	4.369800	H	3.752033	6.263603	0.538908
C	1.869211	1.591415	-2.418473	H	2.000162	-3.603887	3.268378	H	4.555248	5.086496	-0.515322

H	0.232973	5.077790	-0.055220
H	1.219438	6.367950	0.651642
H	0.995217	6.278955	-1.104014
H	-4.040191	3.976378	0.340326
H	-3.953925	4.089041	-1.406731
H	-4.274139	1.573562	0.311274
H	-5.517418	2.364375	-0.635136
H	-4.184995	1.740691	-2.740816
H	-4.962292	0.423087	-1.837294
H	-4.483118	-1.957253	1.251317
H	-2.883650	-1.262622	1.659385
H	-2.995592	-2.609684	0.497107
H	-0.493049	-2.319940	0.759524
H	-1.800878	4.203286	-2.459065
H	-0.399456	3.371714	-1.786713
H	-1.754332	2.424054	-2.397998

IV$^{\alpha\delta}{}_{7CC\text{-}\gamma(S)}$

G = -2040.655918 kcal.mol^{-1}

C	-1.574805	1.395340	3.269258
C	-0.796338	0.360290	2.704962
C	-1.278564	-0.965362	2.653205
C	-2.539360	-1.235895	3.193378
C	-3.309704	-0.231823	3.767189
C	-2.827945	1.071955	3.797252
N	0.470636	0.674738	2.113761
C	1.571927	0.683573	2.861956
C	1.470324	0.327844	4.326107
C	-0.488908	-2.081474	1.986655
C	-0.346981	-3.324396	2.874650
C	-1.108238	2.843781	3.260207
C	-1.293623	3.547336	4.610327
C	2.853939	1.012610	2.375446
C	3.266901	1.371934	1.083717
C	4.736520	1.664734	0.895943
N	2.454886	1.464654	0.022260
Zn	0.545562	1.122981	0.192746
O	-1.008934	0.997336	-0.748376
C	-1.411526	1.616104	-1.942710
C	-2.854894	1.186960	-2.241660
C	-3.829021	1.545774	-1.122086
C	-5.232008	1.044735	-1.411962
O	-6.122547	1.290292	-0.301781
C	-6.696142	2.503922	-0.271899
O	-7.461834	2.666980	0.817202
C	-7.556659	1.606528	1.768836
C	2.986358	1.797813	-1.266435
C	3.431033	0.764617	-2.122686
C	3.841771	1.104126	-3.415034
C	3.826330	2.422136	-3.856628
C	3.405360	3.429543	-2.996810
C	2.984377	3.144380	-1.694231
C	3.453895	-0.693570	-1.685228
C	4.813942	-1.359412	-1.938235
C	2.523455	4.276951	-0.788274
C	3.562647	5.401857	-0.683474
C	-0.498127	1.280590	-3.119633
C	1.166911	4.833362	-1.244873
C	2.328374	-1.493303	-2.357989
C	-1.115075	-2.441625	0.629657
C	-1.814522	3.620711	2.137624
O	-6.574546	3.371181	-1.101270
H	-5.247803	-0.041833	-1.536330
H	1.017977	-0.660376	4.452639
H	2.450924	0.331325	4.803980
H	0.821009	1.034954	4.851758
H	5.276167	1.593180	1.841162
H	5.185218	0.965184	0.183832
H	4.883553	2.666686	0.481542
H	3.644662	0.981103	3.115111
H	-3.438563	1.856619	4.235853
H	-4.285209	-0.464052	4.186212
H	-2.925130	-2.251381	3.158650
H	4.175203	0.319355	-4.088935
H	4.144453	2.663477	-4.867118
H	3.399169	4.459745	-3.343170
H	4.821914	-2.372569	-1.522226
H	5.032949	-1.445423	-3.007941

H	5.633950	-0.798829	-1.477870
H	2.339029	-2.535101	-2.018693
H	1.345012	-1.071677	-2.130712
H	2.444584	-1.493273	-3.447575
H	0.295586	-4.066249	2.388078
H	0.094439	-3.081097	3.846747
H	-1.313668	-3.804976	3.060279
H	-2.122833	-2.851144	0.764835
H	-1.197421	-1.561007	-0.015326
H	-0.512967	-3.199330	0.114965
H	-0.853647	4.549825	4.576882
H	-2.351362	3.668555	4.867013
H	-0.815118	2.995388	5.426011
H	-1.433027	4.646031	2.073301
H	-1.673694	3.133577	1.167644
H	-2.893173	3.674946	2.322592
H	3.236212	6.152486	0.044300
H	4.538870	5.023489	-0.363652
H	3.704444	5.915617	-1.640316
H	0.823306	5.623629	-0.568447
H	1.234478	5.259147	-2.252076
H	0.400808	4.052065	-1.269732
H	-6.575143	1.350956	2.176533
H	-8.203524	1.986732	2.560710
H	-8.001449	0.712619	1.323014
H	3.273548	-0.720283	-0.605706
H	0.520483	-1.703107	1.794008
H	2.388318	3.863367	0.216456
H	-0.036292	2.847186	3.037261
H	-1.419968	2.717256	-1.823089
H	-3.177161	1.649079	-3.185095
H	-2.854460	0.099008	-2.400869
H	-3.468174	1.111423	-0.184848
H	-3.865955	2.634402	-0.993726
H	-5.651812	1.517782	-2.304486
H	-0.826413	1.784324	-4.036378
H	0.533041	1.590352	-2.919146
H	-0.501007	0.200162	-3.302663

$I_{7CC\text{-}\gamma(S,si)}$

G = -2040.632608 kcal.mol^{-1}

C	1.831032	3.185359	-1.658391
C	2.008074	1.834914	-1.269697
C	2.437304	0.865012	-2.203101
C	2.682961	1.266119	-3.520326
C	2.527087	2.589701	-3.913103
C	2.107786	3.535826	-2.983623
N	1.702539	1.447944	0.072898
Zn	-0.116632	0.736882	0.508911
O	-1.233561	-0.168594	-0.710929
C	-1.726476	-1.453245	-0.474878
C	2.638218	-0.593805	-1.819588
C	1.565720	-1.486940	-2.459347
C	1.386829	4.255600	-0.668889
C	0.357139	5.226411	-1.261280
C	2.653691	1.469220	1.004999
C	4.085068	1.788133	0.625734
C	2.450553	1.155775	2.361244
C	1.321581	0.656954	3.034678
C	1.491267	0.509324	4.533504
N	0.160251	0.344570	2.455043
C	-0.868893	-0.292827	3.221559
C	-1.827152	0.472755	3.923526
C	-2.823736	-0.198806	4.641045
C	-2.885340	-1.584550	4.674512
C	-1.943729	-2.328344	3.971703
C	-0.930352	-1.710628	3.233610
C	-1.810605	1.994489	3.945608
C	-3.104680	2.585371	3.369458
C	0.089805	-2.561143	2.485207
C	-0.489813	-3.876872	1.951374
C	1.327988	-2.865732	3.344728
C	-1.576465	2.540071	5.363548
O	-1.467558	2.479807	0.352924
C	-2.304604	2.519912	-0.538260
O	-1.957843	2.705570	-1.804282
C	-2.546340	2.036144	-2.981127
C	-3.651356	1.062663	-2.604755

C	-4.925741	1.744196	-2.102878
C	-4.584573	2.895204	-1.173334
O	-3.596238	2.499761	-0.205025
C	4.047450	-1.094777	-2.165630
C	2.582507	5.049670	-0.118116
H	0.825858	-0.240561	4.961909
H	2.524378	0.256018	4.782272
H	1.265621	1.467339	5.014872
H	4.614078	2.252349	1.461112
H	4.607571	0.854541	0.385238
H	4.156927	2.433626	-0.249790
H	3.322292	1.296870	2.990656
H	-3.563260	0.381541	5.186972
H	-3.665019	-2.085801	5.242007
H	-2.000695	-3.412425	3.994966
H	3.010074	0.527360	-4.247997
H	2.734248	2.884876	-4.938530
H	1.991178	4.570503	-3.294306
H	4.191323	-2.114670	-1.792064
H	4.213489	-1.118166	-3.248262
H	4.823788	-0.459772	-1.726954
H	1.709674	-2.532692	-2.163457
H	0.566236	-1.170609	-2.146466
H	1.617326	-1.441285	-3.553506
H	2.027062	-3.504066	2.792470
H	1.864316	-1.958859	3.630640
H	1.042031	-3.394776	4.261168
H	-0.684730	-4.593644	2.757112
H	-1.422861	-3.720730	1.403672
H	0.227459	-4.349655	1.272220
H	-1.478129	3.631206	5.341488
H	-2.417786	2.299433	6.023483
H	-0.673707	2.127801	5.822857
H	-3.045382	3.679574	3.354839
H	-3.277478	2.245101	2.347548
H	-3.973315	2.310621	3.979290
H	2.239964	5.818448	0.583888
H	3.294003	4.411878	0.411563
H	3.122330	5.552688	-0.929065
H	-0.037292	5.875572	-0.471829
H	0.801341	5.880474	-2.020559
H	-0.478864	4.690831	-1.715961
H	-2.529948	-1.691256	-1.195526
H	-0.962028	-2.240643	-0.599849
H	-2.161431	-1.580337	0.530583
H	2.518815	-0.668579	-0.733872
H	0.428238	-1.972797	1.623999
H	0.908230	3.740199	0.169255
H	-0.985014	2.327293	3.309143
C	-1.383227	1.359743	-3.677642
H	-2.939969	2.858876	-3.592064
H	-3.875042	0.450586	-3.484888
H	-3.236026	0.388615	-1.847454
H	-5.513565	2.145968	-2.937856
H	-5.558366	1.015327	-1.585760
H	-4.206332	3.761006	-1.727025
H	-5.441314	3.217153	-0.577952
H	-0.576311	2.071174	-3.866659
H	-1.007030	0.558441	-3.036165
H	-1.716742	0.943348	-4.634122

TS($\mathbf{I}_{7CC\text{-}\gamma(S,si)} \rightarrow \mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)}$)

G = -2040.620686 kcal.mol^{-1}

C	1.892719	3.231482	-1.587090
C	2.092104	1.888342	-1.190269
C	2.533402	0.918871	-2.118879
C	2.767399	1.315207	-3.439395
C	2.585197	2.633071	-3.841185
C	2.154420	3.576828	-2.916567
N	1.787053	1.495118	0.151897
Zn	-0.021519	0.800015	0.580209
O	-1.117727	-0.094203	-0.746303
C	-1.812458	-1.283518	-0.487542
C	2.746289	-0.536703	-1.730044
C	1.691412	-1.441308	-2.384010
C	1.423768	4.309242	-0.618666
C	0.153684	5.013398	-1.114694
C	2.720937	1.551761	1.099500

C	4.130075	1.966158	0.738642	C	2.528610	5.340408	-0.339526	H	-1.451368	3.663282	5.431851
C	2.510359	1.207460	2.448552	H	0.910655	-0.314784	4.981538	H	-2.522792	2.379171	5.996037
C	1.383001	0.675415	3.099326	H	2.568581	0.321909	4.867868	H	-0.776482	2.124521	5.995958
C	1.525744	0.499467	4.596524	H	1.205966	1.417931	5.101443	H	-2.809592	3.767699	3.292881
N	0.232007	0.358167	2.499814	H	4.671408	2.320260	1.617968	H	-2.903343	2.358954	2.222650
C	-0.820471	-0.261406	3.247338	H	4.673316	1.102940	0.336434	H	-3.829047	2.391249	3.742250
C	-1.755656	0.524460	3.957076	H	4.146799	2.738715	-0.031322	H	2.177710	6.091361	0.377291
C	-2.788168	-0.124586	4.643177	H	3.367777	1.365101	3.092942	H	3.429128	4.878445	0.075967
C	-2.902686	-1.507633	4.640813	H	-3.514777	0.470346	5.190728	H	2.818924	5.866726	-1.256120
C	-1.980253	-2.270742	3.933091	H	-3.709653	-1.991937	5.184258	H	-0.201861	5.723060	-0.359061
C	-0.934556	-1.674701	3.222543	H	-2.079421	-3.351936	3.929479	H	0.340488	5.581056	-2.033863
C	-1.688116	2.044271	3.999483	H	3.103756	0.576877	-4.163377	H	-0.640270	4.290071	-1.308354
C	-2.882214	2.674286	3.267884	H	2.779782	2.923801	-4.870276	H	-2.630199	-1.411362	-1.213123
C	0.062822	-2.540141	2.461155	H	2.014718	4.607670	-3.232493	H	-1.149114	-2.156582	-0.588628
C	-0.551461	-3.830663	1.905878	H	4.313345	-2.043740	-1.686650	H	-2.265412	-1.313145	0.514753
C	1.293333	-2.887603	3.315343	H	4.345612	-1.040189	-3.138420	H	2.614696	-0.611095	-0.645622
C	-1.601151	2.578038	5.437557	H	4.929268	-0.383580	-1.606521	H	0.417627	-1.947330	1.609248
O	-1.549000	2.204268	0.157897	H	1.823427	-2.481182	-2.062459	H	1.175542	3.818001	0.326841
C	-2.155289	1.691903	-0.803811	H	0.682207	-1.115371	-2.114800	H	-0.781378	2.354153	3.470314
O	-1.849892	2.137788	-2.025123	H	1.780216	-1.419436	-3.476588	C	-1.929669	0.426253	-3.774655
C	-2.511310	1.725128	-3.250053	H	1.976727	-3.534588	2.753808	H	-2.209038	2.541597	-3.914483
C	-4.048233	1.725499	-3.176397	H	1.851593	-1.997667	3.613441	H	-4.418929	2.009010	-4.167890
C	-4.587095	2.682112	-2.113129	H	0.994694	-3.422396	4.224271	H	-4.416050	0.712270	-2.979089
C	-4.480405	2.030152	-0.732125	H	-0.766009	-4.555122	2.699631	H	-4.029936	3.625168	-2.142075
O	-3.377238	1.109746	-0.658017	H	-1.480782	-3.640583	1.362067	H	-5.636813	2.929913	-2.306553
C	4.164594	-1.023749	-2.058077	H	0.152543	-4.311592	1.218680	H	-4.397860	2.769238	0.073349

H	-5.350972	1.400219	-0.533887
H	-0.841988	0.491787	-3.842894
H	-2.183613	-0.409831	-3.121106
H	-2.334684	0.229126	-4.773526

II$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)}$

G = -2040.641216 kcal.mol^{-1}

C	-1.622971	0.415470	3.979644
C	-0.556996	-0.292309	3.384005
C	-0.472519	-1.699722	3.489773
C	-1.459349	-2.372338	4.216983
C	-2.505539	-1.686155	4.824281
C	-2.582221	-0.304740	4.698847
N	0.427869	0.418638	2.621180
C	1.602729	0.720860	3.191329
C	1.814825	0.383135	4.649457
C	0.624635	-2.500438	2.801099
C	1.303572	-3.511073	3.735672
C	-1.762675	1.925672	3.861931
C	-1.665028	2.618070	5.229290
C	2.689544	1.319064	2.533483
C	2.842677	1.703747	1.187150
C	4.194331	2.241012	0.781000
N	1.875831	1.616840	0.276081
Zn	0.086358	0.923601	0.772087
O	-2.306588	-0.433133	-1.665401
C	-2.261517	0.159171	-2.962408
C	-3.369982	1.189694	-3.211573
C	-3.179036	2.496150	-2.436787
C	-3.587541	2.397112	-0.964732
H	-4.653852	2.622544	-0.853870
C	2.116176	2.030057	-1.073756
C	2.506398	1.070618	-2.033205
C	2.663794	1.481279	-3.360545
C	2.445526	2.800289	-3.739056
C	2.061367	3.733662	-2.783284
C	1.890036	3.374759	-1.443436
C	2.729834	-0.389681	-1.668901
C	4.107921	-0.899864	-2.111558
C	1.429001	4.419874	-0.437954
C	2.278001	5.697463	-0.475625
O	-1.172592	1.245833	-0.571148
C	-2.232151	0.426789	-0.549729
O	-3.464482	1.099303	-0.401487
O	-2.103655	-0.426933	0.564055
C	-3.176993	-1.331659	0.804127
C	-0.058187	4.745907	-0.643524
C	1.611279	-1.273965	-2.240809
C	0.075662	-3.206782	1.551536
C	-3.064262	2.313693	3.145308
H	1.928556	-0.697451	4.784092
H	2.712266	0.870253	5.033755
H	0.956272	0.685281	5.254454
H	4.883908	2.259199	1.626063
H	4.628355	1.626366	-0.013836
H	4.105566	3.253567	0.376251
H	3.560784	1.483829	3.155776
H	-3.405149	0.229684	5.166503
H	-3.260109	-2.227609	5.388513
H	-1.408234	-3.454285	4.306160
H	2.959535	0.752233	-4.110695
H	2.571974	3.100043	-4.775912
H	1.884698	4.763080	-3.084299
H	4.263228	-1.927012	-1.763748
H	4.206837	-0.906552	-3.202431
H	4.917532	-0.281612	-1.710298
H	1.748981	-2.317303	-1.935331
H	0.623748	-0.945083	-1.903285
H	1.613649	-1.244141	-3.336401
H	2.152067	-3.983688	3.229239
H	1.676940	-3.037843	4.649681
H	0.619649	-4.312370	4.035623
H	-0.685735	-3.945581	1.827061
H	-0.385639	-2.494970	0.861250
H	0.876886	-3.734737	1.022139
H	-1.726622	3.705662	5.112414
H	-2.481675	2.310268	5.891655
H	-0.722557	2.387818	5.736513

H	-3.110602	3.399333	3.002782				C	1.187051	4.048598	-2.794732
H	-3.143107	1.832016	2.166633	TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)} \rightarrow \mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(S,si)}$)			C	1.192889	3.555088	-1.486603
H	-3.942040	2.023387	3.733890	G = -2040.627973 kcal.mol^{-1}			C	2.151812	-0.126196	-2.201204
H	1.969984	6.380570	0.323395	C	-1.149307	0.641137	4.325217	C	0.989242	-0.999008	-2.699668
H	3.343721	5.483323	-0.343837	C	-0.322000	-0.186581	3.535108	C	0.828344	4.467702	-0.319614
H	2.163771	6.234483	-1.423406	C	-0.434163	-1.593533	3.593819	C	2.061591	5.108615	0.338794
H	-0.410403	5.448731	0.120403	C	-1.373019	-2.148276	4.468286	C	2.806339	1.218542	2.081067
H	-0.222434	5.207318	-1.624080	C	-2.183391	-1.347266	5.264415	C	1.847900	0.661587	2.950846
H	-0.668243	3.839166	-0.594457	C	-2.069392	0.035289	5.186216	C	2.309631	0.320261	4.347262
H	-3.287208	-2.029770	-0.031227	N	0.587651	0.410848	2.602829	C	-0.165477	5.571580	-0.701833
H	-2.917952	-1.872707	1.714978	Zn	-0.030357	0.797044	0.776553	C	3.464965	-0.532867	-2.884865
H	-4.112497	-0.785263	0.952965	O	-1.601309	-0.015001	0.275671	O	-3.054478	1.729829	0.083374
H	2.688419	-0.469120	-0.577602	C	-2.573167	0.495915	-0.492625	C	-2.833057	2.917802	-0.655476
H	1.392885	-1.796837	2.465850	O	-3.656187	-0.389729	-0.568265	C	-3.867125	3.128664	-1.764166
H	1.532978	3.988012	0.562741	C	-4.250891	-0.713454	0.677841	C	-4.196973	1.825719	-2.495285
H	-0.927123	2.288252	3.253880	C	0.398319	-2.510298	2.709356	C	-2.973732	0.997424	-2.887037
C	-2.347068	-1.007400	-3.936217	C	-0.471008	-3.142318	1.610194	H	-2.336927	1.604901	-3.544624
H	-1.290455	0.663569	-3.079409	C	-1.094220	2.159514	4.239372	O	-2.087609	0.698615	-1.784601
H	-3.366604	1.413739	-4.285904	C	-0.844470	2.814084	5.605001	C	1.136163	-3.591695	3.510989
H	-4.341545	0.733508	-2.982401	N	1.546539	1.670143	0.046364	C	-2.371916	2.716667	3.592003
H	-2.127838	2.793473	-2.509755	C	2.687256	1.654840	0.751263	H	-2.883087	3.733602	0.073894
H	-3.767808	3.298579	-2.899818	C	3.974304	2.083556	0.082114	H	-0.252785	2.424922	3.590828
H	-3.027428	3.127552	-0.366862	C	1.542112	2.196953	-1.287888	H	-2.906143	-1.799473	5.938231
H	-2.226370	-0.660903	-4.967322	C	1.835532	1.351545	-2.379455	H	3.801101	1.311199	2.500419
H	-1.564378	-1.740118	-3.722318	C	1.802568	1.895607	-3.667629	H	0.346763	3.837605	0.439355
H	-3.316389	-1.509399	-3.849151	C	1.492815	3.232410	-3.878614	H	0.141109	-3.764728	0.947123

H	1.158037	-1.895986	2.214815	H	2.022290	1.256566	-4.518913	C	-0.533015	-0.186854	3.345553
H	2.241304	-0.757832	4.523532	H	1.479148	3.638144	-4.886624	C	-0.517712	-1.601169	3.385089
H	1.785550	-4.176176	2.850278	H	0.929752	5.088241	-2.971919	C	-1.490597	-2.255423	4.146717
H	1.758849	-3.160847	4.302073	H	2.641694	5.676083	-0.397787	C	-2.447184	-1.547231	4.865072
H	0.439469	-4.291988	3.984626	H	1.750975	5.802890	1.127555	C	-2.437360	-0.157956	4.833670
H	1.668779	0.797527	5.094296	H	2.720782	4.367780	0.795494	N	0.385477	0.502987	2.491354
H	3.340492	0.636876	4.511696	H	-1.025690	5.179274	-1.250665	Zn	-0.103820	0.823102	0.607334
H	-1.243993	-3.784360	2.048154	H	-0.535360	6.066320	0.202185	O	-1.189620	-0.405313	-0.410109
H	-1.474062	-3.229157	4.520427	H	0.303756	6.346034	-1.318996	C	-2.272168	0.288798	-0.687912
H	0.070825	2.439256	6.074551	H	-4.792043	3.538344	-1.341014	O	-3.472245	-0.292163	-0.310690
H	-2.712548	0.660982	5.799757	H	-3.479065	3.881880	-2.463488	C	-3.482688	-0.938136	0.953096
H	-1.671466	2.628290	6.298760	H	-4.841720	1.207965	-1.864583	C	0.512239	-2.426301	2.625019
H	-0.746869	3.899749	5.495394	H	-4.759453	2.045674	-3.410898	C	-0.120246	-3.167519	1.437337
H	-2.305184	3.806232	3.489868	C	-3.350270	-0.285498	-3.617963	C	-1.525302	2.068339	4.081187
H	-3.250736	2.496080	4.208670	H	-5.027889	-1.450517	0.461029	C	-1.322458	2.645431	5.490074
H	-2.547004	2.285485	2.601362	H	-4.706213	0.168837	1.141766	N	1.539128	1.737154	-0.023908
H	0.047878	-0.739001	-2.207919	H	-3.518007	-1.145657	1.365766	C	2.607860	1.770113	0.775739
H	2.269911	-0.314849	-1.128845	H	-0.970380	-2.378434	1.006666	C	3.959243	2.167331	0.219848
H	1.199808	-2.058421	-2.514485	H	-1.823442	2.912866	-1.084735	C	1.647518	2.190213	-1.380410
H	4.375246	1.245791	-0.499894	H	-3.886430	-0.053676	-4.545271	C	1.966394	1.275740	-2.408530
H	0.846829	-0.871794	-3.779124	H	-2.450198	-0.851150	-3.873929	C	2.047727	1.752185	-3.721177
H	3.827522	2.912128	-0.611932	H	-3.983821	-0.911822	-2.986486	C	1.826533	3.088939	-4.022151
H	4.724240	2.363655	0.824027					C	1.497521	3.975932	-3.003031
H	3.394888	-0.450107	-3.974824	$\mathbf{II}^{\delta\alpha}{}_{7CC\text{-}\gamma(S,si)}$				C	1.390250	3.552902	-1.674801
H	4.306171	0.088659	-2.561319	G = -2040.631466 kcal.mol^{-1}				C	2.228551	-0.199928	-2.145564
H	3.704820	-1.576289	-2.653587	C	-1.491797	0.546514	4.081088	C	1.180970	-1.089045	-2.832032

C	1.015864	4.556719	-0.588716
C	2.243031	5.269268	0.003285
C	2.609502	1.398266	2.134288
C	1.606817	0.816081	2.928090
C	1.977981	0.500907	4.358535
C	0.009478	5.611755	-1.068733
C	3.647416	-0.609074	-2.570671
O	-2.101610	1.589986	0.151254
C	-2.250002	2.826739	-0.548166
C	-3.682456	3.153791	-0.956358
C	-4.417623	2.014496	-1.674283
C	-3.552579	1.171894	-2.613254
H	-3.158636	1.823881	-3.404727
O	-2.342301	0.649626	-2.016388
C	1.252922	-3.411157	3.541869
C	-2.824512	2.604404	3.462215
H	-1.880102	3.594676	0.138482
H	-0.694690	2.414973	3.457853
H	-3.193879	-2.076322	5.451129
H	3.558896	1.541368	2.637150
H	0.546919	3.989024	0.223734
H	0.641857	-3.741418	0.897645
H	1.257391	-1.735174	2.218192
H	2.020472	-0.581615	4.515900
H	2.052753	-3.914958	2.988340
H	1.703055	-2.909883	4.405053
H	0.583791	-4.188979	3.925899
H	1.227088	0.887056	5.052865
H	2.949401	0.925305	4.615862
H	-0.884072	-3.875607	1.780233
H	-1.497055	-3.342001	4.176939
H	-0.394880	2.288544	5.948676
H	-3.181051	0.394485	5.402544
H	-2.146796	2.371825	6.157873
H	-1.279136	3.739537	5.451956
H	-2.813208	3.700416	3.440890
H	-3.699425	2.296510	4.046163
H	-2.952098	2.240171	2.439128
H	0.171978	-0.849372	-2.488506
H	2.146727	-0.366938	-1.066557
H	1.377064	-2.143643	-2.607163
H	4.487729	1.263008	-0.103393
H	1.217649	-0.971650	-3.921229
H	3.884592	2.828125	-0.643614
H	4.570911	2.644265	0.989014
H	3.778884	-0.523992	-3.655149
H	4.414227	0.012434	-2.097475
H	3.839840	-1.652519	-2.298263
H	2.292099	1.057176	-4.520346
H	1.902186	3.439681	-5.047900
H	1.313927	5.018269	-3.245989
H	2.806945	5.785071	-0.782173
H	1.929448	6.018581	0.738953
H	2.920524	4.577355	0.507052
H	-0.838504	5.164266	-1.594497
H	-0.376589	6.176442	-0.213329
H	0.474210	6.338344	-1.744301
H	-4.262688	3.449032	-0.074416
H	-3.626606	4.040172	-1.603003
H	-4.869932	1.350326	-0.936273
H	-5.237591	2.430396	-2.272401
C	-4.336615	0.037167	-3.260317
H	-4.509577	-1.278233	1.103874
H	-3.210205	-0.252832	1.762037
H	-2.806293	-1.795566	0.965418
H	-0.585918	-2.472199	0.732855
H	-1.599129	2.820813	-1.430365
H	-5.165827	0.434894	-3.855788
H	-3.683973	-0.540674	-3.920307
H	-4.737820	-0.632756	-2.496500

TS($\mathbf{II}^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)} \rightarrow \mathbf{III}^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)}$)

G = -2040.625136 kcal.mol^{-1}

C	-1.543217	0.368814	4.070165
C	-0.645372	-0.387949	3.282388
C	-0.703425	-1.798973	3.275394
C	-1.656715	-2.433717	4.077573
C	-2.528795	-1.704387	4.876205

C	-2.466513	-0.315890	4.865848	C	3.866548	-0.493188	-1.481446	H	4.597877	-0.137560	-2.216167
N	0.313618	0.291016	2.459580	C	1.197923	4.507413	-0.498487	H	4.060310	0.011903	-0.533563
C	1.538138	0.509496	2.936343	C	2.132545	5.726643	-0.516626	H	2.191267	-2.234385	-2.835695
C	1.917084	-0.014034	4.304550	O	-1.850108	2.063398	0.516029	H	1.190183	-1.012262	-3.633669
C	0.209795	-2.645174	2.400877	C	-2.638743	1.136595	0.088514	H	2.930030	-1.089403	-3.949120
C	0.961033	-3.723736	3.193788	O	-3.601578	1.435081	-0.824424	H	1.673361	-4.245957	2.545601
C	-1.522775	1.890898	4.094000	O	-3.159655	0.355121	1.079411	H	1.517759	-3.299035	4.035085
C	-0.906709	2.426510	5.396195	C	-4.068351	-0.670069	0.709425	H	0.277803	-4.477549	3.600283
C	2.562138	1.185914	2.242943	C	-0.266537	4.952008	-0.621145	H	-1.346109	-3.967672	1.630613
C	2.602854	1.706316	0.940547	C	2.164945	-1.192785	-3.171428	H	-1.093712	-2.508329	0.661850
C	3.878127	2.432923	0.567999	C	-0.585210	-3.276895	1.249539	H	0.076907	-3.844109	0.584533
N	1.601716	1.632996	0.055930	C	-2.916278	2.492659	3.873231	H	-0.895021	3.522290	5.391029
Zn	-0.176790	0.989685	0.659204	H	2.167718	-1.078646	4.237127	H	-1.487883	2.103575	6.267787
O	-1.536756	0.053250	-0.629684	H	2.791773	0.511124	4.692383	H	0.122538	2.083163	5.537469
C	-1.371760	-0.235015	-2.027624	H	1.097382	0.073507	5.019404	H	-2.842007	3.581829	3.781970
C	-2.222317	0.600618	-2.995641	H	4.715409	2.087844	1.177691	H	-3.365553	2.100809	2.959026
C	-2.197435	2.103956	-2.712948	H	4.131393	2.316681	-0.486863	H	-3.588293	2.282076	4.713315
C	-3.309711	2.489431	-1.741703	H	3.752125	3.505732	0.753153	H	1.922146	6.375859	0.340035
H	-4.253877	2.631261	-2.275710	H	3.477754	1.316090	2.807754	H	3.187187	5.436645	-0.473782
C	1.790915	2.125585	-1.273806	H	-3.154153	0.253150	5.485909	H	1.993549	6.328582	-1.421212
C	2.160839	1.211639	-2.293857	H	-3.256062	-2.215243	5.501870	H	-0.502809	5.700469	0.143784
C	2.291046	1.692693	-3.599761	H	-1.712769	-3.519401	4.077150	H	-0.458223	5.404110	-1.601300
C	2.057586	3.029522	-3.906192	H	2.574774	1.009567	-4.394370	H	-0.945552	4.106580	-0.483563
C	1.698268	3.912641	-2.897081	H	2.158829	3.379987	-4.929845	H	-3.607635	-1.346937	-0.017335
C	1.566973	3.489323	-1.569423	H	1.519557	4.956977	-3.139624	H	-4.288615	-1.215944	1.627805
C	2.432442	-0.258083	-1.985313	H	4.041307	-1.563605	-1.325102	H	-4.989772	-0.253307	0.291994

H	1.754743	-0.544537	-1.170763
H	0.956714	-1.979510	1.956319
H	1.306859	4.019988	0.475520
H	-0.893969	2.223822	3.263291
C	-1.594597	-1.724029	-2.270487
H	-0.326336	0.004490	-2.262537
H	-1.814882	0.403179	-3.994388
H	-3.256311	0.235172	-3.004958
H	-1.219695	2.389580	-2.311614
H	-2.331012	2.676152	-3.638645
H	-3.077212	3.404493	-1.188895
H	-1.405829	-1.980978	-3.319116
H	-0.928923	-2.326516	-1.647902
H	-2.627983	-2.002666	-2.037316

TS(**II**$^{6\alpha}{}_{7CC\text{-}\gamma(S,si)}$→**III**$^{6\alpha}{}_{7CC\text{-}\gamma(S,si)}$)

G = -2040.630014 kcal.mol^{-1}

C	1.576721	3.623764	-1.613848
C	1.763602	2.248105	-1.325887
C	2.042280	1.325985	-2.359690
C	2.151313	1.806311	-3.669020
C	1.994278	3.153629	-3.963173
C	1.706833	4.049181	-2.939198
N	1.627787	1.793889	0.027698
C	2.698328	1.747927	0.823214
C	2.684278	1.352566	2.175116
C	1.660773	0.795686	2.960141
C	2.039385	0.413007	4.373143
C	2.242464	-0.161476	-2.106994
C	3.659490	-0.613945	-2.493201
C	1.259032	4.640282	-0.522429
C	0.293597	5.738497	-0.988787
Zn	-0.097804	1.040509	0.678949
O	-1.101696	-0.312521	-0.407876
C	-2.174657	0.313285	-0.722744
O	-3.375167	-0.175126	-0.320367
C	-3.394020	-0.859670	0.928710
N	0.422206	0.557927	2.527302
C	-0.519297	-0.123840	3.360037
C	-1.479802	0.621624	4.082090
C	-2.452476	-0.070490	4.811341
C	-2.488017	-1.459601	4.833454
C	-1.528358	-2.180117	4.131389
C	-0.528303	-1.538856	3.393929
C	-1.474919	2.143446	4.105596
C	-2.773690	2.727892	3.533125
C	0.504733	-2.380016	2.655209
C	1.201034	-3.383706	3.586664
O	-1.943706	1.795849	0.289613
C	-2.025732	3.018438	-0.418178
C	-3.447024	3.392637	-0.831536
C	-4.226963	2.269617	-1.527291
C	-3.430398	1.426855	-2.523361
O	-2.231753	0.813069	-1.977112
H	-1.624297	3.809887	0.228618
C	-0.109065	-3.105868	1.448796
C	-1.211308	2.684752	5.518999
C	4.070948	2.082268	0.276363
C	1.192067	-1.007150	-2.841535
C	2.525871	5.294644	0.052938
H	-0.652833	2.477943	3.464870
H	-3.255175	-1.978965	5.401601
H	3.641564	1.438516	2.676812
H	0.776172	4.092877	0.295368
H	0.654133	-3.700489	0.933632
H	1.271667	-1.701834	2.268288
H	2.227031	-0.664095	4.440216
H	2.013766	-3.892072	3.056518
H	1.624562	-2.897490	4.471475
H	0.509156	-4.157089	3.937978
H	1.235580	0.639085	5.077259
H	2.946525	0.932562	4.686590
H	-0.902060	-3.793027	1.767460
H	-1.553301	-3.266631	4.156777
H	-0.273905	2.301746	5.934752
H	-3.195096	0.492090	5.371554
H	-2.016382	2.408992	6.209276
H	-1.149604	3.778616	5.503999

H	-2.732934	3.823319	3.541916
H	-3.644430	2.428062	4.127513
H	-2.925170	2.397369	2.501775
H	0.181307	-0.734310	-2.531768
H	2.115886	-0.338392	-1.034133
H	1.342098	-2.069773	-2.619419
H	4.033541	2.728066	-0.600590
H	1.272203	-0.883089	-3.927661
H	4.688379	2.552653	1.045336
H	4.571849	1.153052	-0.017964
H	3.826555	-0.518691	-3.572029
H	4.431948	-0.025094	-1.989169
H	3.808530	-1.666860	-2.229691
H	2.366734	1.105535	-4.471539
H	2.089726	3.506280	-4.986667
H	1.576095	5.101099	-3.175438
H	3.096609	5.794000	-0.738256
H	2.257957	6.048906	0.801453
H	3.182372	4.568270	0.535783
H	-0.581688	5.326384	-1.498260
H	-0.053224	6.321515	-0.128830
H	0.779035	6.441999	-1.674139
H	-4.017178	3.717299	0.047005
H	-3.369432	4.266512	-1.493249
H	-4.662924	1.605571	-0.779497
H	-5.065961	2.705461	-2.084172
H	-3.008941	2.090840	-3.288470
C	-4.281253	0.366395	-3.210001
H	-4.430784	-1.165336	1.078417
H	-3.085723	-0.199057	1.742896
H	-2.745546	-1.736861	0.902958
H	-0.530636	-2.397661	0.730263
H	-1.388215	2.978480	-1.314050
H	-5.078637	0.841050	-3.791657
H	-3.666354	-0.227415	-3.891766
H	-4.734631	-0.303961	-2.476159

III$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)}$

G = -2040.638429 kcal.mol^{-1}

C	2.212694	1.290212	-2.322312
C	1.766788	2.158943	-1.292036
C	1.490050	3.518101	-1.565197
C	1.647511	3.980804	-2.877135
C	2.077942	3.141399	-3.894682
C	2.361460	1.809311	-3.611080
N	1.558038	1.620796	0.018159
Zn	-0.156747	0.692025	0.465074
O	-1.302643	-0.298320	-0.660665
C	-1.178345	-0.475084	-2.047573
C	-1.250491	-1.962515	-2.396165
C	1.057799	4.505253	-0.488553
C	-0.362987	5.034075	-0.729027
C	2.551742	-0.170741	-2.041767
C	2.383547	-1.084398	-3.261795
C	2.516356	1.725200	0.942129
C	3.774958	2.516251	0.649699
C	2.456936	1.164804	2.228822
C	1.428950	0.462523	2.883893
C	1.797096	-0.105494	4.238919
N	0.215078	0.240166	2.377998
C	-0.765295	-0.406086	3.200106
C	-0.876163	-1.813024	3.198474
C	-1.852600	-2.408316	4.004876
C	-2.692023	-1.644142	4.804798
C	-2.577585	-0.257363	4.790419
C	-1.632885	0.389157	3.988681
C	0.013059	-2.697998	2.338316
C	-0.789207	-3.312978	1.182925
C	-1.554468	1.911376	3.978288
C	-2.927635	2.583480	4.102972
C	-0.618708	2.453515	5.070905
C	0.720357	-3.789905	3.154038
C	-2.261641	0.301403	-2.819745
C	-2.205495	1.819460	-2.574073
C	-3.385478	2.376292	-1.791851
O	-3.746639	1.569384	-0.648351
C	-2.894601	1.515459	0.361548
O	-1.897407	2.220393	0.496305

O	-3.258316	0.671375	1.311254
C	-4.222216	-0.347624	1.014817
C	2.043590	5.678862	-0.372000
C	3.975562	-0.337042	-1.485036
H	-4.298434	2.363608	-2.392490
H	2.095012	-1.153617	4.118930
H	2.642410	0.433129	4.671452
H	0.963387	-0.090172	4.941732
H	4.630346	2.086658	1.176159
H	4.000701	2.569803	-0.415741
H	3.649741	3.541708	1.014732
H	3.357679	1.297614	2.817060
H	-3.243948	0.336316	5.409287
H	-3.435194	-2.124783	5.435932
H	-1.948571	-3.491149	4.008535
H	2.701976	1.159288	-4.410861
H	2.197283	3.521546	-4.905764
H	1.433785	5.023480	-3.098552
H	4.200289	-1.398686	-1.332773
H	4.714633	0.065512	-2.187134
H	4.106117	0.167583	-0.526225
H	2.458898	-2.131725	-2.952359
H	1.415363	-0.947214	-3.751310
H	3.168391	-0.915181	-4.007980
H	1.425089	-4.339701	2.520616
H	1.277877	-3.373093	3.999019
H	0.009431	-4.519348	3.557692
H	-1.599547	-3.946127	1.563446
H	-1.221301	-2.530586	0.552553
H	-0.143332	-3.941123	0.557933
H	-0.620597	3.549464	5.062880
H	-0.946488	2.125432	6.064363
H	0.414035	2.126609	4.930355
H	-2.832599	3.656381	3.904547
H	-3.641836	2.165786	3.389524
H	-3.347740	2.481732	5.110423
H	1.781177	6.313193	0.481842
H	3.074749	5.338582	-0.239659
H	2.020510	6.310018	-1.267392
H	-0.632608	5.762210	0.044414
H	-0.441180	5.536443	-1.699990
H	-1.091921	4.222204	-0.691581
H	-3.845669	-0.964314	0.196667
H	-4.300839	-0.932574	1.930252
H	-5.188094	0.091568	0.754934
H	1.856669	-0.519880	-1.267613
H	0.787254	-2.061685	1.897064
H	1.048128	3.973791	0.468028
H	-1.140690	2.201033	3.007528
H	-0.209969	-0.089976	-2.411629
H	-2.140879	0.092461	-3.889808
H	-3.243377	-0.099198	-2.534098
H	-1.275603	2.076420	-2.058880
H	-2.186951	2.369683	-3.522908
H	-3.198574	3.399682	-1.452884
H	-1.160745	-2.134184	-3.475457
H	-0.450293	-2.511685	-1.892260
H	-2.206594	-2.380991	-2.060698

III$^{6\alpha}{}_{7CC\text{-}\gamma(S,si)}$

G = -2040.64134 kcal.mol^{-1}

C	1.770337	3.671404	-1.671802
C	1.888710	2.298564	-1.337502
C	2.154851	1.334801	-2.336550
C	2.331968	1.770031	-3.654400
C	2.246347	3.113609	-3.991267
C	1.961898	4.050208	-3.003661
N	1.702216	1.894368	0.024767
C	2.758486	1.790735	0.832811
C	2.704851	1.410542	2.187724
C	1.655454	0.862624	2.945475
C	2.018147	0.434841	4.350964
C	2.255720	-0.154355	-2.038027
C	3.659828	-0.704052	-2.333271
C	1.461187	4.730254	-0.619504
C	0.601503	5.879706	-1.160660
Zn	-0.116489	1.452273	0.731676
O	-1.767801	2.328804	0.513525

C	-1.917065	3.353150	-0.422608	H	-1.559903	4.322213	-0.028536	H	1.380233	-0.899794	-3.897890
C	-3.381583	3.550563	-0.828867	H	-0.798560	2.526904	3.433292	H	4.775671	2.509473	1.078174
C	-4.116492	2.283442	-1.279456	H	-3.290481	-2.100177	5.102149	H	4.624569	1.088926	0.049735
C	-3.434421	1.463421	-2.372850	H	3.654759	1.466461	2.708073	H	3.895417	-0.636330	-3.401360
O	-2.204485	0.812441	-1.905229	H	0.894313	4.235510	0.178010	H	4.437665	-0.158039	-1.791742
C	-2.146791	0.035890	-0.843666	H	0.929675	-3.601993	0.873764	H	3.725633	-1.759974	-2.048039
O	-3.315256	-0.447542	-0.440998	H	1.372357	-1.559308	2.206528	H	2.542290	1.037382	-4.429501
C	-3.300659	-1.230020	0.764626	H	2.339244	-0.611914	4.364765	H	2.393336	3.431838	-5.019994
N	0.416062	0.676073	2.494055	H	2.201603	-3.693941	3.056669	H	1.884133	5.098738	-3.275319
C	-0.531076	-0.069542	3.259435	H	1.673566	-2.729230	4.447441	H	3.377429	5.762546	-0.748386
C	-1.556678	0.611622	3.958388	H	0.667108	-4.049210	3.851416	H	2.477941	6.087093	0.743204
C	-2.537250	-0.143053	4.611458	H	1.169291	0.523450	5.031598	H	3.318890	4.548160	0.538950
C	-2.517995	-1.532541	4.589891	H	2.845745	1.038612	4.729572	H	-0.270339	5.513419	-1.709050
C	-1.490180	-2.190189	3.923255	H	-0.656170	-3.772761	1.635383	H	0.246713	6.501244	-0.331781
C	-0.481067	-1.486424	3.258070	H	-1.465657	-3.277262	3.922173	H	1.171720	6.535181	-1.828712
C	-1.590423	2.129099	4.075157	H	-0.327500	2.187210	5.870531	H	-3.937029	3.971432	0.018857
C	-2.914587	2.727298	3.584630	H	-3.324959	0.372678	5.154695	H	-3.414147	4.305403	-1.628416
C	0.627736	-2.273833	2.569313	H	-2.061844	2.216982	6.209983	H	-4.308308	1.640332	-0.418785
C	1.331535	-3.235699	3.539618	H	-1.260552	3.663885	5.582358	H	-5.101446	2.566985	-1.672989
C	-4.346604	0.463542	-3.068673	H	-2.897708	3.816953	3.701845	H	-3.021126	2.142884	-3.126002
C	0.112064	-3.045347	1.346198	H	-3.769563	2.350698	4.158318	H	-4.342105	-1.496917	0.941592
C	-1.290022	2.570564	5.516770	H	-3.056896	2.506110	2.523920	H	-2.909247	-0.642671	1.596421
C	4.156496	2.045646	0.306277	H	0.196939	-0.579526	-2.616629	H	-2.694351	-2.125929	0.627644
C	1.202097	-0.954269	-2.817775	H	2.054505	-0.295255	-0.971566	H	-0.311719	-2.364262	0.605088
C	2.736072	5.308896	0.016104	H	1.237704	-2.011027	-2.530434	H	-1.330611	3.167943	-1.341496
O	-1.068640	-0.278314	-0.340724	H	4.168399	2.670382	-0.586597	H	-5.106981	1.006207	-3.639173

H	-3.775744	-0.153002	-3.769109
H	-4.851543	-0.189342	-2.354263

TS(**III**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S,si)}$→**IV**$^{\alpha\delta}{}_{7CC\text{-}\gamma(S)}$)

G = -2040.636141 kcal.mol^{-1}

C	2.309460	1.334274	-2.357927
C	1.886694	2.118510	-1.255063
C	1.596650	3.492708	-1.411111
C	1.739828	4.061136	-2.682175
C	2.162063	3.309222	-3.769081
C	2.444236	1.957602	-3.601570
N	1.708559	1.484450	0.018129
Zn	0.018087	0.538643	0.442679
O	-1.326597	-0.073718	-0.655695
C	-1.163071	-0.306942	-2.037935
C	-1.001501	-1.803130	-2.306655
C	1.146540	4.381432	-0.259163
C	-0.294067	4.878445	-0.449504
C	2.633600	-0.147623	-2.204372
C	2.406066	-0.958336	-3.485174
C	2.667890	1.562639	0.943337
C	3.936884	2.338044	0.662815
C	2.587538	0.991341	2.225898
C	1.516189	0.364137	2.884208
C	1.806130	-0.144375	4.279285
N	0.302580	0.175692	2.355078
C	-0.730166	-0.384857	3.178732
C	-0.871473	-1.786138	3.273825
C	-1.882215	-2.300761	4.092909
C	-2.729319	-1.460315	4.802881
C	-2.593274	-0.081117	4.679409
C	-1.610411	0.488003	3.864145
C	0.009331	-2.746480	2.487579
C	-0.776462	-3.357678	1.317622
C	-1.514419	2.003647	3.719238
C	-2.846450	2.720669	3.963409
C	-0.435304	2.619710	4.625325
C	0.620521	-3.849466	3.362856
C	-2.366504	0.247407	-2.814886
C	-2.573944	1.758250	-2.610894
C	-3.909312	2.111090	-1.974453
O	-4.161168	1.323954	-0.795928
C	-3.472811	1.667389	0.298066
O	-2.803207	2.669025	0.431039
O	-3.652413	0.807800	1.300538
C	-4.248143	-0.466642	1.034350
C	2.093674	5.576043	-0.061916
C	4.070527	-0.377308	-1.707490
H	-4.745285	1.862815	-2.634502
H	1.921014	-1.233595	4.257280
H	2.730984	0.285849	4.667014
H	0.992228	0.073984	4.972867
H	4.778194	1.904539	1.208303
H	4.179627	2.378361	-0.399505
H	3.816994	3.369033	1.013279
H	3.488087	1.092280	2.820197
H	-3.275604	0.567388	5.219269
H	-3.501455	-1.876484	5.444822
H	-2.002636	-3.377788	4.176444
H	2.771062	1.376008	-4.457678
H	2.270615	3.771852	-4.746362
H	1.517423	5.116457	-2.817360
H	4.281752	-1.450313	-1.638073
H	4.794232	0.063238	-2.402646
H	4.240598	0.056705	-0.720223
H	2.480534	-2.028067	-3.265275
H	1.420611	-0.770735	-3.920426
H	3.162091	-0.735658	-4.246552
H	1.324181	-4.451453	2.777715
H	1.160016	-3.439215	4.222652
H	-0.144673	-4.530876	3.749842
H	-1.621477	-3.950930	1.685886
H	-1.169647	-2.578928	0.658256
H	-0.136265	-4.020978	0.724392
H	-0.451590	3.711739	4.536574
H	-0.618969	2.368861	5.676720
H	0.571722	2.287453	4.364310
H	-2.756158	3.767703	3.658433

H	-3.653400	2.270699	3.382136
H	-3.126721	2.715528	5.023717
H	1.820882	6.131898	0.841686
H	3.138344	5.264238	0.032182
H	2.036504	6.275038	-0.903725
H	-0.577266	5.539145	0.377463
H	-0.392328	5.451492	-1.378690
H	-1.014593	4.057767	-0.471791
H	-3.659324	-0.994180	0.281855
H	-4.212807	-0.997825	1.985433
H	-5.282755	-0.354309	0.699420
H	1.958569	-0.547325	-1.436244
H	0.836392	-2.168836	2.061327
H	1.168364	3.783500	0.657501
H	-1.235681	2.206540	2.678752
H	-0.267536	0.212090	-2.423711
H	-2.229616	0.019988	-3.879318
H	-3.257155	-0.304527	-2.488679
H	-1.777092	2.157244	-1.977575
H	-2.517650	2.299188	-3.563469
H	-3.959030	3.171670	-1.710872
H	-0.884745	-2.015982	-3.375731
H	-0.126512	-2.199010	-1.781550
H	-1.882537	-2.344184	-1.943659

TS(**III**$^{6\alpha}{}_{7CC\text{-}\gamma(S,si)}$→**IV**$^{6\alpha}{}_{7CC\text{-}\gamma(S)}$)

G = -2040.637865 kcal.mol^{-1}

C	1.849892	3.874715	-1.385734
C	2.035043	2.477281	-1.236704
C	2.312828	1.658438	-2.352286
C	2.430391	2.265195	-3.608059
C	2.283046	3.636034	-3.766282
C	1.991674	4.428511	-2.660752
N	1.875820	1.899599	0.065207
C	2.940197	1.707665	0.845998
C	2.878654	1.238918	2.171632
C	1.792462	0.761194	2.923639
C	2.105694	0.347694	4.343841
C	2.477674	0.149219	-2.244254
C	3.829773	-0.321130	-2.802336
C	1.507067	4.765640	-0.196575
C	0.654746	5.983928	-0.572995

Zn	0.071213	1.424899	0.718960
O	-1.579263	1.950503	0.101954
C	-1.664034	2.673928	-1.102331
C	-3.100304	3.128023	-1.367165
C	-4.154531	2.017889	-1.392027
C	-3.946354	0.938377	-2.452810
O	-2.766321	0.119081	-2.197710
C	-2.575779	-0.586373	-1.086751
O	-3.680318	-0.725003	-0.340512
C	-3.500520	-1.427011	0.893185
N	0.542930	0.644681	2.463730
C	-0.463159	0.013484	3.263986
C	-1.439005	0.812773	3.904064
C	-2.466426	0.177477	4.608964
C	-2.534725	-1.207334	4.698085
C	-1.558468	-1.980976	4.081040

C	-0.510672	-1.399501	H	0.916712	4.157405	H	-3.545817	2.659156
3.359240		0.500836			3.719927			
C	-1.390042	2.333889	H	0.683736	-3.733557	H	-2.689478	2.604015
3.883051		1.069394			2.157076			
C	-2.623460	2.937099	H	1.312443	-1.681428	H	0.357414	-0.364068
3.196963		2.287994			2.491576			
C	0.520120	-2.311328	H	2.256491	-0.733970	H	2.444382	-0.117828
2.704012		4.411788			1.182765			
C	1.163422	-3.273475	H	1.981190	-3.827920	H	1.475312	-1.675021
3.715325		3.242474			2.869029			
C	-5.175609	0.080571	H	1.566362	-2.753229	H	4.346868	2.803030
2.724274		4.589990			0.402430			
C	-0.084400	-3.107563	H	0.440511	-4.010871	H	1.282042	-0.332570
1.538077		4.080976			4.005673			
C	-1.207101	2.905597	H	1.286929	0.601237	H	5.026766	2.183392
5.297361		5.021095			1.121787			
C	4.328485	1.975659	H	3.019160	0.834644	H	4.689970	1.086095
0.308514		4.690064			0.219468			
C	1.326684	-0.591866	H	-0.878050	-3.775738	H	3.891424	-0.168769
2.941645		1.894111			3.885518			
C	2.760206	5.236424	H	-1.609140	-3.064136	H	4.670755	0.212904
0.559986		4.157856			2.348850			
O	-1.504031	-1.095539	H	-0.315227	2.500762	H	3.965482	-1.391990
0.834366		5.786707			2.616015			
H	-1.034768	3.579040	H	-3.222272	0.782953	H	2.641621	1.646033
1.083575		5.102769			4.476162			
H	-0.511067	2.629297	H	-2.067629	2.678745	H	2.384901	4.087766
3.300294		5.936420			4.749393			
H	-3.340050	-1.681823	H	-1.104569	3.995612	H	1.861674	5.497825
5.252576		5.256837			2.795511			
H	3.830807	1.218564	H	-2.559919	4.031462	H	3.429648	5.789827
2.689073		3.201636			0.108439			

H	2.479711	5.903959	1.382460
H	3.321119	4.403560	0.989267
H	-0.214029	5.706843	-1.177290
H	0.292200	6.476302	0.335202
H	1.232662	6.728895	-1.131495
H	-3.387255	3.848137	-0.590124
H	-3.113789	3.674704	-2.321901
H	-4.223804	1.549416	-0.407947
H	-5.135216	2.469782	-1.591247
H	-3.653858	1.423162	-3.391659
H	-4.492997	-1.487251	1.340053
H	-2.823743	-0.879572	1.551351
H	-3.102098	-2.426993	0.710364
H	-0.506599	-2.453244	0.771857
H	-1.312438	2.075412	-1.957168
H	-5.958068	0.700880	-3.173254
H	-4.932779	-0.719442	-3.429989
H	-5.567954	-0.365326	-1.808784

Propagation step of the ROP of 7CC-γMe.

$\mathbf{V}^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.679412 kcal.mol^{-1}

C	2.723967	3.173283	-1.466283
C	2.727089	1.860102	-0.936520
C	3.286873	0.787445	-1.669216
C	3.830185	1.050988	-2.930768
C	3.816397	2.331085	-3.470640
C	3.267214	3.377004	-2.738356
N	2.099175	1.602078	0.321510
C	2.736947	1.879390	1.457212
C	4.162008	2.387627	1.413460
C	3.357344	-0.624053	-1.102510
C	4.785801	-0.968281	-0.651161
C	2.149210	4.363617	-0.707685
C	3.131973	5.543051	-0.653185
C	2.167376	1.775637	2.739048
C	0.889727	1.354253	3.149809
C	0.672765	1.386617	4.650870
N	-0.080708	0.945078	2.331782
Zn	0.163321	1.093494	0.335183
O	-0.048941	-0.956223	-0.482477
C	-1.129747	-1.481046	-0.710831
O	-1.284615	-2.259977	-1.781008
C	-1.951518	-3.565727	-1.786193
C	-2.818478	-3.620018	-3.031199
C	-1.276386	0.366942	2.851928
C	-1.256092	-0.938119	3.401356
C	-2.464816	-1.511264	3.812476
C	-3.667294	-0.826548	3.698873
C	-3.673061	0.461150	3.170474
C	-2.496579	1.080823	2.739583
C	0.023212	-1.752779	3.559795
C	0.216725	-2.246087	5.002051
C	-2.527567	2.505739	2.203928
C	-2.109316	3.514620	3.285419
O	-1.088961	1.940013	-0.776783
C	-3.879666	2.913005	1.612245
C	0.069505	-2.940875	2.588062
C	2.842230	-1.683915	-2.084133
C	0.800765	4.810545	-1.291663
O	-2.162442	-1.240617	0.085381

C	-3.499493	-1.532410	-0.361403
C	-3.844695	-2.995063	-0.129196
C	-2.663195	-3.901968	-0.480794
H	4.671445	2.192391	2.359331
H	4.729848	1.933971	0.599084
H	4.172291	3.470123	1.245703
H	1.055010	2.327745	5.056201
H	-0.377726	1.284723	4.924096
H	1.231310	0.578923	5.135241
H	2.824043	2.069879	3.550951
H	4.273395	0.237170	-3.499044
H	4.237028	2.514535	-4.455906
H	3.261229	4.378022	-3.162010
H	-4.612978	0.999789	3.099417
H	-4.594360	-1.284887	4.034381
H	-2.458879	-2.513131	4.235622
H	-2.121828	4.533003	2.881290
H	-2.798033	3.481515	4.138047
H	-1.100960	3.318382	3.657523
H	-3.781649	3.878211	1.106116
H	-4.231940	2.186016	0.874198
H	-4.655286	3.027598	2.379148
H	2.744122	6.326714	0.006668
H	4.117152	5.241820	-0.281630
H	3.277800	5.995807	-1.640147
H	0.908515	5.106217	-2.342124
H	0.060942	4.006767	-1.226695
H	0.417414	5.677830	-0.741227
H	4.821443	-1.974746	-0.218431
H	5.482685	-0.942881	-1.496826
H	5.154296	-0.267476	0.103738
H	2.849481	-2.670390	-1.606803
H	1.817722	-1.470888	-2.397173
H	3.471381	-1.752294	-2.978798
H	1.197248	-2.722176	5.113371
H	0.151065	-1.427746	5.724831
H	-0.538622	-2.989765	5.279175
H	0.983776	-3.525671	2.740655
H	-0.784181	-3.611239	2.743630
H	0.061935	-2.596165	1.551625
H	-1.806674	2.564989	1.381613
H	1.960111	4.046936	0.322595
H	0.871914	-1.110111	3.310869
H	2.713010	-0.653894	-0.218596
H	-3.576542	-1.253239	-1.416547
H	-4.128800	-0.862238	0.224641
H	-4.112921	-3.152345	0.919924
H	-4.729670	-3.242127	-0.726776
H	-1.930307	-3.874760	0.333035
H	-2.993872	-4.944274	-0.551618
H	-1.120080	-4.269895	-1.906415
H	-3.188590	-4.639573	-3.176291
H	-3.679092	-2.949049	-2.965920
H	-2.232460	-3.339452	-3.909782
C	-1.542913	1.554547	-2.033004
C	-0.422392	1.502307	-3.075283
C	-2.686871	2.505766	-2.430567
C	-3.419461	2.159733	-3.737464
C	-2.951074	2.930964	-4.958936
O	-3.343088	4.306577	-4.769225
C	-3.000272	5.232665	-5.665057
O	-2.290700	4.715089	-6.690181
C	-1.897236	5.675687	-7.671694
O	-3.304180	6.394693	-5.554991
H	-1.270684	6.450784	-7.223547
H	-1.336254	5.117682	-8.421896
H	-2.773625	6.148468	-8.122077
H	-1.866268	2.879814	-5.084743
H	-3.420164	2.552697	-5.874214

H	-4.495823	2.340261	-3.631936
H	-3.311536	1.088890	-3.962275
H	-3.395634	2.500216	-1.596316
H	-2.293532	3.528226	-2.478968
H	-0.771248	1.111824	-4.039404
H	0.384282	0.848720	-2.729702
H	0.006140	2.496952	-3.234267
H	-1.996043	0.535657	-2.008461

$\mathbf{V}^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.675001 kcal.mol^{-1}

C	2.933047	3.267457	-1.346131
C	2.820336	1.899861	-0.992732
C	3.315541	0.890684	-1.849193
C	3.913215	1.271793	-3.054991
C	4.013942	2.607370	-3.422728
C	3.526422	3.591060	-2.569719
N	2.133201	1.541821	0.208830
C	2.745913	1.667502	1.384222
C	4.223805	1.993199	1.429898
C	3.256352	-0.583731	-1.476004
C	4.646548	-1.113849	-1.090440
C	2.412116	4.387479	-0.451932
C	3.439607	5.513512	-0.268370
C	2.103596	1.578500	2.632718
C	0.744434	1.405987	2.950373
C	0.385124	1.654717	4.401273
N	-0.213691	1.108607	2.070211
Zn	0.163177	1.188621	0.109401
O	-0.131866	-0.890320	-0.704279
C	-1.187892	-1.325665	-1.138621
O	-1.242290	-1.861300	-2.358781
C	-1.932546	-3.106371	-2.718443
C	-2.669871	-2.854951	-4.021490
C	-1.546540	0.873813	2.534521
C	-1.928104	-0.446711	2.881906
C	-3.237756	-0.664055	3.319321
C	-4.161113	0.374449	3.391812
C	-3.778599	1.657832	3.025515
C	-2.474459	1.935923	2.600873
C	-0.948077	-1.611320	2.783277
C	-0.120694	-1.805635	4.064931
C	-2.103865	3.365023	2.231837
C	-2.399822	4.347335	3.374978
O	-0.922099	1.955898	-1.215628
C	-2.799204	3.809488	0.936200
C	-1.627008	-2.939558	2.427549
C	2.646557	-1.447896	-2.586837
C	1.080134	4.952272	-0.969170
O	-2.297203	-1.226343	-0.416946
C	-3.589044	-1.379916	-1.045972
C	-3.978951	-2.842102	-1.174220
C	-2.780134	-3.692853	-1.595372
H	4.381398	3.074145	1.345720
H	4.658924	1.666352	2.376721
H	4.765352	1.526331	0.605086
H	0.099083	2.706640	4.519481
H	-0.458492	1.052114	4.739088
H	1.242058	1.471747	5.053091
H	2.750265	1.748808	3.486162
H	4.307411	0.504888	-3.716759
H	4.475474	2.882425	-4.367483
H	3.609008	4.635225	-2.859824
H	-4.501799	2.467949	3.078842
H	-5.174985	0.180538	3.732690
H	-3.546373	-1.666404	3.601488
H	-2.023695	5.345259	3.124196
H	-3.475985	4.442121	3.558134
H	-1.932921	4.033820	4.314294
H	-2.548746	4.853018	0.711953

H	-2.480417	3.196470	0.087573
H	-3.889451	3.744787	1.036072
H	3.084201	6.230120	0.480133
H	4.411027	5.130693	0.061622
H	3.603539	6.071832	-1.196423
H	1.193922	5.356199	-1.981934
H	0.301733	4.183418	-0.990149
H	0.736885	5.767957	-0.321787
H	4.588355	-2.168261	-0.797152
H	5.345541	-1.038701	-1.931402
H	5.076415	-0.557761	-0.251812
H	2.569227	-2.488039	-2.250986
H	1.642911	-1.106412	-2.849450
H	3.263539	-1.443178	-3.492648
H	0.516540	-2.692482	3.971861
H	0.532239	-0.955864	4.270286
H	-0.774531	-1.952684	4.932541
H	-0.867357	-3.687906	2.176082
H	-2.204759	-3.344479	3.266456
H	-2.298241	-2.827247	1.573114
H	-1.025156	3.389877	2.046828
H	2.214003	3.964701	0.537434
H	-0.252396	-1.367412	1.973075
H	2.608902	-0.673948	-0.598893
H	-3.557260	-0.888037	-2.018549
H	-4.270662	-0.827468	-0.400097
H	-4.369015	-3.221001	-0.223840
H	-4.796677	-2.903035	-1.899941
H	-2.133403	-3.873288	-0.728799
H	-3.115460	-4.681486	-1.928732
H	-1.104536	-3.798918	-2.909449
H	-3.058129	-3.802479	-4.408140
H	-3.507985	-2.163496	-3.903647
H	-1.984757	-2.439841	-4.765128
C	-0.494021	2.019815	-2.545511
C	-1.640945	2.453995	-3.466699
C	-2.784915	1.448394	-3.405410
C	-4.008145	1.740409	-4.263136
O	-4.960800	0.654459	-4.021273
C	-5.810120	0.685889	-2.996635
O	-5.963051	1.915285	-2.475137
C	-6.866069	1.987867	-1.369208
C	-3.756569	1.728785	-5.758805
O	-6.387361	-0.303814	-2.603928
H	0.340462	2.728353	-2.682872
H	-1.992289	3.446961	-3.155671
H	-1.252399	2.549005	-4.489781
H	-3.098465	1.385308	-2.357699
H	-2.403270	0.458575	-3.691430
H	-4.474593	2.683286	-3.965982
H	-6.913551	3.042809	-1.099555
H	-6.492261	1.399297	-0.527782
H	-7.853718	1.617536	-1.653164
H	-0.124000	1.042492	-2.911589
H	-3.072893	2.537311	-6.031172
H	-3.308824	0.779474	-6.069439
H	-4.690757	1.868045	-6.309861

$\mathbf{V}^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.667596 kcal.mol^{-1}

C	2.757689	3.199412	-1.435356
C	2.737637	1.850422	-1.003031
C	3.290491	0.827078	-1.806267
C	3.852056	1.176261	-3.038782
C	3.861104	2.492021	-3.483999
C	3.317018	3.489703	-2.683114
N	2.087446	1.517791	0.226519
C	2.711931	1.734259	1.382291
C	4.162163	2.169247	1.385196
C	3.328734	-0.624541	-1.350162

C	4.748156	-1.035070	-0.926948	O	-1.024552	1.609487	-1.164656	H	-3.589743	4.265121	3.579435
C	2.167670	4.331748	-0.602427	C	-2.879043	3.531458	0.996165	H	-2.035808	3.957249	4.360398
C	3.114632	5.535532	-0.496993	C	-1.426701	-3.073982	2.594633	H	-2.679259	4.573256	0.718946
C	2.103634	1.647640	2.648180	C	2.792214	-1.590650	-2.413574	H	-2.534161	2.893521	0.175980
C	0.767316	1.394471	3.003908	C	0.795833	4.767659	-1.139650	H	-3.964714	3.419143	1.103621
C	0.423216	1.659156	4.455433	O	-2.184415	-1.477535	-0.352243	H	2.715562	6.268655	0.212481
N	-0.189601	1.009749	2.155869	C	-3.456292	-1.551962	-1.063629	H	4.112670	5.241068	-0.156177
Zn	0.144582	1.019011	0.186672	C	-3.862067	-3.011180	-1.210982	H	3.232378	6.048446	-1.457826
O	-0.007847	-1.109505	-0.486866	C	-2.682382	-3.868866	-1.675643	H	0.874866	5.114727	-2.176480
C	-1.027013	-1.558454	-0.991640	H	4.233272	3.259583	1.301064	H	0.075282	3.944734	-1.106720
O	-0.949522	-2.128492	-2.194347	H	4.646821	1.877079	2.319315	H	0.397210	5.594418	-0.539946
C	-1.814026	-3.173318	-2.707594	H	4.714967	1.746292	0.544693	H	4.759538	-2.072996	-0.575178
H	-2.416867	-2.730189	-3.507839	H	0.009934	2.670701	4.544830	H	5.447630	-0.958810	-1.767475
C	-1.496722	0.729017	2.665225	H	-0.329383	0.972497	4.844614	H	5.131205	-0.405252	-0.118540
C	-1.811744	-0.595729	3.057115	H	1.314858	1.608534	5.083503	H	2.766454	-2.609799	-2.012493
C	-3.091181	-0.850979	3.559916	H	2.755998	1.890245	3.479407	H	1.776877	-1.325585	-2.715944
C	-4.050084	0.153447	3.649134	H	4.289784	0.399824	-3.660795	H	3.426917	-1.608172	-3.306976
C	-3.735765	1.440056	3.230781	H	4.294988	2.741046	-4.448856	H	0.730444	-2.736237	4.127957
C	-2.463298	1.756032	2.742338	H	3.326595	4.518273	-3.034128	H	0.660292	-1.000736	4.430241
C	-0.791166	-1.723648	2.948919	H	-4.488586	2.221809	3.294216	H	-0.591203	-2.063238	5.096602
C	0.050101	-1.882563	4.225923	H	-5.038874	-0.068582	4.042322	H	-0.643138	-3.798070	2.345634
C	-2.164241	3.184994	2.311222	H	-3.345639	-1.856452	3.882864	H	-1.993493	-3.495616	3.432789
C	-2.509677	4.205826	3.405201	H	-2.173965	5.205782	3.109511	H	-2.098899	-2.984823	1.737832

H	-1.087931	3.256019	2.123976
H	2.006821	3.955959	0.412491
H	-0.110792	-1.456147	2.133949
H	2.679236	-0.711147	-0.474386
H	-3.298184	-1.101724	-2.048436
C	-4.435283	-0.710682	-0.275229
H	-4.253375	-3.390127	-0.260485
H	-4.683072	-3.058511	-1.936129
H	-2.056832	-4.162502	-0.824853
H	-3.043552	-4.802112	-2.122178
H	-1.115206	-3.879555	-3.162977
C	-0.586914	1.634595	-2.494438
C	-1.642812	2.257742	-3.414466
C	-2.937289	1.450772	-3.424759
C	-4.070980	2.028811	-4.262813
O	-5.232728	1.160698	-4.095043
C	-6.090395	1.322990	-3.089918
O	-5.916874	2.484094	-2.430114
C	-6.846070	2.707590	-1.367706
C	-3.803839	2.056206	-5.756310
O	-6.941350	0.504956	-2.824978
H	0.344874	2.210531	-2.620635
H	-1.845323	3.281891	-3.073240
H	-1.221096	2.329625	-4.426232
H	-3.279203	1.363206	-2.388224
H	-2.729605	0.434786	-3.791487
H	-4.330800	3.029952	-3.908260
H	-6.590706	3.684163	-0.956370
H	-6.750145	1.935298	-0.600885
H	-7.871202	2.705943	-1.745884
H	-0.365006	0.617815	-2.874690
H	-2.958997	2.713964	-5.977332
H	-3.567787	1.053263	-6.126067
H	-4.678692	2.426167	-6.297989
H	-5.398076	-0.689604	-0.794902
H	-4.577639	-1.120162	0.728457
H	-4.059953	0.310115	-0.175882

$\mathbf{V}^{\alpha\delta,\alpha\delta}{}_{\gamma CC\text{-}\gamma(R)}$

G = -2500.666477 kcal.mol^{-1}

C	-2.230733	1.751220	3.071231
C	-1.273292	0.710707	3.098743
C	-1.568663	-0.518430	3.743533
C	-2.828869	-0.675482	4.330337
C	-3.783620	0.333658	4.292142
C	-3.476784	1.536170	3.668070
N	-0.020433	0.895498	2.432043
Zn	0.067524	0.919403	0.410847
O	-1.485683	1.186065	-0.605975
C	-1.535156	1.492407	-1.973567
C	-3.000805	1.380505	-2.461255
C	-3.193927	0.765551	-3.852285
C	-2.621375	1.549040	-5.019575
O	-3.308371	2.814439	-5.074633
C	-2.971108	3.722147	-5.993505
O	-3.526959	4.787202	-6.095537
C	-0.568166	-1.664066	3.864868
C	-1.098317	-2.970269	3.256104
C	-1.927198	3.117728	2.475185
C	-2.941352	3.523476	1.399165
C	1.089628	1.102303	3.132779
C	1.044203	1.316579	4.632182
C	2.383605	1.194119	2.578122
C	2.801078	1.369661	1.253127
C	4.299824	1.447547	1.045674
N	1.982095	1.456610	0.196385
C	2.502915	2.001247	-1.022176
C	2.532131	3.413549	-1.171940
C	3.049795	3.949687	-2.354290
C	3.512982	3.132048	-3.379198

C	3.458151	1.753171	-3.229331	H	4.660210	0.469618	0.706809	H	0.760893	6.085424	0.200157
C	2.961021	1.162621	-2.061904	H	4.580657	2.173970	0.281750	H	4.342937	-2.024784	-1.870596
C	2.029629	4.351874	-0.079192	H	1.340646	2.349168	4.847009	H	4.822456	-0.763641	-3.012616
C	1.225188	5.538456	-0.627483	H	0.055696	1.149494	5.056976	H	5.034090	-0.503915	-1.280149
C	2.950854	-0.354213	-1.953457	H	1.765356	0.666262	5.135454	H	2.016447	-2.073703	-2.898370
C	2.060749	-0.987706	-3.030930	H	3.180560	1.225433	3.313230	H	1.038685	-0.605668	-2.977639
C	4.368869	-0.941078	-2.030620	H	3.818169	1.114004	-4.031842	H	2.448656	-0.787698	-4.036740
C	3.177805	4.876081	0.799013	H	3.911111	3.569747	-4.290871	H	0.600229	-2.696351	5.384075
O	0.127976	-1.283884	-0.204812	H	3.085305	5.028404	-2.478176	H	0.213379	-1.025704	5.822138
C	-0.914228	-1.794126	-0.581016	H	-4.214064	2.334872	3.654352	H	-1.032247	-2.272051	5.910664
O	-1.978981	-1.817116	0.209169	H	-4.755148	0.188078	4.757216	H	-0.326596	-3.747282	3.301238
C	-3.320381	-1.917643	-0.343241	H	-3.062105	-1.610038	4.834962	H	-1.968238	-3.342455	3.809784
C	-3.684655	-3.390394	-0.475535	H	-1.554244	5.153319	3.152835	H	-1.391399	-2.829539	2.215533
C	-2.521956	-4.185365	-1.075678	H	-2.787473	4.305673	4.096701	H	-0.946271	3.058047	1.992694
C	-1.814662	-3.447677	-2.198810	H	-1.079347	3.915878	4.330828	H	1.362350	3.768020	0.564187
H	-2.530228	-3.058911	-2.932086	H	-2.681886	4.505692	0.987903	H	0.332401	-1.387765	3.308599
O	-0.974238	-2.336644	-1.800153	H	-2.933040	2.796479	0.582714	H	2.524865	-0.617586	-0.981220
C	-0.172188	-1.920901	5.329200	H	-3.956539	3.598908	1.805472	H	-3.294855	-1.444288	-1.330213
C	-1.829427	4.182155	3.579174	H	2.792719	5.565451	1.559027	C	-4.216369	-1.118452	0.576819
C	-0.969784	2.883652	-2.260046	H	3.701839	4.070210	1.317633	H	-3.955871	-3.800517	0.503435
O	-1.954828	3.302131	-6.774736	H	3.910847	5.420992	0.192934	H	-4.573756	-3.467756	-1.113037
C	-1.549808	4.247723	-7.766740	H	1.861265	6.251915	-1.163220	H	-1.790789	-4.442043	-0.301014
H	4.816280	1.689601	1.976380	H	0.433138	5.215045	-1.307025	H	-2.880498	-5.137475	-1.483000

H	-1.127197	-4.117227	-2.722558
H	-1.209694	5.174797	-7.298870
H	-0.732802	3.772498	-8.310168
H	-2.377689	4.476692	-8.442371
H	-1.546799	1.718949	-4.906970
H	-2.780071	1.016344	-5.963811
H	-4.264027	0.610157	-4.039861
H	-2.720851	-0.226590	-3.882243
H	-3.528090	0.751844	-1.736839
H	-3.488612	2.362138	-2.425404
H	-1.063620	3.167607	-3.313856
H	0.089356	2.930938	-1.993988
H	-1.515726	3.623148	-1.664086
H	-0.938947	0.760444	-2.558731
H	-5.246686	-1.146486	0.207848
H	-4.194118	-1.528677	1.589914
H	-3.876121	-0.081895	0.616150

TS($\mathbf{V}^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VI}^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.664979 kcal.mol^{-1}

C	2.696023	3.027869	-1.483885
C	2.715721	1.681940	-1.032080
C	3.314864	0.671580	-1.816017
C	3.898012	1.027950	-3.037407
C	3.901133	2.342374	-3.482576
C	3.301573	3.329037	-2.707209
N	2.098116	1.368989	0.222331
C	2.823366	1.480777	1.345375
C	4.328141	1.632308	1.252072
C	3.364817	-0.783702	-1.376644
C	4.808810	-1.287559	-1.229963
C	2.047654	4.140332	-0.666296
C	3.046273	4.818334	0.286896
C	2.306319	1.436680	2.645682
C	0.982444	1.293015	3.113856
C	0.824705	1.475500	4.609432
N	-0.062077	1.011251	2.344123
Zn	0.230773	0.699639	0.376676
O	-0.020021	-1.379895	0.024024
C	-1.060590	-1.425932	-0.661957
O	-1.051521	-1.694878	-2.003161
C	-0.917640	-3.091936	-2.373587
C	-1.230612	-3.144988	-3.857915
C	-1.366982	0.838118	2.905092
C	-1.715317	-0.360325	3.571052
C	-3.026891	-0.502448	4.037974
C	-3.973633	0.497180	3.864393
C	-3.616452	1.673329	3.213828
C	-2.322956	1.867233	2.723790
C	-0.729451	-1.495156	3.818800
C	-0.561497	-1.782380	5.319933
C	-1.942172	3.184026	2.061791
C	-1.304455	4.148409	3.075270
O	-1.271611	0.539223	-0.850022
C	-3.107656	3.875613	1.348417
C	-1.137621	-2.780435	3.085945
C	2.587220	-1.684690	-2.344812
C	1.373413	5.212639	-1.532203
O	-2.209605	-1.749104	-0.033688
C	-3.337777	-2.084606	-0.848041
C	-3.249576	-3.533459	-1.351900
C	-1.799816	-4.002454	-1.515290
H	4.733750	2.089510	2.156643
H	4.779311	0.638622	1.150689
H	4.638952	2.217619	0.385847
H	1.389071	2.352371	4.938533
H	-0.217406	1.588355	4.908515
H	1.239588	0.609086	5.134963
H	3.041424	1.579412	3.430381
H	4.365865	0.257154	-3.644906

H	4.365856	2.599596	-4.430744
H	3.299221	4.354911	-3.063594
H	-4.358617	2.455073	3.085279
H	-4.986014	0.364355	4.236878
H	-3.307088	-1.420105	4.549143
H	-1.029451	5.091739	2.589967
H	-2.008952	4.377508	3.882928
H	-0.401801	3.728039	3.525189
H	-2.737124	4.719414	0.757159
H	-3.631507	3.192665	0.674501
H	-3.838161	4.281310	2.057420
H	2.559770	5.640784	0.823379
H	3.440480	4.126400	1.033638
H	3.891963	5.235764	-0.271641
H	2.108513	5.843156	-2.044935
H	0.716377	4.777608	-2.289459
H	0.772480	5.876029	-0.901420
H	4.818489	-2.307674	-0.830529
H	5.323845	-1.307529	-2.196926
H	5.398098	-0.655259	-0.559450
H	2.608197	-2.722263	-1.992435
H	1.543894	-1.370603	-2.420648
H	3.029131	-1.666042	-3.347914
H	0.227841	-2.525429	5.479972
H	-0.304115	-0.884499	5.888740
H	-1.483446	-2.188555	5.750833
H	-0.391566	-3.564991	3.258282
H	-2.101382	-3.154851	3.451023
H	-1.219466	-2.606378	2.012757
H	-1.180821	2.958102	1.304993
H	1.274143	3.671316	-0.047056
H	0.242479	-1.191783	3.418019
H	2.876942	-0.855422	-0.399880
H	-3.402628	-1.379073	-1.678372
H	-4.204478	-1.938138	-0.199889
H	-3.744588	-4.207197	-0.644151
H	-3.801084	-3.614320	-2.295922
H	-1.348721	-4.093274	-0.521756
H	-1.779047	-5.007035	-1.953470
H	0.131034	-3.372401	-2.211827
H	-1.047845	-4.151829	-4.245272
H	-2.274534	-2.881849	-4.053319
H	-0.594274	-2.443935	-4.404147
C	-1.685230	1.189054	-2.031050
C	-0.829888	2.423237	-2.286294
C	-3.190804	1.533511	-1.959699
C	-3.979895	1.319752	-3.256521
C	-3.586493	2.196702	-4.431606
O	-3.810492	3.567103	-4.047451
C	-3.564274	4.556553	-4.909883
O	-3.094717	4.099131	-6.088578
C	-2.814490	5.124397	-7.044548
O	-3.748834	5.717340	-4.641933
H	-2.061251	5.815542	-6.658673
H	-2.441666	4.607879	-7.929283
H	-3.720496	5.687030	-7.282775
H	-2.535822	2.062810	-4.707783
H	-4.195525	1.966335	-5.312181
H	-5.048413	1.471581	-3.060623
H	-3.868465	0.278749	-3.591449
H	-3.629931	0.899430	-1.183277
H	-3.325281	2.568412	-1.624369
H	-1.145915	2.962907	-3.184969
H	0.223265	2.152263	-2.402863
H	-0.924917	3.116984	-1.442903
H	-1.531807	0.481688	-2.864797

TS($\mathbf{V}^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VI}^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.662531 kcal.mol^{-1}

C	2.725672	2.964502	-1.678883

C	2.663236	1.654810	-1.143476	C	-2.114257	-0.278490	3.022155	H	1.175961	1.787221	4.935596
C	3.226309	0.563652	-1.845131	C	-3.421395	-0.374214	3.509851	H	2.625113	1.978871	3.330759
C	3.829276	0.805259	-3.083570	C	-4.281770	0.717225	3.505081	H	4.273734	-0.023901	-3.627442
C	3.875229	2.081161	-3.631368	C	-3.839609	1.933937	2.999006	H	4.342871	2.245858	-4.598371
C	3.327124	3.146755	-2.928010	C	-2.538950	2.086923	2.507989	H	3.371270	4.145609	-3.354575
N	1.985020	1.424272	0.095690	C	-1.211265	-1.504033	3.065771	H	-4.512380	2.788281	2.995526
C	2.592101	1.723170	1.247081	C	-0.743041	-1.814521	4.496474	H	-5.291257	0.620229	3.896228
C	4.040329	2.164354	1.246337	C	-2.110318	3.436092	1.950284	H	-3.769539	-1.325027	3.904635
C	3.238775	-0.843753	-1.267029	C	-2.315810	4.581748	2.951080	H	-1.915221	5.517815	2.546723
C	4.624277	-1.199717	-0.705220	O	-1.074259	0.678431	-1.437052	H	-3.377554	4.747062	3.164446
C	2.160869	4.178627	-0.951636	C	-2.839332	3.733712	0.632233	H	-1.816629	4.384088	3.904759
C	3.196752	5.304313	-0.812453	C	-1.884293	-2.738672	2.452849	H	-2.476740	4.669764	0.192065
C	1.973468	1.707294	2.508034	C	2.787243	-1.898148	-2.282905	H	-2.688716	2.927386	-0.090581
C	0.627216	1.508805	2.868132	C	0.894366	4.707617	-1.638753	H	-3.918022	3.838616	0.793909
C	0.287224	1.844062	4.304199	O	-2.394195	-1.417261	-0.763844	H	2.801101	6.109488	-0.183824
N	-0.332447	1.105376	2.034682	C	-3.353685	-1.745898	-1.778000	H	4.128863	4.948498	-0.363085
Zn	0.121852	0.717410	0.130352	C	-3.297688	-3.239455	-2.128151	H	3.448987	5.744272	-1.783355
O	-0.231052	-1.295744	-0.261387	C	-1.888957	-3.820055	-1.962461	H	1.104033	5.021253	-2.667607
C	-1.111298	-1.249418	-1.154324	H	4.104962	3.256248	1.185914	H	0.114751	3.942762	-1.674851
O	-0.859889	-1.622647	-2.443987	H	4.527012	1.859308	2.175550	H	0.495526	5.574101	-1.099231
C	-0.782267	-3.052522	-2.689618	H	4.595198	1.757505	0.399875	H	4.616715	-2.208351	-0.277061
C	-0.810164	-3.203451	-4.199659	H	-0.095674	2.869421	4.359735	H	5.385914	-1.174846	-1.493229
C	-1.670878	0.972055	2.530155	H	-0.486996	1.193467	4.712298	H	4.936015	-0.506271	0.081235

H	2.710077	-2.875600	-1.794369
H	1.809352	-1.642949	-2.697833
H	3.498235	-2.005087	-3.110054
H	-0.099026	-2.701070	4.502208
H	-0.174305	-0.989472	4.934529
H	-1.596115	-2.017858	5.154200
H	-1.165270	-3.563342	2.395054
H	-2.728860	-3.086883	3.058908
H	-2.243697	-2.522864	1.445012
H	-1.039909	3.377784	1.728673
H	1.873864	3.866150	0.056867
H	-0.329286	-1.283234	2.458569
H	2.525535	-0.868703	-0.437916
H	-3.174749	-1.125055	-2.656632
H	-4.320157	-1.471213	-1.350745
H	-3.975062	-3.803855	-1.478110
H	-3.665223	-3.374631	-3.151961
H	-1.647187	-3.853236	-0.895042
H	-1.868578	-4.858268	-2.313488
H	0.186949	-3.395235	-2.305637
H	-0.646347	-4.249732	-4.474903
H	-1.769838	-2.881765	-4.615031
H	-0.021868	-2.599636	-4.656798
C	-0.819265	1.256206	-2.700283
C	-1.867648	2.299462	-3.097474
C	-3.270081	1.713797	-3.246082
C	-4.370212	2.751049	-3.452255
O	-5.647142	2.069765	-3.602012
C	-6.337120	1.623522	-2.551246
O	-5.754223	1.929291	-1.374617
C	-6.466220	1.473906	-0.220789
C	-4.224347	3.582067	-4.714827
O	-7.373282	1.015575	-2.669083
H	0.174782	1.725252	-2.725253
H	-1.881465	3.097842	-2.343897
H	-1.539807	2.761615	-4.038415
H	-3.499900	1.149910	-2.337302
H	-3.295652	1.012124	-4.091343
H	-4.428706	3.405198	-2.576219
H	-5.780475	1.594790	0.617449
H	-6.753674	0.426784	-0.335468
H	-7.369433	2.072003	-0.070239
H	-0.804280	0.455053	-3.453716
H	-3.317226	4.190651	-4.669118
H	-4.166859	2.937381	-5.597601
H	-5.081457	4.250359	-4.833103

TS($\mathbf{V}^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VI}^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.656092 kcal.mol^{-1}

C	2.693341	3.037308	-1.600948
C	2.680236	1.717478	-1.085266
C	3.234038	0.649376	-1.828123
C	3.777439	0.922842	-3.087589
C	3.773459	2.207522	-3.615751
C	3.235790	3.251046	-2.871613
N	2.049524	1.455381	0.172178
C	2.679209	1.771951	1.307334
C	4.116550	2.243395	1.260120
C	3.296193	-0.768871	-1.280513
C	4.725477	-1.134152	-0.849827
C	2.127886	4.225896	-0.831912
C	3.116652	5.399201	-0.763551
C	2.093643	1.745115	2.583746
C	0.767437	1.483709	2.980157
C	0.441335	1.812248	4.420411
N	-0.188509	1.023104	2.174119
Zn	0.218984	0.681574	0.255580
O	-0.068555	-1.310765	-0.207514
C	-1.044079	-1.243802	-0.999036
O	-0.932648	-1.611265	-2.312177

C	-0.928130	-3.030620	-2.557532
H	-1.102254	-3.109688	-3.634614
C	-1.500436	0.789395	2.700825
C	-1.830495	-0.488160	3.210778
C	-3.120563	-0.688744	3.711883
C	-4.071642	0.324597	3.698768
C	-3.738015	1.568758	3.177712
C	-2.458006	1.827724	2.678657
C	-0.827688	-1.634057	3.251481
C	-0.340645	-1.915045	4.681897
C	-2.144767	3.203109	2.108193
C	-2.477006	4.337935	3.086678
O	-1.051936	0.668386	-1.272658
C	-2.865465	3.411482	0.768349
C	-1.393577	-2.916004	2.626812
C	2.755326	-1.802303	-2.275184
C	0.790537	4.693169	-1.423040
O	-2.271365	-1.425476	-0.467960
C	-3.370674	-1.669596	-1.372542
C	-3.377330	-3.150266	-1.803716
C	-1.987307	-3.791037	-1.770339
H	4.161793	3.325730	1.098527
H	4.616783	2.030424	2.207193
H	4.672548	1.772966	0.447250
H	-0.025421	2.802806	4.471842
H	-0.266113	1.106487	4.857510
H	1.347232	1.838874	5.028766
H	2.754040	2.047827	3.388229
H	4.213182	0.110988	-3.663934
H	4.193874	2.396934	-4.599782
H	3.240604	4.256627	-3.284396
H	-4.483228	2.360266	3.163953
H	-5.068495	0.144949	4.092844
H	-3.383601	-1.661533	4.119018
H	-2.161315	5.301899	2.672677
H	-3.553047	4.404056	3.281573
H	-1.976281	4.203021	4.050732
H	-2.600888	4.381954	0.332746
H	-2.602039	2.626402	0.053888
H	-3.952979	3.392347	0.902659
H	2.733160	6.179900	-0.097699
H	4.097195	5.086259	-0.391427
H	3.270653	5.858365	-1.746102
H	0.906473	5.000764	-2.468288
H	0.043377	3.896266	-1.389599
H	0.398433	5.549123	-0.862139
H	4.752521	-2.146817	-0.432142
H	5.414376	-1.104706	-1.701872
H	5.109522	-0.449008	-0.088060
H	2.730466	-2.791854	-1.806036
H	1.740300	-1.548337	-2.589211
H	3.386174	-1.880288	-3.168066
H	0.381958	-2.738852	4.683318
H	0.147587	-1.045646	5.131226
H	-1.174496	-2.202215	5.332899
H	-0.610978	-3.680624	2.569715
H	-2.212473	-3.332381	3.224953
H	-1.762717	-2.721630	1.618239
H	-1.068785	3.243989	1.910521
H	1.928272	3.903297	0.194311
H	0.036623	-1.336380	2.651116
H	2.659808	-0.811336	-0.391968
H	-3.221561	-1.033433	-2.246815
C	-4.633560	-1.258282	-0.642172
H	-4.036181	-3.722864	-1.139750
H	-3.811482	-3.216726	-2.808831
H	-1.661820	-3.884846	-0.729198
H	-2.034696	-4.810627	-2.171366
H	0.070119	-3.426255	-2.336180

C	-0.730569	1.219783	-2.537521
C	-1.775107	2.214545	-3.050612
C	-3.145325	1.590006	-3.300804
C	-4.194193	2.550007	-3.856110
O	-5.444445	1.819208	-4.003510
C	-6.328778	1.716565	-3.011947
O	-5.993284	2.446633	-1.927771
C	-6.952499	2.393531	-0.869175
C	-3.886653	3.087858	-5.242713
O	-7.327356	1.044075	-3.101194
H	0.244073	1.725862	-2.504688
H	-1.873576	3.044075	-2.338550
H	-1.376249	2.644105	-3.979578
H	-3.519888	1.187863	-2.354350
H	-3.049442	0.748119	-4.000004
H	-4.354010	3.376925	-3.158120
H	-6.551478	3.026664	-0.077810
H	-7.077621	1.368721	-0.512171
H	-7.920712	2.770359	-1.207828
H	-0.633160	0.400282	-3.263195
H	-2.982145	3.701766	-5.225136
H	-3.736156	2.266804	-5.950707
H	-4.712866	3.706050	-5.604004
H	-5.505574	-1.412714	-1.285565
H	-4.761818	-1.851055	0.268738
H	-4.587581	-0.203724	-0.359484

TS($\mathbf{V}^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)}\rightarrow\mathbf{VI}^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R}$

G = -2500.655125 kcal.mol^{-1}

C	-2.310845	1.849257	2.749849
C	-1.333721	0.842639	2.943918
C	-1.655993	-0.352061	3.629622
C	-2.962425	-0.512483	4.104811
C	-3.929855	0.465184	3.918957
C	-3.598800	1.637345	3.247429
N	-0.034630	1.032396	2.375930
Zn	0.256577	0.704233	0.411509
O	-1.267526	0.524820	-0.796229
C	-1.653040	1.162758	-1.995544
C	-3.167429	1.472403	-1.981575
C	-3.900864	1.232206	-3.306124
C	-3.488194	2.117958	-4.467901
O	-3.767671	3.481708	-4.096259
C	-3.514433	4.477432	-4.949447
O	-3.745265	5.632300	-4.691924
C	-0.647701	-1.465209	3.885311
C	-1.029951	-2.762248	3.159002
C	-1.958383	3.163125	2.067077
C	-3.136651	3.814058	1.336630
C	1.007876	1.340343	3.138877
C	0.850361	1.541215	4.632095
C	2.327915	1.495227	2.665131
C	2.842324	1.526416	1.363031
C	4.346412	1.687582	1.269510
N	2.116539	1.394006	0.242941
C	2.726734	1.700234	-1.016944
C	2.710116	3.044712	-1.473533
C	3.308712	3.338889	-2.701956
C	3.898253	2.346818	-3.477939
C	3.891735	1.033942	-3.028127
C	3.315069	0.684171	-1.801773
C	2.073433	4.164265	-0.656414
C	1.372142	5.219875	-1.521697
C	3.364788	-0.769250	-1.356403
C	2.610142	-1.680030	-2.333371
C	4.809921	-1.261312	-1.182672
C	3.090899	4.861546	0.262202
O	0.039391	-1.366500	0.053421
C	-1.013498	-1.424975	-0.616031
O	-2.139793	-1.786754	0.028549

C	-3.307123	-2.104070	-0.756185	H	-3.222330	-1.427025	4.631942	H	-1.984591	-3.155249	3.528674
C	-3.204278	-3.546583	-1.290513	H	-1.088929	5.098655	2.566460	H	-1.118210	-2.595291	2.085100
C	-1.757360	-4.010975	-1.471646	H	-2.062808	4.388047	3.865684	H	-1.188583	2.942447	1.317466
C	-0.903985	-3.078860	-2.321376	H	-0.440412	3.765005	3.530682	H	1.317550	3.699630	-0.012859
H	-1.216332	-3.104442	-3.369760	H	-2.784214	4.658610	0.735410	H	0.317944	-1.145060	3.482511
O	-1.016524	-1.688655	-1.960987	H	-3.638048	3.108274	0.669061	H	2.860770	-0.840588	-0.388016
C	-0.473121	-1.740461	5.387800	H	-3.882173	4.211017	2.034887	H	-3.340515	-1.403931	-1.594797
C	-1.348164	4.158847	3.067023	H	2.611358	5.684439	0.804240	C	-4.506701	-1.889699	0.146009
C	-0.819460	2.417795	-2.218685	H	3.513776	4.180778	1.003430	H	-3.702640	-4.231462	-0.593959
O	-2.980620	4.033547	-6.105647	H	3.916613	5.281568	-0.323650	H	-3.753152	-3.608386	-2.238430
C	-2.689613	5.066146	-7.050485	H	2.090780	5.845854	-2.062505	H	-1.293811	-4.125617	-0.486312
H	4.740364	2.210669	2.143253	H	0.698761	4.769519	-2.255174	H	-1.736437	-5.002578	-1.939484
H	4.807268	0.693279	1.245258	H	0.783577	5.890033	-0.886347	H	0.150016	-3.375040	-2.267971
H	4.659422	2.213123	0.366986	H	4.820857	-2.282507	-0.785952	H	-1.977090	5.781210	-6.632258
H	1.410899	2.424740	4.949535	H	5.343532	-1.273124	-2.139732	H	-2.260717	4.560716	-7.915991
H	-0.192241	1.653304	4.929923	H	5.379826	-0.625736	-0.498775	H	-3.601166	5.599489	-7.331185
H	1.268599	0.683434	5.169034	H	2.626080	-2.714118	-1.970689	H	-2.424184	2.014866	-4.703178
H	3.063387	1.657711	3.445756	H	1.567991	-1.369370	-2.434755	H	-4.055789	1.868117	-5.370578
H	4.352031	0.258843	-3.635888	H	3.072667	-1.670768	-3.327226	H	-4.979897	1.354208	-3.151422
H	4.357876	2.598437	-4.430085	H	0.332772	-2.464742	5.551157	H	-3.746353	0.193827	-3.631495
H	3.308996	4.363817	-3.061287	H	-0.235549	-0.833993	5.951731	H	-3.621488	0.832156	-1.219190
H	-4.356513	2.402619	3.110218	H	-1.385200	-2.165281	5.821729	H	-3.339053	2.505344	-1.657287
H	-4.937578	0.318771	4.298902	H	-0.267159	-3.530122	3.333156	H	-1.121029	2.953405	-3.124727

H	0.242769	2.172338	-2.306223
H	-0.955856	3.105657	-1.376057
H	-1.451539	0.459584	-2.821855
H	-5.429098	-2.119929	-0.397023
H	-4.448977	-2.543636	1.021447
H	-4.551111	-0.855644	0.495806

VI$^{a\delta,\delta a}{}_{7CC\text{-}\gamma(R)}$

G = -2500.681477 kcal.mol^{-1}

Zn	0.331982	0.344617	0.500475
O	-0.459413	-0.324150	-1.083206
O	-2.072688	0.208307	0.328583
C	-3.445080	0.430000	0.664004
H	-3.805767	1.325183	0.146571
C	-1.762488	-0.022034	-1.059936
H	-3.248667	-1.246291	3.426774
C	-2.673189	-0.883588	4.282950
N	1.404926	1.990805	0.628171
C	-1.179227	-0.753959	3.961594
N	1.018730	-0.629099	2.067353
H	-1.063953	0.064171	3.240272
C	2.073448	-0.149906	2.734489
C	2.641998	1.118488	2.524235
H	3.467702	1.359339	3.183579
H	3.957521	3.299444	0.771301
C	3.224150	3.336661	1.584099
C	2.352048	2.102723	1.560823
O	-2.103314	1.170957	-1.714750
C	-2.398824	1.146924	-3.118632
C	-1.208977	0.683735	-3.947916
O	-2.582474	-1.024621	-1.583412
C	-2.620762	-2.240275	-0.829174
C	-3.586713	-2.106254	0.380367
C	-4.347667	-0.779361	0.370277
C	0.488153	-1.917515	2.394927
C	-0.591752	-2.000657	3.308572
C	-1.110732	-3.264800	3.604051
C	-0.606243	-4.413932	3.003539
C	0.433159	-4.311788	2.088662
C	1.002676	-3.074177	1.769689
C	2.771414	-1.022012	3.755220
C	1.268217	3.000366	-0.381216
C	0.302173	4.017601	-0.224471
C	0.142285	4.948765	-1.255171
C	0.899779	4.879627	-2.417838
C	1.848223	3.872435	-2.557299
C	2.057257	2.923550	-1.552028
C	-0.569814	4.126384	1.017534
C	-2.060490	4.046765	0.660030
C	3.095250	1.829495	-1.761951
C	2.610337	0.798358	-2.792162
C	2.133242	-3.013205	0.752080
C	3.278514	-3.977407	1.092379
C	-0.424640	-0.349298	5.238597
C	-2.866225	2.571090	-3.425889
C	-3.400414	2.791869	-4.850152
C	-2.384683	3.287098	-5.864208
O	-1.957623	4.600975	-5.450529
C	-1.063039	5.175072	-6.254952
O	-0.615410	4.712261	-7.280342
O	-0.740287	6.368958	-5.733421
C	0.189597	7.115627	-6.519842
C	-3.052920	-3.326024	-1.800926
C	4.466974	2.391345	-2.162145
C	1.611039	-3.270337	-0.670238
C	-0.272070	5.403031	1.817675
H	1.129094	6.569242	-6.636395
H	-0.220582	7.325492	-7.511222
H	0.354636	8.044537	-5.973828
H	-2.825094	3.360657	-6.864231

H	-1.505451	2.641172	-5.934301
H	-0.371325	1.380020	-3.846758
H	-1.486634	0.610065	-5.004954
H	-3.236581	0.455516	-3.282593
H	-3.836080	1.863808	-5.244564
H	-4.218535	3.520786	-4.824752
H	-2.049301	3.270527	-3.216079
H	-2.363608	-3.383460	-2.647766
H	-4.057264	-3.119923	-2.187299
H	-3.071842	-4.298826	-1.299384
H	-4.311237	-2.929343	0.360433
H	-3.421949	0.639806	1.736542
H	-3.021918	-2.209932	1.312437
H	-4.834062	-0.654944	-0.601365
H	-5.144781	-0.804522	1.123806
H	-0.876441	-0.302175	-3.618507
H	-3.658586	2.804659	-2.706576
H	3.224367	1.303118	-0.810668
H	-0.481122	6.300167	1.224414
H	3.485171	-1.676581	3.241578
H	3.649100	-3.827721	2.111661
H	0.815571	-5.210550	1.611874
H	-1.607215	-2.453148	-0.473253
H	3.766553	3.413976	2.527835
H	2.635002	4.243725	1.432643
H	3.331472	-0.414891	4.469025
H	2.078768	-1.667310	4.297037
H	2.437714	3.817410	-3.469060
H	0.739566	5.599558	-3.215162
H	-0.598841	5.736810	-1.149015
H	-1.931857	-3.353178	4.308739
H	-1.029282	-5.385397	3.244743
H	-0.902905	0.520316	5.703289
H	-0.433144	-1.166686	5.968728
H	0.614589	-0.082678	5.037594
H	-3.075514	0.092006	4.575826
H	-2.853262	-1.564975	5.122139
H	-0.897083	5.446720	2.716715
H	0.774275	5.452789	2.135132
H	-2.380938	4.925946	0.089625
H	-2.267990	3.161112	0.054712
H	-2.670654	4.006536	1.569698
H	5.209595	1.586955	-2.200661
H	4.440842	2.856328	-3.153507
H	4.822596	3.146993	-1.453869
H	3.343173	-0.009530	-2.901921
H	1.651982	0.360760	-2.498592
H	2.479995	1.264180	-3.775758
H	4.115351	-3.829637	0.401309
H	2.967334	-5.023995	1.005306
H	1.168021	-4.270017	-0.747004
H	0.852006	-2.536686	-0.958439
H	2.431251	-3.213589	-1.394947
H	-0.336450	3.270853	1.659814
H	2.544567	-1.998557	0.771132

VI$^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.680281 kcal.mol^{-1}

Zn	-0.162194	0.779661	0.355091
O	-2.248530	1.367932	-0.605204
C	-3.358500	2.219168	-0.908879
C	-4.687028	1.479493	-1.035812
C	-4.903677	0.389579	0.013965
C	-3.828022	-0.724504	-0.055060
O	-2.090824	0.499650	-2.774430
C	-4.436182	-2.110691	0.075487
C	-0.897937	1.025845	-3.337139
C	-1.161693	1.294347	-4.810783
C	-0.811098	0.887424	-7.908781
O	-3.682783	-2.634442	-8.015565

C	-3.414728	-1.563813	-7.528297	C	2.060919	1.534726	2.505160	H	4.274409	2.631718	1.902420
O	-2.222120	-0.985251	-7.679400	C	0.917845	0.905569	3.029830	H	4.285351	2.062320	0.219572
C	-1.899180	0.279504	-7.040595	C	1.001968	0.506286	4.486644	H	1.721281	1.130154	5.020715
C	-1.482296	0.021172	-5.595561	C	2.042665	3.742082	-2.962889	H	0.036519	0.556599	4.991601
O	-4.268291	-0.818546	-6.796039	C	-1.385238	-1.390161	3.109583	H	1.346439	-0.532063	4.555169
C	-5.554722	-1.412148	-6.611529	C	1.032338	4.477428	-0.771154	H	2.843538	1.728373	3.228878
C	-2.525295	-1.932890	3.712157	C	-0.407135	4.746306	-1.231006	H	3.461539	0.830296	-3.946642
N	-0.175093	0.606515	2.323088	N	1.555424	1.739827	0.141844	H	2.916381	3.077856	-4.814840
H	-2.606808	-3.011437	3.817573	C	2.361367	1.926981	1.190372	H	1.820457	4.734972	-3.345745
C	1.990074	2.126172	-1.167265	C	3.700246	2.593132	0.975813	H	-4.266681	0.884844	4.403568
C	1.702576	3.425319	-1.643872	C	3.031045	-0.206678	-1.490886	H	-4.425114	-1.563219	4.651337
H	1.862500	6.282801	-1.694319	C	4.540801	-0.457952	-1.626359	H	-1.585501	4.118840	4.393398
C	1.832801	5.786669	-0.718350	C	-2.057744	0.163831	-1.422559	H	-2.133179	2.789436	5.427951
C	-3.551413	-1.121862	4.179465	O	-3.160223	-0.685834	-1.314986	H	-0.555927	2.705112	4.627643
C	-3.457771	0.259152	4.038361	C	-2.268510	2.371003	3.291549	H	-3.491966	4.088393	2.797347
C	-2.348176	0.854753	3.431203	C	-3.631015	3.033162	3.055579	H	-4.260741	3.006474	3.951784
C	-0.289014	-2.321192	2.610398	C	0.186434	-3.295077	3.698675	H	1.372831	6.485096	-0.010886
C	-0.735420	-3.088489	1.356306	C	2.235132	-1.314422	-2.197047	H	2.867905	5.620038	-0.403448
C	2.645860	1.180482	-1.989094	C	-1.591517	3.028853	4.505712	H	-0.426333	5.143081	-2.252332
C	2.963823	1.548929	-3.300449	H	-4.183436	2.554166	2.243007	H	-1.001825	3.829178	-1.216007
C	2.660276	2.813106	-3.792453	H	-3.094593	-0.580310	0.745649	H	-0.892589	5.480313	-0.577848
O	-0.909504	-0.349260	-0.973637	H	0.569106	-1.703251	2.326173	H	4.804974	-1.423632	-1.182071
C	-1.303441	0.013460	2.975578	H	3.567945	3.614738	0.606272	H	4.851476	-0.484943	-2.676326

H	5.133295	0.315834	-1.127208
H	2.541947	-2.298058	-1.823588
H	1.160266	-1.206615	-2.026063
H	2.416978	-1.302184	-3.277988
H	1.046867	-3.870660	3.340970
H	0.483073	-2.774127	4.614818
H	-0.595074	-4.014147	3.966878
H	0.070611	-3.741580	1.002931
H	-1.602316	-3.721846	1.576661
H	-1.002566	-2.409304	0.541356
H	-1.641575	2.579339	2.416638
H	0.981203	4.079104	0.247296
H	2.786088	-0.255795	-0.424963
H	-3.153453	2.777420	-1.831131
H	-3.387305	2.931564	-0.078532
H	-5.490618	2.224776	-0.975185
H	-4.744960	1.022953	-2.027368
H	-4.920914	0.811015	1.025858
H	-5.895873	-0.048532	-0.154030
H	-4.982994	-2.196198	1.019949
H	-5.133644	-2.297538	-0.748097
H	-3.659711	-2.878856	0.049611
H	-0.607539	1.956696	-2.832030
H	-1.993667	2.006372	-4.897536
H	-0.272357	1.790626	-5.216910
H	-2.294369	-0.504520	-5.084881
H	-0.611965	-0.648112	-5.596333
H	-2.792056	0.913147	-7.060220
H	-6.120559	-0.704236	-6.005512
H	-5.465568	-2.370644	-6.094676
H	-6.046891	-1.573442	-7.573887
H	-0.077422	0.312068	-3.214690
H	-0.535584	1.879419	-7.540318
H	0.081957	0.254567	-7.906371
H	-1.157086	0.988889	-8.940939

VI$^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.679246 kcal.mol^{-1}

C	0.491448	3.681075	-1.394111
C	1.185344	2.639458	-0.739792
C	2.202480	1.919330	-1.402753
C	2.489193	2.241898	-2.732556
C	1.803041	3.252424	-3.394868
C	0.816551	3.965011	-2.723411
N	0.818905	2.276206	0.597422
C	1.384463	2.906396	1.626282
C	2.406826	3.986193	1.360693
C	2.972947	0.799494	-0.718990
C	2.541227	-0.569292	-1.263981
C	-0.612936	4.468209	-0.704286
C	-0.446097	5.986354	-0.850977
C	1.095122	2.629469	2.975448
C	0.259884	1.657008	3.546015
C	0.251605	1.598035	5.056190
N	-0.491231	0.783089	2.859392
Zn	-0.518639	0.843235	0.913887
O	-1.255778	0.168842	-0.641651
C	-2.178997	-0.801129	-0.717261
O	-3.464720	-0.362183	-0.312405
C	-4.497645	-0.161009	-1.270116
C	-4.316430	1.076497	-2.141595
C	-5.475108	1.232368	-3.128344
C	-5.393557	2.503313	-3.969927
C	-4.229799	2.542004	-4.942997
C	-1.213637	-0.223411	3.587548
C	-2.570577	-0.013895	3.915832
C	-3.247397	-1.021499	4.611419
C	-2.612889	-2.202434	4.975427
C	-1.276801	-2.394600	4.642354
C	-0.553167	-1.419997	3.950274

C	-3.312498	1.266107	3.558210	H	2.795902	-2.214972	4.514953	H	-4.609291	-1.049007	-1.902406
C	-3.747176	2.043307	4.810267	H	-3.150753	-4.762258	1.098510	H	3.235524	3.593484	0.763693
C	0.903131	-1.684468	3.590662	H	-3.103922	-3.225359	1.994021	H	1.968575	4.804391	0.781289
C	1.740552	-2.132397	4.796590	H	-1.598286	-4.078433	1.612211	H	2.804780	4.390733	2.292250
O	-1.813670	-1.845851	0.167256	H	0.066860	-2.822886	-1.108118	H	-0.767385	1.549252	5.446599
C	-2.506200	-3.076771	-0.077868	H	0.423439	-2.403560	1.582309	H	0.763478	0.697327	5.409633
C	-1.792065	-3.895542	-1.190507	H	0.636964	-3.688432	2.776310	H	0.755376	2.467244	5.481241
C	-0.664980	-3.112530	-1.866975	H	-10.239401	3.221196	-3.763301	H	1.626109	3.246281	3.690070
C	-1.168610	-1.870818	-2.611499	H	-10.567121	3.673564	-5.466489	H	3.264524	1.689676	-3.257251
O	-2.324942	-1.289942	-2.021560	H	-5.376035	3.375785	-3.308100	H	2.038849	3.486879	-4.429383
C	-2.595499	-3.828202	1.237938	H	-4.260008	3.457226	-5.540625	H	0.284280	4.758012	-3.241989
C	1.010620	-2.710194	2.452463	H	-4.265430	1.685055	-5.623173	H	-4.291500	-0.872801	4.874608
C	-4.520984	0.984657	2.654262	H	-3.280035	2.514130	-4.403090	H	-3.157208	-2.971345	5.517100
C	4.493396	0.977740	-0.828126	H	-6.422429	1.260644	-2.575855	H	-0.784838	-3.321819	4.924168
C	-1.989127	4.017449	-1.212679	H	-5.519486	0.367068	-3.803069	H	-4.241741	2.978247	4.524881
O	-6.589043	2.603099	-4.790438	H	-1.502687	-2.143828	-3.617956	H	-4.457400	1.463916	5.410502
C	-7.650227	3.171352	-4.217464	H	-4.253173	1.960513	-1.495880	H	-2.899572	2.297136	5.454715
O	-7.718167	3.623806	-3.094966	H	-0.141381	-3.758369	-2.583152	H	-4.999959	1.925481	2.360050
O	-8.649771	3.165582	-5.111204	H	-1.368140	-4.811376	-0.759740	H	-4.221270	0.449916	1.749435
C	-9.861436	3.754724	-4.639516	H	-2.528204	-4.215410	-1.938003	H	-5.274409	0.383471	3.176082
H	2.718376	0.823697	0.345767	H	-3.521042	-2.825904	-0.404917	H	-1.208933	6.508385	-0.263370
H	-2.621022	1.905086	2.998586	H	-0.378277	-1.117220	-2.707278	H	0.536330	6.325084	-0.505696
H	-0.570003	4.236589	0.364898	H	-5.407521	-0.061302	-0.666619	H	-0.560359	6.310790	-1.890910

H	-2.105177	4.251419	-2.277089
H	-2.114837	2.937885	-1.094982
H	-2.792500	4.525811	-0.667404
H	5.008822	0.199681	-0.254537
H	4.838837	0.900770	-1.864638
H	4.816298	1.950579	-0.443357
H	3.053779	-1.379710	-0.733573
H	1.461969	-0.710032	-1.154541
H	2.782529	-0.660167	-2.329174
H	1.668574	-1.427435	5.631028
H	1.425938	-3.113830	5.167359
H	2.054871	-2.838185	2.145144
H	1.332976	-0.746981	3.224415
H	-3.362761	0.987560	-2.669937
H	-9.707004	4.803701	-4.373070

VI$^{a\delta,a\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.674144 kcal.mol^{-1}

C	-0.085225	-2.050343	2.803356
C	-0.238937	-0.692972	3.159735
C	-1.247534	-0.288876	4.063006
C	-2.089172	-1.267168	4.600714
C	-1.947358	-2.608079	4.262770
C	-0.952844	-2.988952	3.370044
N	0.591191	0.297630	2.545054
C	1.712845	0.695596	3.139903
C	2.121008	0.064900	4.449990
C	-1.460687	1.172697	4.432080
C	-1.530619	1.396052	5.949054
C	0.969949	-2.509330	1.807836
C	1.877495	-3.607462	2.379786
Zn	0.039234	1.085124	0.812904
O	-1.449156	0.200927	0.179846
C	-2.283715	0.616909	-0.778164
O	-1.532832	1.186044	-1.817554
C	-2.234172	1.593575	-3.002929
C	-1.938411	0.592261	-4.112917
O	-3.033618	-0.431484	-1.328999
C	-3.609824	-1.365309	-0.412807
C	-4.247002	-0.741137	0.822934
C	-5.182053	0.434878	0.537203
C	-4.579497	1.467799	-0.431197
O	-3.169831	1.624251	-0.250061
C	-5.197576	2.844874	-0.249950
N	1.452489	2.380877	0.562080
C	1.468483	3.253274	-0.580333
C	2.126355	2.842278	-1.760557
C	2.106583	3.701212	-2.863473
C	1.462253	4.932298	-2.813428
C	0.817057	5.318295	-1.644523
C	0.804333	4.497311	-0.512195
C	2.825711	1.494649	-1.870225
C	4.272721	1.619868	-2.366630
C	0.070891	4.956812	0.740428
C	-1.451011	4.934547	0.531206
C	-1.815939	3.033383	-3.298568
C	-2.499106	3.671132	-4.520083
C	-1.712614	3.582223	-5.816777
O	-0.521794	4.378058	-5.640774
C	0.441845	4.371043	-6.559270
O	0.120923	3.630411	-7.637213
C	1.131326	3.592256	-8.648435
C	0.529356	6.343964	1.212039
C	2.445758	2.471666	1.460058
C	2.561664	1.693238	2.621870
C	3.541478	3.484533	1.223485
C	2.027160	0.536854	-2.767561
C	-2.714155	1.735203	3.744000
C	0.321037	-2.964860	0.491916
O	1.479366	4.974768	-6.419087

H	-4.356813	-1.897289	-1.013410
H	4.060032	3.284709	0.281152
H	3.128852	4.494009	1.139209
H	4.270306	3.468707	2.034750
H	1.372680	0.263752	5.223551
H	2.185298	-1.022970	4.353152
H	3.084375	0.446967	4.790577
H	3.438299	1.902102	3.222668
H	2.599167	3.404574	-3.785491
H	1.450702	5.566759	-3.693881
H	0.306904	6.277730	-1.610549
H	-2.872654	-0.971640	5.293594
H	-2.611657	-3.353254	4.692200
H	-0.847564	-4.037357	3.102934
H	-1.590056	2.466844	6.172053
H	-2.414773	0.923218	6.389965
H	-0.650869	0.993197	6.461556
H	-2.840870	2.797418	3.983047
H	-2.660344	1.633297	2.655980
H	-3.612758	1.207183	4.083440
H	0.044346	6.601591	2.159947
H	1.612529	6.385566	1.365463
H	0.268073	7.124361	0.489327
H	-1.743228	5.628349	-0.265590
H	-1.814131	3.939322	0.256996
H	-1.968299	5.244259	1.446675
H	4.763072	0.640233	-2.357818
H	4.315865	1.998155	-3.393357
H	4.863065	2.297418	-1.741098
H	2.496885	-0.453176	-2.791667
H	0.996576	0.425550	-2.418591
H	1.990612	0.913614	-3.796422
H	2.669056	-3.856438	1.664609
H	2.354032	-3.295733	3.315016
H	1.320340	-4.528367	2.583703
H	1.088279	-3.242639	-0.239963
H	-0.315988	-3.842199	0.654044
H	-0.297842	-2.171312	0.063138
H	-0.601530	1.739480	4.059004
H	0.303649	4.247784	1.541765
H	1.605812	-1.647791	1.578749
H	2.860362	1.054208	-0.868375
H	-4.771147	1.121515	-1.453748
H	-5.428127	0.922755	1.489507
H	-6.133002	0.085600	0.112131
H	-3.445653	-0.408597	1.485926
H	-4.789913	-1.531368	1.356777
H	-2.846483	-2.087353	-0.098821
H	2.054937	3.161725	-8.253984
H	0.727394	2.965818	-9.443860
H	1.340784	4.597756	-9.021095
H	-1.425175	2.555671	-6.058099
H	-2.286433	3.983998	-6.659239
H	-2.687684	4.732984	-4.325782
H	-3.483834	3.216637	-4.695790
H	-2.050387	3.617104	-2.404077
H	-0.727285	3.082158	-3.408371
H	-2.516513	0.814541	-5.016826
H	-2.206770	-0.410659	-3.774746
H	-0.873812	0.600555	-4.368725
H	-3.310851	1.583573	-2.800924
H	-6.285635	2.793219	-0.363378
H	-4.974927	3.233033	0.749174
H	-4.804335	3.550315	-0.987384

TS($\mathbf{VI}^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VII}^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.665665 kcal.mol^{-1}

Zn	0.256978	0.300972	0.526997
O	0.138393	-0.712946	-1.209448
O	-1.628333	0.420112	-0.184204

C	-2.968959	0.430147	0.253078	C	-0.812088	-2.003454	3.278296	C	-1.631607	5.329037	-6.326322
H	-3.503192	1.300771	-0.161295	C	-1.347526	-3.261213	3.571519	O	-2.027711	4.952960	-7.406752
C	-0.988595	-0.342373	-1.681900	C	-0.762942	-4.426676	3.087429	O	-0.682132	6.251910	-6.118984
H	-3.461821	-1.248385	3.040785	C	0.379125	-4.346076	2.301726	C	-0.127810	6.799988	-7.316029
C	-2.997174	-0.863567	3.953308	C	0.967021	-3.114985	1.990564	C	-2.788631	-3.435350	-2.120737
N	1.397697	1.928109	0.630419	C	2.516627	-0.952701	3.986697	C	4.352434	2.062053	-1.855616
C	-1.474551	-0.741691	3.818146	C	1.280317	2.957881	-0.359791	C	1.952327	-3.514871	-0.307221
N	0.895946	-0.654272	2.148456	C	0.460526	4.082429	-0.111828	C	-0.055697	5.636229	1.836437
H	-1.264420	0.060321	3.099572	C	0.325233	5.045563	-1.116377	H	0.346591	6.020098	-7.917469
C	1.909129	-0.146993	2.857488	C	0.985739	4.920664	-2.333021	H	-0.901495	7.286350	-7.915829
C	2.519180	1.095045	2.615272	C	1.796593	3.814677	-2.558130	H	0.612868	7.529341	-6.988003
H	3.309707	1.349782	3.311721	C	1.956681	2.814863	-1.593339	H	-3.996718	4.334695	-5.581094
H	3.462399	3.640903	0.699200	C	-0.296719	4.261669	1.196583	H	-2.763189	3.097101	-5.855566
C	3.145962	3.300314	1.686779	C	-1.798859	4.018297	0.994197	H	-1.352996	0.876959	-5.199205
C	2.297484	2.050912	1.605220	C	2.875687	1.636830	-1.886477	H	-3.128531	0.874250	-5.119153
O	-0.940667	0.679484	-2.563971	C	2.544820	0.950813	-3.218079	H	-3.008407	0.806012	-2.622196
C	-2.145613	1.149566	-3.203733	C	2.232384	-3.094404	1.143484	H	-4.171603	2.757336	-3.742498
C	-2.215107	0.558614	-4.604358	C	3.339998	-3.971261	1.748222	H	-3.536331	4.272308	-3.136599
O	-1.938181	-1.244586	-2.037318	C	-0.876670	-0.307836	5.166762	H	-1.148472	3.006960	-3.632356
C	-2.093821	-2.423004	-1.224761	C	-2.071129	2.673635	-3.145392	H	-2.223844	-3.586859	-3.044680
C	-2.897951	-2.111751	0.056077	C	-3.282387	3.402086	-3.751912	H	-3.797167	-3.098520	-2.383942
C	-3.755066	-0.850587	-0.072577	C	-3.080323	3.892188	-5.174761	H	-2.872668	-4.395966	-1.603831
C	0.361146	-1.937159	2.485766	O	-2.057470	4.905323	-5.134711	H	-3.532598	-2.977159	0.279448

H	-2.957119	0.563279	1.343768	H	0.185185	-0.065960	5.086827	Zn	-0.369032	1.007160	0.346519
H	-2.214385	-2.007282	0.903685	H	-3.431806	0.118005	4.169965	O	-2.055932	1.554621	-0.588767
H	-4.182053	-0.795269	-1.079964	H	-3.281054	-1.525361	4.779200	C	-3.173933	2.409186	-0.456232
H	-4.606589	-0.900246	0.617524	H	-0.535412	5.687152	2.820047	C	-4.502406	1.717603	-0.749571
H	-2.216831	-0.532061	-4.549058	H	1.010882	5.844357	1.968508	C	-4.793331	0.462926	0.077601
H	-1.960105	2.945763	-2.092389	H	-2.225728	4.758812	0.307957	C	-3.725748	-0.635388	-0.066699
H	2.725584	0.896629	-1.094797	H	-1.975174	3.025338	0.573080	O	-1.961158	0.440094	-2.848465
H	-0.474559	6.445073	1.228031	H	-2.338302	4.094063	1.945636	C	-4.300991	-2.029372	0.109260
H	3.332163	-1.571156	3.595123	H	5.002726	1.200520	-2.044960	C	-0.695799	0.736911	-3.438892
H	3.534567	-3.724163	2.796571	H	4.561134	2.813012	-2.626331	C	-0.939531	1.059268	-4.903230
H	0.831997	-5.259075	1.923508	H	4.637924	2.489596	-0.889628	C	-0.723199	0.643125	-8.011832
H	-1.094763	-2.781304	-0.961918	H	3.172840	0.062073	-3.345025	O	-4.175616	-2.312705	-8.099100
H	4.026750	3.133318	2.309231	H	1.499247	0.639467	-3.245903	C	-3.711335	-1.317306	-7.600490
H	2.567797	4.116552	2.133834	H	2.737924	1.609541	-4.072847	O	-2.438465	-0.955226	-7.773046
H	2.941777	-0.292690	4.745966	H	4.272797	-3.842185	1.188736	C	-1.884825	0.222599	-7.127908
H	1.797194	-1.624388	4.456625	H	3.079879	-5.034641	1.704892	C	-1.490928	-0.127504	-5.695428
H	2.315830	3.719138	-3.508217	H	1.537874	-4.528992	-0.349312	O	-4.401248	-0.450175	-6.831019
H	0.857348	5.672894	-3.106202	H	1.252336	-2.828400	-0.790169	C	-5.769518	-0.808235	-6.626354
H	-0.310626	5.910009	-0.942216	H	2.881425	-3.513109	-0.888583	C	-2.433556	-2.070807	3.648537
H	-2.242247	-3.331626	4.182690	H	0.063659	3.502317	1.897957	N	-0.284219	0.671750	2.316152
H	-1.198451	-5.394106	3.322832	H	2.600610	-2.064144	1.117110	H	-2.440942	-3.155803	3.712895
H	-1.392000	0.582880	5.543430					C	1.917450	2.128679	-1.202161
H	-0.989386	-1.102711	5.912924	TS($\mathbf{VI}^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VII}^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)				C	1.583853	3.356435	-1.819115

G = -2500.672381 kcal.mol^{-1}

H	1.923725	6.156331	-1.806384
C	1.608434	5.700189	-0.861378
C	-3.501729	-1.349723	4.165104
C	-3.497709	0.039327	4.084398
C	-2.439719	0.730969	3.487126
C	-0.192666	-2.272971	2.513679
C	-0.611839	-3.082806	1.277708
C	2.689845	1.161825	-1.889806
C	3.090459	1.440696	-3.200149
C	2.764122	2.641656	-3.820584
O	-0.912548	-0.405342	-0.991094
C	-1.353944	-0.019626	2.968937
C	1.924727	1.667526	2.481595
C	0.815429	0.980692	3.006071
C	0.956049	0.538072	4.447401
C	2.022648	3.590344	-3.126716
C	-1.342869	-1.430643	3.049229
C	0.777739	4.430959	-1.103797
C	-0.511302	4.768505	-1.864529
N	1.428225	1.839253	0.111508
C	2.227267	2.040718	1.161687
C	3.586867	2.669585	0.952974
C	3.098510	-0.163205	-1.257725
C	4.616435	-0.390017	-1.328314
C	-1.974646	0.045905	-1.556286
O	-3.178079	-0.557039	-1.390229
C	-2.455516	2.254676	3.423462
C	-3.866560	2.851735	3.362396
C	0.385874	-3.203672	3.590633
C	2.351816	-1.348221	-1.888533
C	-1.696924	2.896811	4.597436
H	-4.484534	2.381127	2.592890
H	-2.921118	-0.479773	0.656989
H	0.603700	-1.590115	2.201185
H	3.548139	3.479470	0.221760
H	3.982911	3.055040	1.894104
H	4.295079	1.928246	0.567879
H	1.621178	1.209877	4.994218
H	-0.001041	0.479047	4.966500
H	1.403652	-0.461880	4.474655
H	2.703900	1.884294	3.203179
H	3.675383	0.702666	-3.742989
H	3.094939	2.840326	-4.836535
H	1.777586	4.534293	-3.606941
H	-4.336430	0.595338	4.491858
H	-4.335975	-1.866261	4.632165
H	-1.777880	3.988461	4.547849
H	-2.119982	2.572003	5.554848
H	-0.634820	2.646697	4.591514
H	-3.806783	3.922219	3.139892
H	-4.390714	2.755591	4.319914
H	1.019111	6.444368	-0.314269
H	2.510065	5.492505	-0.277144
H	-0.296811	5.213423	-2.842630
H	-1.115971	3.872110	-2.024377
H	-1.111442	5.490812	-1.300024
H	4.890855	-1.289576	-0.766825
H	4.956321	-0.534975	-2.359562
H	5.178972	0.452708	-0.913593
H	2.670171	-2.288610	-1.424303
H	1.270596	-1.253127	-1.758280
H	2.567133	-1.420924	-2.961128
H	1.280313	-3.710408	3.212551
H	0.661444	-2.660287	4.499936
H	-0.331095	-3.980731	3.877119
H	0.230278	-3.681729	0.912899
H	-1.427399	-3.773340	1.521609
H	-0.937999	-2.429129	0.464384
H	-1.928581	2.539151	2.503992

H	0.491388	4.030277	-0.126071
H	2.819202	-0.129292	-0.200154
H	-3.075724	3.272953	-1.131557
H	-3.183348	2.806068	0.568461
H	-5.301030	2.452986	-0.585195
H	-4.534394	1.451571	-1.810700
H	-4.896166	0.704100	1.142367
H	-5.764130	0.062710	-0.243643
H	-4.774017	-2.116737	1.092061
H	-5.054641	-2.230010	-0.659501
H	-3.517606	-2.786929	0.033182
H	-0.238649	1.590583	-2.929138
H	-1.633859	1.907703	-4.964944
H	0.015263	1.399773	-5.320348
H	-2.373942	-0.512785	-5.176778
H	-0.750549	-0.937840	-5.724547
H	-2.651525	1.004343	-7.118734
H	-6.184375	-0.028911	-5.986809
H	-5.842979	-1.782752	-6.137825
H	-6.304020	-0.848691	-7.578668
H	-0.028989	-0.123571	-3.327192
H	-0.273870	1.568415	-7.640971
H	0.046814	-0.134439	-8.032324

TS($\mathbf{VI}^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VII}^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.672491 kcal.mol^{-1}

C	2.900990	0.716350	-1.002391
C	2.050912	1.794263	-0.653744
C	1.853746	2.873326	-1.550765
C	2.500908	2.830470	-2.790842
C	3.326206	1.771509	-3.149013
C	3.527194	0.729384	-2.252315
N	1.356643	1.753085	0.598485
C	1.871213	2.349614	1.672903
C	3.176656	3.116087	1.590651
C	1.031927	4.106718	-1.196142
C	1.941024	5.334255	-1.010002
C	3.191123	-0.424011	-0.035852
C	3.068232	-1.807961	-0.685522
C	1.299007	2.331497	2.958628
C	0.241129	1.567647	3.474960
C	0.093088	1.615308	4.982378
N	-0.573628	0.806230	2.740182
Zn	-0.474783	0.904781	0.746455
O	-1.459679	1.986704	-0.700168
C	-2.380968	1.220665	-1.103074

O	-3.618021	1.454417	-0.621384
C	-4.776582	0.907574	-1.265555
C	-5.349011	1.883529	-2.284617
C	-6.631218	1.339761	-2.917109
C	-7.333734	2.339052	-3.834013
C	-6.546133	2.722272	-5.073153
C	-1.429392	-0.138082	3.386677
C	-0.880869	-1.323974	3.931057
C	-1.749249	-2.260283	4.502426
C	-3.118472	-2.039201	4.553151
C	-3.643533	-0.865284	4.023304
C	-2.824138	0.098963	3.429577
C	0.612950	-1.629601	3.912847
C	1.145710	-2.010201	5.302715
C	-3.422743	1.382955	2.872848
C	-3.275631	2.556908	3.854279
O	-1.807657	-0.303606	-0.123256
C	-1.991826	-1.542737	-0.761515
C	-0.924630	-1.821035	-1.847274
C	-0.279889	-0.554311	-2.408036
C	-1.209871	0.463093	-3.058109
O	-2.435543	0.713131	-2.355328
C	-2.094764	-2.680551	0.245783

C	-4.890948	1.240882	2.463719	H	-6.283141	1.834021	-5.656297	H	-4.714790	-0.697893	4.070260
C	0.953604	-2.731350	2.899576	H	-5.624429	3.240588	-4.796145	H	-3.776337	-2.776861	5.004977
C	-0.049950	4.424395	-2.236315	H	-7.338449	1.064959	-2.125374	H	-1.342079	-3.179715	4.915302
C	4.582021	-0.263640	0.598693	H	-6.416625	0.428911	-3.491600	H	-3.735234	3.459670	3.436683
O	-8.561534	1.740461	-4.323502	H	-1.556594	0.104510	-4.031776	H	-3.773733	2.333798	4.805024
C	-9.622676	1.834615	-3.519075	H	-5.549854	2.837364	-1.780566	H	-2.228878	2.787300	4.063704
O	-9.666460	2.375013	-2.435181	H	0.464189	-0.822475	-3.168959	H	-5.202336	2.126507	1.901960
O	-10.649675	1.224726	-4.124758	H	-0.124531	-2.444225	-1.424737	H	-5.047188	0.363081	1.830565
C	-11.868700	1.248018	-3.380704	H	-1.377991	-2.416740	-2.650823	H	-5.554261	1.157971	3.332836
H	2.451971	-0.366214	0.770147	H	-2.961549	-1.476230	-1.278093	H	1.353747	6.195381	-0.672206
H	-2.863829	1.639668	1.966108	H	-0.677200	1.408509	-3.201703	H	2.733812	5.158482	-0.278499
H	0.522706	3.906505	-0.249052	H	-5.492509	0.732345	-0.457882	H	2.421929	5.612365	-1.954942
H	2.237768	-2.094820	5.281251	H	-4.541139	-0.051043	-1.732804	H	0.381923	4.638974	-3.220569
H	-2.337660	-3.623983	-0.257522	H	3.887240	2.719029	2.321950	H	-0.754909	3.596976	-2.324738
H	-2.870076	-2.466363	0.985811	H	3.630871	3.075101	0.601438	H	-0.613329	5.312151	-1.927958
H	-1.148976	-2.817139	0.778065	H	3.002549	4.164607	1.852643	H	4.770957	-1.061894	1.325315
H	0.287129	-0.058514	-1.616803	H	-0.902342	1.317779	5.312826	H	5.365843	-0.313127	-0.165804
H	0.689584	-2.428963	1.882598	H	0.816773	0.944597	5.457386	H	4.683758	0.694716	1.114692
H	0.414448	-3.658354	3.124409	H	0.303853	2.625568	5.342994	H	3.180315	-2.592169	0.070659
H	-11.745980	0.747462	-2.416650	H	1.838110	2.916926	3.696584	H	2.097728	-1.941667	-1.170829
H	-12.595472	0.716192	-3.994803	H	4.188583	-0.088993	-2.524383	H	3.843999	-1.974797	-1.440754
H	-7.606821	3.229186	-3.256755	H	3.820385	1.765033	-4.116940	H	0.876168	-1.268174	6.060389
H	-7.135348	3.388952	-5.708389	H	2.361872	3.654866	-3.485515	H	0.752533	-2.976477	5.636729

H	2.026679	-2.954118	2.918010
H	1.143482	-0.728318	3.592692
H	-4.587238	2.072634	-3.047467
H	-12.198188	2.275421	-3.205201

TS($\mathbf{VI}^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)} \rightarrow \mathbf{VII}^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$).

G = -2500.663089 kcal.mol^{-1}

C	1.770144	0.436860	-2.534393
C	1.128632	1.444602	-1.777566
C	0.535670	2.559837	-2.413430
C	0.627215	2.665403	-3.805361
C	1.267470	1.688579	-4.559185
C	1.821175	0.583628	-3.924264
N	1.078503	1.344666	-0.346536
C	2.115965	1.795948	0.355316
C	3.307460	2.409756	-0.349277
C	-0.161974	3.663969	-1.631891
C	0.674449	4.952908	-1.602953
C	2.416331	-0.789553	-1.903349
C	1.698792	-2.082341	-2.317692
Zn	-0.446884	0.449103	0.597404
O	-2.309768	0.492824	-0.191321
C	-3.654176	0.715027	0.186048
C	-3.965066	2.205780	0.238617
N	0.172582	0.661965	2.489503
C	1.389529	1.168782	2.726750
C	2.240082	1.713924	1.756178
C	-0.597453	0.184149	3.597506
C	-1.561602	1.044765	4.182930
C	-2.331257	0.555399	5.242345
C	-2.172509	-0.743419	5.715232
C	-1.223589	-1.573171	5.134456
C	-0.415213	-1.132316	4.080279
C	-1.753406	2.477107	3.692184
C	-3.146226	3.047740	3.987290
C	0.628716	-2.082635	3.507414
C	-0.014389	-3.235808	2.722251
C	1.956694	1.138156	4.131637
C	1.555692	-2.638878	4.599756
C	-0.698971	3.442955	4.259905
O	-0.900491	-1.427393	-0.087005
C	-1.916840	-1.195619	-0.819436
O	-3.094225	-1.847373	-0.656088
C	-3.428116	-2.343662	0.647655
C	-3.357696	-1.314737	1.762807
C	-4.054971	0.018932	1.502180
O	-1.662498	-0.972945	-2.127752
C	-2.734661	-0.921661	-3.094209
C	-2.276597	0.068425	-4.161651
C	-3.346491	0.373481	-5.210281
C	-2.877746	1.325131	-6.294848
O	-2.559999	2.584564	-5.671723
C	-2.060168	3.583755	-6.396875
O	-1.709578	4.632942	-5.910134
C	-2.988554	-2.323796	-3.633988
C	-1.564660	3.954871	-2.180139
C	3.912981	-0.889245	-2.239317
O	-1.998510	3.286544	-7.708625
C	-1.468299	4.333906	-8.526287
H	-4.447992	-2.719299	0.518412
H	3.814758	3.118981	0.308070
H	4.026984	1.626090	-0.609316
H	3.029482	2.911918	-1.276068
H	1.191655	1.268817	4.898024
H	2.432514	0.167791	4.310836
H	2.720790	1.908171	4.255302
H	3.172543	2.106359	2.145296
H	2.315708	-0.181873	-4.517372
H	1.336752	1.789375	-5.639559
H	0.188050	3.525725	-4.302886

H	-3.072855	1.199029	5.704463
H	-2.785975	-1.103416	6.536903
H	-1.099103	-2.586014	5.509103
H	-0.917414	4.467831	3.939663
H	-0.707738	3.425260	5.355745
H	0.309422	3.203381	3.919534
H	-3.276135	3.997603	3.458750
H	-3.951336	2.377064	3.673950
H	-3.278685	3.256661	5.054974
H	0.162941	5.728126	-1.021263
H	1.659115	4.792972	-1.153710
H	0.826325	5.342630	-2.615636
H	-1.538817	4.361973	-3.195507
H	-2.167469	3.043665	-2.201200
H	-2.073696	4.686525	-1.542265
H	4.370689	-1.721139	-1.692577
H	4.069812	-1.075643	-3.307768
H	4.459194	0.024213	-1.984924
H	2.165143	-2.946244	-1.829930
H	0.645575	-2.052429	-2.035009
H	1.765680	-2.238534	-3.400952
H	2.373416	-3.210011	4.146939
H	1.993200	-1.844982	5.212988
H	1.021551	-3.316717	5.274710
H	0.757989	-3.926039	2.364271
H	-0.702988	-3.807492	3.355520
H	-0.558427	-2.865156	1.850114
H	-1.619080	2.459149	2.602768
H	-0.271994	3.315880	-0.599529
H	1.245031	-1.517042	2.801618
H	2.320388	-0.696747	-0.817067
H	-4.271447	0.273424	-0.610683
H	-3.821933	0.675455	2.348592
H	-5.146753	-0.106509	1.500348
H	-2.309629	-1.129763	2.001491
H	-3.785103	-1.780250	2.659731
H	-2.774428	-3.192304	0.879226
H	-0.451491	4.586477	-8.216457
H	-1.472620	3.942722	-9.543696
H	-2.091967	5.228256	-8.456691
H	-1.985757	0.939592	-6.800277
H	-3.656323	1.482809	-7.048496
H	-4.239954	0.794437	-4.731338
H	-3.667356	-0.544120	-5.719126
H	-1.974725	0.994509	-3.665656
H	-1.375592	-0.330013	-4.645079
H	-3.811003	-2.324404	-4.356399
H	-3.252522	-3.002884	-2.821916
H	-2.090414	-2.703679	-4.132005
H	-3.635797	-0.540976	-2.601900
H	-5.007623	2.371614	0.533864
H	-3.324088	2.708256	0.970375
H	-3.804151	2.674629	-0.734083

VII$^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.682348 kcal.mol^{-1}

Zn	-0.071517	0.452069	0.736988
O	-0.043503	-0.783352	-1.144954
O	-1.876699	0.779499	0.300276
C	-3.026686	0.300044	0.921705
H	-3.786188	1.102185	0.975688
C	-0.956408	-0.468611	-1.906742
H	-3.395631	-1.351654	3.694239
C	-2.788137	-0.976256	4.522849
N	1.232840	1.968516	0.641276
C	-1.312590	-0.817041	4.135307
N	0.827691	-0.633627	2.168510
H	-1.237772	0.020403	3.430513
C	1.907089	-0.143483	2.785510
C	2.474477	1.118156	2.543182

H	3.305923	1.367302	3.192570
H	3.226541	3.772756	0.668810
C	2.995748	3.362741	1.652839
C	2.178915	2.091106	1.570614
O	-0.891139	0.644134	-2.613560
C	-2.014059	1.100903	-3.423934
C	-1.859878	0.534352	-4.825425
O	-2.020588	-1.208212	-2.174226
C	-2.271083	-2.413702	-1.391411
C	-2.679204	-2.074492	0.043274
C	-3.657322	-0.892863	0.185235
C	0.342155	-1.934536	2.517244
C	-0.731819	-2.042870	3.438926
C	-1.237511	-3.313725	3.727266
C	-0.714210	-4.455990	3.130984
C	0.343085	-4.337762	2.239914
C	0.896712	-3.092250	1.921583
C	2.644628	-0.980221	3.811850
C	1.104977	2.983516	-0.361692
C	0.244706	4.084502	-0.152102
C	0.130066	5.043818	-1.163872
C	0.849005	4.939464	-2.348545
C	1.694923	3.852348	-2.538863
C	1.834536	2.855309	-1.568224
C	-0.560990	4.258472	1.127275
C	-2.061033	4.059161	0.866316
C	2.783654	1.690274	-1.822346
C	2.553875	1.029940	-3.188024
C	2.091660	-3.048730	0.977815
C	3.271877	-3.867037	1.527789
C	-0.506023	-0.426997	5.385130
C	-1.977944	2.619956	-3.311347
C	-3.142404	3.334745	-4.016540
C	-2.834698	3.834451	-5.417259
O	-1.829084	4.856899	-5.294869
C	-1.316748	5.288542	-6.449685
O	-1.620672	4.905707	-7.557313
O	-0.401545	6.225477	-6.168771
C	0.236344	6.784874	-7.318325
C	-3.339343	-3.157915	-2.172879
C	4.254279	2.118580	-1.692127
C	1.734206	-3.537837	-0.432711
C	-0.298724	5.614514	1.798776
H	0.764328	6.012813	-7.884019
H	-0.495313	7.264661	-7.973549
H	0.940792	7.521448	-6.932109
H	-3.722852	4.269643	-5.888888
H	-2.459308	3.048428	-6.078837
H	-0.940978	0.900029	-5.293923
H	-2.708530	0.824084	-5.452431
H	-2.931061	0.721614	-2.964789
H	-4.023041	2.681201	-4.078500
H	-3.452033	4.198342	-3.418449
H	-1.020846	2.995165	-3.687712
H	-3.020730	-3.332940	-3.204355
H	-4.277503	-2.594779	-2.190820
H	-3.529614	-4.126399	-1.701794
H	-3.100500	-2.992107	0.469748
H	-2.846170	-0.008526	1.964390
H	-1.773443	-1.869774	0.619804
H	-3.990770	-0.552615	-0.802771
H	-4.561510	-1.201596	0.725812
H	-1.829726	-0.557830	-4.795904
H	-1.991387	2.852744	-2.243396
H	2.585035	0.934812	-1.056291
H	-0.664069	6.445481	1.185310
H	3.469038	-1.509796	3.322165
H	3.531570	-3.582762	2.551523
H	0.759529	-5.232631	1.783870

H	-1.340389	-2.989935	-1.382117
H	3.924472	3.197224	2.201994
H	2.420829	4.127244	2.188104
H	3.082255	-0.341287	4.582494
H	2.007438	-1.726778	4.286608
H	2.258314	3.772367	-3.465129
H	0.739099	5.690444	-3.125749
H	-0.534478	5.891671	-1.016686
H	-2.058118	-3.413322	4.430833
H	-1.125972	-5.433568	3.367535
H	-0.972337	0.429903	5.884255
H	-0.474899	-1.256969	6.100257
H	0.520459	-0.147713	5.141942
H	-3.197372	-0.008591	4.830570
H	-2.913230	-1.660029	5.370303
H	-0.818666	5.667462	2.761673
H	0.767711	5.784606	1.979431
H	-2.437431	4.801600	0.152322
H	-2.243136	3.054233	0.472736
H	-2.629472	4.176959	1.796727
H	4.918780	1.267288	-1.879208
H	4.500124	2.900089	-2.420417
H	4.485056	2.506839	-0.696438
H	3.182389	0.137385	-3.281923
H	1.511270	0.731207	-3.309725
H	2.819134	1.700139	-4.013923
H	4.158009	-3.726568	0.899093
H	3.042897	-4.938560	1.535232
H	1.373693	-4.573008	-0.413913
H	0.967510	-2.904006	-0.881841
H	2.618340	-3.508920	-1.079844
H	-0.247204	3.475463	1.825257
H	2.412386	-2.006051	0.890960

VII$^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.687616 kcal.mol^{-1}

Zn	-0.604853	1.439142	0.530355
O	-2.041375	2.288970	-0.297188
C	-3.178652	2.918415	0.202677
C	-4.453097	2.354541	-0.433539
C	-4.868160	0.954515	0.031912
C	-3.824282	-0.148060	-0.122779
O	-1.945205	0.160310	-3.068949
C	-4.383607	-1.533366	0.150680
C	-0.605026	0.246151	-3.589493
C	-0.712563	0.528320	-5.075616
C	-0.312219	-0.176040	-8.134418
O	-4.317456	-2.306487	-8.379129
C	-3.682821	-1.405156	-7.890331
O	-2.350357	-1.345876	-7.960214
C	-1.601539	-0.269749	-7.336954
C	-1.403595	-0.590258	-5.857034
O	-4.217240	-0.356336	-7.231938
C	-5.644040	-0.382087	-7.144471
C	-2.261565	-2.237590	3.535224
N	-0.325015	0.744398	2.394815
H	-2.218979	-3.321695	3.467197
C	1.736442	2.204643	-1.192260
C	1.336016	3.363545	-1.898187
H	1.694977	6.147322	-2.055379
C	1.386869	5.746962	-1.082792
C	-3.311540	-1.637516	4.216669
C	-3.362122	-0.250784	4.312765
C	-2.380798	0.558317	3.732011
C	-0.107066	-2.202876	2.239738
C	-0.595161	-2.984512	1.011832
C	2.548642	1.225136	-1.818322
C	2.921726	1.419777	-3.151919
C	2.524196	2.548947	-3.859780
O	-1.141194	-0.200361	-0.983381

C	-1.315337	-0.068339	3.035489	H	3.425636	3.559786	0.121136	H	4.829065	-0.483774	-2.253379
C	1.877146	1.769934	2.485330	H	3.842037	3.284075	1.829250	H	5.100214	0.639987	-0.919552
C	0.821023	1.011938	3.024098	H	4.211312	2.062163	0.610609	H	2.612470	-2.173030	-1.065831
C	1.091026	0.446644	4.403536	H	1.662355	1.160726	5.001999	H	1.190675	-1.178200	-1.433590
C	1.742235	3.509201	-3.229429	H	0.182127	0.175313	4.940411	H	2.441494	-1.441324	-2.666750
C	-1.248020	-1.477998	2.940356	H	1.704665	-0.455985	4.307646	H	1.521773	-3.567761	2.706447
C	0.532916	4.479477	-1.245247	H	2.684882	1.974368	3.179513	H	0.974746	-2.624106	4.103899
C	-0.762268	4.784833	-2.007385	H	3.540424	0.673349	-3.643561	H	0.007494	-3.977583	3.515802
N	1.281701	1.991276	0.145321	H	2.833297	2.685104	-4.892891	H	0.244169	-3.495588	0.527156
C	2.124964	2.173420	1.161820	H	1.446644	4.400805	-3.776371	H	-1.327689	-3.749011	1.294955
C	3.474273	2.812489	0.915443	H	-4.181631	0.211915	4.854003	H	-1.053349	-2.317786	0.277909
C	3.018798	-0.035241	-1.100670	H	-4.085463	-2.245657	4.677331	H	-1.981127	2.513364	3.004749
C	4.535149	-0.246336	-1.225154	H	-1.772275	3.650174	5.223476	H	0.245963	4.138603	-0.246165
C	-2.080264	-0.041314	-1.766112	H	-2.043604	2.097765	6.033149	H	2.786861	0.073942	-0.037448
O	-3.367851	-0.116794	-1.501172	H	-0.599708	2.344919	5.038370	H	-3.145988	4.002323	-0.016827
C	-2.453762	2.072775	3.890728	H	-3.882892	3.700018	3.894454	H	-3.269203	2.840261	1.299272
C	-3.888713	2.608256	3.975294	H	-4.357817	2.361649	4.934435	H	-5.288528	3.038522	-0.228470
C	0.641257	-3.141561	3.199611	H	0.815828	6.527716	-0.568254	H	-4.310517	2.348921	-1.520511
C	2.266541	-1.278611	-1.596498	H	2.294491	5.556968	-0.500901	H	-5.138674	0.978249	1.096092
C	-1.665700	2.564893	5.116450	H	-0.564983	5.108166	-3.035977	H	-5.775314	0.650699	-0.508135
H	-4.525555	2.214974	3.177882	H	-1.407504	3.903094	-2.021263	H	-4.753676	-1.586080	1.178478
H	-2.965963	0.047121	0.521178	H	-1.306309	5.595446	-1.509704	H	-5.209892	-1.758078	-0.531466
H	0.602073	-1.447080	1.888606	H	4.853257	-1.085054	-0.596473	H	-3.612815	-2.298731	0.030438

H	-0.068559	1.043645	-3.070258
H	-1.250342	1.474764	-5.213825
H	0.308732	0.690491	-5.438640
H	-2.385828	-0.774019	-5.411212
H	-0.828229	-1.521939	-5.773830
H	-2.175972	0.656637	-7.439213
H	-5.918868	0.504464	-6.572844
H	-5.981699	-1.287036	-6.633957
H	-6.091435	-0.350327	-8.140974
H	-0.090452	-0.700450	-3.396159
H	0.307332	0.648805	-7.771628
H	0.259978	-1.105254	-8.051114
H	-0.529508	-0.000604	-9.191256

VII$^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.683585 kcal.mol^{-1}

C	-0.223366	-0.321457	3.569114
C	-0.350425	-1.731505	3.614972
C	-1.167686	-2.295510	4.600487
C	-1.831480	-1.507795	5.533644
C	-1.659137	-0.129227	5.507882
C	-0.856914	0.488068	4.542948
C	0.413584	-2.658409	2.677672
C	-0.511502	-3.551018	1.840515
C	-0.644422	1.994294	4.612711
C	-1.954403	2.781179	4.476004
N	0.485948	0.308352	2.498285
C	1.807442	0.472652	2.550771
C	2.595159	-0.039479	3.738438
C	2.575570	1.106195	1.558457
C	2.191249	1.751042	0.369235
C	3.307809	2.470831	-0.359481
N	0.943978	1.806284	-0.099496
C	0.659669	2.592394	-1.260945
C	0.489917	3.991035	-1.141423
C	0.154591	4.721186	-2.286811
C	0.005996	4.103426	-3.520846
C	0.182618	2.727860	-3.625842
C	0.500902	1.945836	-2.511540
C	0.644912	4.727321	0.182953
C	-0.714725	5.184835	0.731467
C	0.683107	0.438241	-2.652243
C	-0.056695	-0.150703	-3.857881
Zn	-0.575056	1.093296	0.992365
O	-2.172433	2.054825	1.169637
C	-3.391332	1.828920	0.535622
C	-4.389537	1.111406	1.476628
C	-3.840846	-0.158009	2.129085
C	-4.000175	-1.454520	1.351710
O	-3.757731	-1.373748	-0.081694
C	-2.554576	-1.048655	-0.525560
O	-1.577469	-0.788755	0.162756
C	1.611459	5.916411	0.074785
C	0.097969	2.378608	5.902652
C	2.163701	0.030831	-2.725782
C	1.407538	-3.534242	3.458990
C	-3.991722	3.156506	0.066820
O	-2.461058	-1.064553	-1.850249
C	-3.590864	-1.425502	-2.675253
H	-3.130141	-1.790991	-3.595210
C	-4.505708	-0.237059	-2.933714
C	-5.654842	-0.571201	-3.902165
C	-5.406915	-0.146457	-5.347330
O	-6.636117	-0.467500	-6.044737
C	-6.910891	0.278863	-7.119036
O	-8.063476	-0.160583	-7.637206
C	-8.495541	0.551336	-8.798614
O	-6.245502	1.193447	-7.552947
H	3.068721	-0.995150	3.488918
H	3.393763	0.661636	3.992731

H	0.314022	3.452677	5.911971
H	1.047073	1.841699	6.000390
H	3.637777	1.150549	1.773229
H	4.264781	1.976532	-0.177535
H	3.390060	3.497099	0.015221
H	3.133393	2.531060	-1.434337
H	1.200149	6.715700	-0.551393
H	2.662598	0.527100	-3.566346
H	2.575678	5.626663	-0.355485
H	1.795718	6.345062	1.066019
H	2.704350	0.279966	-1.811098
H	1.065368	4.025750	0.910198
H	2.251756	-1.051441	-2.874955
H	-0.580846	5.719047	1.679619
H	-1.207107	5.869966	0.031154
H	-0.048383	-1.243583	-3.797593
H	-1.374570	4.329830	0.904376
H	0.260653	-0.022081	-1.751350
H	-1.098523	0.179411	-3.891603
H	0.421243	0.124981	-4.805175
H	0.009931	5.795488	-2.206634
H	-0.248503	4.689570	-4.399984
H	0.063858	2.253732	-4.594921
H	2.030188	-4.116231	2.770334
H	-0.005325	2.278909	3.771339
H	-0.502655	2.154272	6.791320
H	-2.672575	2.507268	5.257700
H	-2.403956	2.605514	3.494682
H	-1.759128	3.855443	4.571829
H	-2.151575	0.485577	6.257291
H	-2.462157	-1.967934	6.289846
H	0.881654	-4.244029	4.107405
H	1.966483	-0.195936	4.615872
H	-1.127677	-4.197910	2.475571
H	0.980762	-2.033528	1.981071
H	2.067993	-2.939194	4.095612
H	-1.274884	-3.376807	4.643280
H	-1.169255	-2.945977	1.214694
H	0.077768	-4.201143	1.183901
H	-3.265808	1.211538	-0.374028
H	-2.792429	0.008640	2.381774
H	-3.317375	3.646441	-0.640839
H	-4.130150	3.825690	0.923212
H	-4.636663	1.822897	2.274602
H	-4.964159	3.012677	-0.420189
H	-4.351129	-0.342505	3.083130
H	-5.328497	0.907065	0.941723
H	-3.353139	-2.235310	1.761188
H	-5.034820	-1.805160	1.378311
H	-7.755005	0.474936	-9.598965
H	-9.430391	0.078498	-9.099224
H	-8.659606	1.607194	-8.568452
C	-4.244338	-0.835688	-6.042086
H	-5.269105	0.939219	-5.399228
H	-6.569269	-0.068921	-3.571358
H	-5.879116	-1.646292	-3.882625
H	-4.917516	0.088430	-1.974409
H	-3.908095	0.600307	-3.313944
H	-4.137598	-2.247073	-2.205428
H	-4.178115	-0.499091	-7.079517
H	-3.297560	-0.583546	-5.554924
H	-4.370923	-1.923257	-6.029259

VII$^{a\delta,a\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.682765 kcal.mol^{-1}

Zn	-0.546213	1.202704	0.985773
C	1.372363	-3.335095	2.571297
C	1.767295	0.428022	2.578275
C	2.591034	1.081614	1.647092
C	2.267097	1.785848	0.472270

N	1.037942	1.904611	-0.027774
N	0.448707	0.272032	2.448149
H	3.500026	-0.339244	3.612717
H	2.499284	0.759738	4.563055
H	0.318952	3.019338	6.307991
H	0.911781	1.348905	6.373019
H	3.643670	1.096849	1.907386
H	4.360840	1.939557	-0.017543
H	3.551951	3.489836	0.220345
H	3.284802	2.597282	-1.273725
H	1.520296	6.815707	-0.319746
H	2.709068	0.657799	-3.566136
C	1.888441	5.982547	0.288973
H	2.848514	5.667604	-0.133037
H	2.071130	6.374428	1.295606
H	2.776800	0.392197	-1.814978
C	2.209148	0.170678	-2.720878
C	0.873809	4.830590	0.345037
H	1.254340	4.090168	1.055599
H	2.255524	-0.912499	-2.881898
C	0.707339	4.143204	-1.003884
C	-0.475525	5.323566	0.888522
H	-0.337557	5.811238	1.860980
H	-0.923890	6.058308	0.209248
H	-0.063515	-0.987259	-3.792730
H	-1.173482	4.490079	1.010578
H	0.320652	0.166776	-1.717647
C	-0.038331	0.106383	-3.819163
H	-1.069700	0.469652	-3.816638
H	0.425103	0.396741	-4.769152
C	0.364069	2.969085	-3.528481
H	0.331443	5.999111	-2.020956
C	0.256863	4.348152	-3.384419
H	0.041719	4.972032	-4.247979
H	0.230595	2.528647	-4.511513
H	1.807519	-3.897291	1.737216
H	0.179795	2.059100	4.064587
C	-0.534606	-1.824978	3.266281
C	-0.564884	1.731659	4.797055
C	0.027766	1.969440	6.194289
H	-0.696973	1.745602	6.984882
H	-2.633484	2.272137	5.245170
C	-1.819329	2.592162	4.584013
C	-1.330348	-2.485467	4.207861
H	-2.162860	2.539356	3.546183
H	-1.600393	3.641627	4.812870
H	-2.069345	0.071997	6.299511
C	-1.890715	-1.809424	5.286988
H	-2.510616	-2.341982	6.003560
C	-1.640484	-0.452837	5.449657
H	1.152943	-4.045279	3.377013
H	1.956123	-0.894524	4.303387
C	2.467897	-0.055672	3.830726
C	0.810824	2.742152	-1.164336
C	0.746813	0.632745	-2.614319
C	0.423499	4.921717	-2.131158
C	-0.862919	-3.625975	1.484502
H	-1.093728	-4.455879	2.161817
C	0.632676	2.141803	-2.434225
C	3.431775	2.484804	-0.198797
C	-0.838156	0.254274	4.547496
H	0.369283	-1.886740	1.347542
C	0.093281	-2.609812	2.120559
H	2.132982	-2.640820	2.935235
H	-1.512582	-3.550928	4.095747
H	-1.804942	-3.161043	1.184740
H	-0.403360	-4.060732	0.590335
C	-0.296425	-0.438146	3.440116
O	-2.065925	2.288429	1.118189

C	-3.284225	2.130555	0.461836
H	-3.189053	1.458493	-0.412217
H	-2.850928	0.406610	2.421043
H	-3.033717	3.880022	-0.791926
C	-3.764088	3.476955	-0.085003
H	-3.873870	4.194125	0.736017
H	-4.576080	2.312870	2.157306
H	-4.731108	3.385688	-0.595271
C	-4.355245	1.540659	1.409563
H	-4.444129	0.186747	3.100018
C	-3.901124	0.282692	2.151024
H	-5.290365	1.363392	0.859025
C	-4.111963	-1.050709	1.451312
H	-3.491654	-1.826666	1.908521
H	-5.158687	-1.360195	1.504718
O	-3.880336	-1.071362	0.014766
C	-2.664633	-0.876551	-0.473141
O	-2.597140	-1.038447	-1.789830
O	-1.661993	-0.610034	0.174326
C	-3.770665	-1.419198	-2.570185
C	-4.528621	-0.149898	-2.956633
C	-5.830552	-0.405797	-3.737128
C	-5.665085	-0.250494	-5.238679
O	-6.941148	-0.529244	-5.834959
C	-6.968368	-0.431134	-7.168666
O	-6.032963	-0.145028	-7.881546
C	-3.239921	-2.240872	-3.729986
O	-8.212083	-0.706493	-7.575519
C	-8.395617	-0.636435	-8.991093
H	-7.746186	-1.351310	-9.502922
H	-9.443065	-0.884353	-9.161938
H	-8.176623	0.368372	-9.361492
H	-4.916904	-0.932769	-5.654477
H	-5.358283	0.768386	-5.500390
H	-6.602190	0.298227	-3.409339
H	-6.223544	-1.407006	-3.519572
H	-4.761723	0.384301	-2.031295
H	-3.855544	0.502389	-3.527707
H	-4.070674	-2.643291	-4.316476
H	-2.650766	-3.083951	-3.359403
H	-2.605991	-1.638504	-4.386407
H	-4.408361	-2.041692	-1.935959

TS(**VII**$^{a\delta,\delta a}{}_{7CC\text{-}\gamma(R)}$→**VIII**$^{a\delta,\delta a}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.679334 kcal.mol^{-1}

C	1.908757	2.862920	-1.590302
C	1.127820	2.896304	-0.410786
C	0.142159	3.893387	-0.226256
C	-0.060406	4.829934	-1.244827
C	0.684254	4.798775	-2.417681
C	1.660502	3.822546	-2.576957
N	1.306777	1.893745	0.599391
C	2.316311	2.007481	1.465523
C	3.211661	3.224634	1.411080
C	-0.683698	4.000190	1.048336
C	-0.460557	5.345219	1.755781
C	3.007979	1.834947	-1.830599
C	4.353634	2.499383	-2.163967
Zn	-0.008350	0.433880	0.812934
N	0.883520	-0.609305	2.254434
C	0.292846	-1.824971	2.730048
C	-0.759027	-1.743449	3.678829
C	-1.370838	-2.928720	4.095391
C	-0.973028	-4.164365	3.595291
C	0.059048	-4.228800	2.670034
C	0.715180	-3.075242	2.224422
C	-1.201291	-0.406575	4.265703
C	-0.322623	0.012851	5.456059
C	1.868675	-3.223138	1.240707
C	1.405464	-3.774311	-0.115449

O	-0.021676	-1.128496	-1.742531	C	-2.175773	3.758062	0.779473	H	-2.808093	-3.344670	0.043323
C	-0.965800	-0.723838	-2.393545	C	2.627686	0.842080	-2.938284	H	-2.502421	-0.740272	1.794482
O	-2.105587	-1.385261	-2.609541	C	2.984951	-4.111346	1.814419	H	-1.516109	-2.162925	0.017012
C	-2.313724	-2.637031	-1.900613	O	-1.675263	5.166823	-7.603751	H	-3.815886	-0.741858	-0.944162
C	-3.514827	-3.274962	-2.575801	H	-3.585188	0.512843	1.176875	H	-4.372346	-1.658238	0.452268
O	-1.758402	0.431271	0.233031	H	-3.339520	-0.738054	3.903572	H	-1.924448	-0.613454	-5.255022
C	-2.818330	-0.222932	0.874103	H	-1.070512	0.350859	3.482422	H	-1.999407	2.645296	-2.501469
C	-3.475520	-1.261049	-0.040444	H	3.517962	1.294184	3.036589	H	3.138729	1.257888	-0.909660
C	-2.497575	-2.392990	-0.403939	H	3.934202	3.140122	0.593672	H	-0.812742	6.184081	1.145476
O	-0.918983	0.447803	-3.020540	H	0.693665	6.344210	-7.823123	H	3.531747	-1.568485	3.346285
C	-2.048841	0.957369	-3.777858	H	-0.591753	7.571939	-7.775005	H	3.314673	-3.774466	2.801631
C	-2.001470	2.468403	-3.580239	H	0.845613	7.747604	-6.718424	H	0.372007	-5.196105	2.285216
C	-3.168394	3.229278	-4.232506	H	-3.738660	4.309880	-6.029520	H	-1.419910	-3.250651	-2.060825
C	-2.851098	3.849711	-5.581416	H	-2.452912	3.126284	-6.299010	H	3.768916	3.333968	2.343102
O	-1.863191	4.873249	-5.358016	H	-0.993877	0.845048	-5.663836	H	2.633244	4.133762	1.231052
C	-1.368210	5.433736	-6.463676	H	-2.764780	0.834152	-5.817472	H	3.240658	-0.325658	4.561285
O	-0.465417	6.350932	-6.090106	H	-2.966587	0.561297	-3.333999	H	2.091051	-1.669037	4.361152
C	0.153688	7.041337	-7.177059	H	-4.039812	2.573292	-4.361437	H	2.247002	3.802103	-3.492119
C	-2.673773	-0.377416	4.692556	H	-3.496784	4.035250	-3.567513	H	0.498097	5.522438	-3.205975
C	2.018873	-0.156647	2.792561	H	-1.045165	2.856118	-3.946121	H	-0.816125	5.600569	-1.114015
C	2.749334	-0.977148	3.834882	H	-3.347380	-3.384316	-3.651072	H	-2.176355	-2.886412	4.821842
C	2.635955	1.058685	2.451966	H	-4.415662	-2.672214	-2.425746	H	-1.466108	-5.072957	3.930497
C	-1.922695	0.479081	-5.215310	H	-3.692061	-4.267405	-2.151260	H	-0.679096	0.960150	5.875857

H	-0.362142	-0.742916	6.248691
H	0.721955	0.150764	5.170420
H	-2.966015	0.648694	4.938140
H	-2.849737	-0.982545	5.589090
H	-1.010951	5.373213	2.702802
H	0.598098	5.517676	1.975497
H	-2.579211	4.502687	0.083320
H	-2.331101	2.758289	0.362093
H	-2.747257	3.836128	1.711982
H	5.147572	1.745783	-2.207075
H	4.323743	2.995497	-3.140176
H	4.642607	3.254012	-1.425305
H	3.439613	0.122085	-3.095276
H	1.722301	0.288223	-2.684956
H	2.457807	1.363515	-3.887355
H	3.852589	-4.110378	1.145573
H	2.653441	-5.150605	1.917180
H	0.928668	-4.754657	-0.000388
H	0.703721	-3.095975	-0.605327
H	2.264781	-3.901045	-0.783662
H	-0.343070	3.215771	1.732263
H	2.287847	-2.227814	1.062345

TS(**VII**$^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$→**VIII**$^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.687746 kcal.mol^{-1}

C	1.436703	3.209849	-1.559195
C	1.849456	2.048634	-0.865737
C	2.635959	1.062161	-1.513087
C	2.978450	1.259376	-2.854481
C	2.568219	2.391283	-3.550850
C	1.804348	3.353213	-2.901676
N	1.436192	1.847206	0.489414
C	2.322477	2.024275	1.474281
C	3.670864	2.633570	1.160873
C	3.108633	-0.207265	-0.812867
C	2.333057	-1.440255	-1.299755
C	0.651386	4.327159	-0.887385
C	-0.716674	4.544991	-1.547551
C	2.113618	1.657901	2.813577
C	1.027516	1.000474	3.421198
C	1.289771	0.485468	4.820144
N	-0.151469	0.790094	2.835115
Zn	-0.433794	1.364507	0.940322
O	-1.968204	1.927853	0.084127
C	-3.143119	2.396308	0.682247
C	-4.380755	1.907093	-0.075172
C	-4.787289	0.459883	0.219112

C	-3.702574	-0.586685	-0.009456
O	-3.255351	-0.437894	-1.379231
C	-1.956788	-0.361493	-1.623200
O	-1.814080	-0.067758	-2.914223
C	-0.469474	0.032011	-3.410657
C	-0.553061	0.385956	-4.883428
C	-1.232703	-0.692725	-5.728393
C	-1.424338	-0.293679	-7.189765
C	-0.130832	-0.131963	-7.969288
C	-1.201853	0.123170	3.545376
C	-1.259880	-1.288967	3.563064
C	-2.347603	-1.903290	4.194609
C	-3.343137	-1.156509	4.808960
C	-3.261436	0.232296	4.805693
C	-2.204083	0.900510	4.181373
C	-0.176741	-2.164373	2.946160
C	0.426952	-3.128360	3.979834
C	-2.131193	2.424148	4.225662
C	-1.229071	2.927011	5.365493
C	-4.202844	-2.009882	0.173200
C	-3.502449	3.101149	4.343675
C	-0.691439	-2.945746	1.729410
C	4.618995	-0.437671	-0.974682

C	1.461879	5.632306	-0.853080	H	-2.408051	-2.988601	4.208760	H	1.258841	-1.324855	-1.137207
O	-1.038452	-0.567479	-0.841484	H	-4.219925	2.717890	3.612669	H	2.504083	-1.609164	-2.369753
O	-2.149167	-1.345674	-7.879533	H	-2.848675	-0.395272	0.642477	H	1.274729	-3.668827	3.544942
C	-3.480544	-1.433124	-7.822933	H	0.625106	-1.507644	2.594667	H	0.779007	-2.604469	4.873749
O	-4.038847	-0.432017	-7.112280	H	4.137842	3.015614	2.070472	H	0.105490	-3.575853	1.318512
C	-5.465128	-0.490052	-7.034725	H	4.345598	1.892284	0.722188	H	-1.522995	-3.603607	2.006652
O	-4.095158	-2.317595	-8.365427	H	1.971349	1.152375	5.353455	H	-1.028114	-2.273328	0.936599
H	-4.038949	0.808212	5.297472	H	1.777160	-0.494006	4.756859	H	-3.158479	3.501920	0.694278
H	3.577671	3.447561	0.438144	H	2.957654	1.837080	3.469892	H	-3.237516	2.076072	1.733105
H	0.377369	0.362173	5.404081	H	3.579896	0.510274	-3.362928	H	-5.232389	2.555204	0.173440
H	-5.663409	0.194437	-0.388103	H	2.851745	2.526819	-4.591307	H	-4.191323	2.030040	-1.147718
H	-4.178123	-1.652479	5.296557	H	1.494307	4.244410	-3.441357	H	-5.098186	0.370265	1.268800
H	-5.033983	-2.218631	-0.508146	H	-1.240936	4.022047	5.401282	H	-4.550355	-2.154605	1.200575
H	-3.405287	-2.732007	-0.020374	H	-0.191221	2.614181	5.240397	H	0.067558	0.799842	-2.848602
H	0.472885	0.565061	-5.224851	H	-3.397300	4.178316	4.179478	H	-1.089414	1.338155	-4.983337
H	-1.246986	5.365684	-1.050924	H	0.911427	6.407476	-0.308816	H	-2.215967	-0.906119	-5.298327
H	-3.934437	2.971334	5.342478	H	2.430438	5.498305	-0.360422	H	-0.651949	-1.624139	-5.692399
H	-1.584141	2.555134	6.333285	H	-0.613500	4.813924	-2.605235	H	-2.014297	0.626983	-7.245352
H	1.654246	6.011627	-1.862918	H	-1.329788	3.643500	-1.462084	H	-5.760320	0.361534	-6.421599
H	-1.676621	2.754996	3.283581	H	4.940209	-1.282579	-0.356090	H	-5.787232	-1.425424	-6.571073
H	0.471054	4.026830	0.149799	H	4.882451	-0.677675	-2.010508	H	-5.908187	-0.418157	-8.031081
H	2.901869	-0.100941	0.255992	H	5.207390	0.438175	-0.682767	H	0.039592	-0.925279	-3.255784
H	-0.304297	-3.876359	4.304897	H	2.669760	-2.337165	-0.767213	H	0.467706	0.684942	-7.556876

H	0.460525	-1.052076	-7.930168
H	-0.343005	0.095243	-9.017292

TS(**VII**$^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$→**VIII**$^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$)

G = -2500.682863 kcal.mol^{-1}

C	-0.086818	-0.162125	3.754002
C	-0.151812	-1.569590	3.886172
C	-0.932941	-2.105907	4.915411
C	-1.625123	-1.291818	5.803079
C	-1.529664	0.088575	5.678862
C	-0.766314	0.678946	4.667339
C	0.600162	-2.524910	2.968145
C	-0.356565	-3.373460	2.119431
C	-0.659268	2.197173	4.618960
C	-2.026062	2.869893	4.437135
N	0.615887	0.431804	2.654607
C	1.935143	0.624291	2.718619
C	2.696140	0.178084	3.946074
C	2.702504	1.229817	1.707754
C	2.316391	1.812204	0.487674
C	3.419395	2.512893	-0.276802
N	1.067651	1.829775	0.014246
C	0.774789	2.550196	-1.188672
C	0.571783	3.947615	-1.132241
C	0.245420	4.619828	-2.314648
C	0.132254	3.942418	-3.521026
C	0.327828	2.565967	-3.559206
C	0.639535	1.839467	-2.405677
C	0.663290	4.733005	0.169480
C	-0.735540	5.085484	0.698810
C	0.822955	0.326584	-2.467983
C	0.117897	-0.319983	-3.664254
Zn	-0.415962	1.158916	1.126537
O	-2.154665	1.740367	1.240234
C	-3.304730	1.477599	0.487527
C	-4.308769	0.667283	1.333917
C	-3.758359	-0.669980	1.840956
C	-4.083577	-1.886760	0.987839
O	-3.946285	-1.705465	-0.443887
C	-2.722175	-1.515897	-0.937680
O	-1.698982	-1.398181	-0.297374
C	1.527328	5.994971	0.037875
C	0.060485	2.738770	5.864374
C	2.302951	-0.089743	-2.472367
C	1.551333	-3.440404	3.755904
C	-3.938766	2.793872	0.035666
O	-2.709917	-1.472898	-2.273769
C	-3.917686	-1.649356	-3.038042
H	-3.565665	-2.028352	-4.000261
C	-4.682773	-0.342466	-3.194515
C	-5.907592	-0.472297	-4.117646
C	-5.666865	-0.014406	-5.553664
O	-6.954887	-0.144047	-6.206444
C	-7.172862	0.675173	-7.239093
O	-8.392953	0.409611	-7.720868
C	-8.773599	1.218880	-8.835193
O	-6.412399	1.514171	-7.669986
H	2.906423	-0.895059	3.894050
H	3.650111	0.702645	4.022360
H	0.183142	3.825171	5.792201
H	1.053826	2.294993	5.986773
H	3.761612	1.302560	1.926321
H	4.390344	2.073515	-0.038704
H	3.454010	3.569977	0.010330
H	3.263057	2.476393	-1.355636
H	1.058731	6.743664	-0.609912
H	2.832576	0.362733	-3.318951
H	2.515733	5.772317	-0.377246
H	1.667312	6.460449	1.019517
H	2.816707	0.197417	-1.553190

H	1.137925	4.091116	0.918273
H	2.386390	-1.178046	-2.568226
H	-0.659312	5.642921	1.639639
H	-1.275526	5.714196	-0.018732
H	0.132063	-1.408024	-3.552623
H	-1.332365	4.186435	0.880093
H	0.366417	-0.092527	-1.562676
H	-0.927278	-0.009427	-3.734809
H	0.618357	-0.081760	-4.610338
H	0.079071	5.693341	-2.287066
H	-0.114743	4.482975	-4.430915
H	0.226097	2.045182	-4.505733
H	2.164815	-4.033429	3.068876
H	-0.047467	2.461031	3.750262
H	-0.509815	2.529813	6.776389
H	-2.704351	2.631632	5.264402
H	-2.483406	2.551814	3.496579
H	-1.909205	3.959343	4.411776
H	-2.055297	0.726616	6.384915
H	-2.226280	-1.730914	6.594908
H	0.996124	-4.142975	4.387158
H	2.119250	0.347919	4.857700
H	-1.008377	-3.984111	2.755318
H	1.201389	-1.925243	2.277419
H	2.222749	-2.877432	4.411521
H	-0.995653	-3.185945	5.022818
H	-0.978642	-2.745929	1.478060
H	0.209664	-4.055535	1.474745
H	-3.066018	0.904788	-0.423954
H	-2.679098	-0.577509	1.978315
H	-3.241118	3.355180	-0.592168
H	-4.184185	3.410865	0.907217
H	-4.567185	1.294933	2.195503
H	-4.858691	2.623498	-0.536757
H	-4.168657	-0.899062	2.832606
H	-5.238725	0.515895	0.767528
H	-3.472639	-2.745624	1.283030
H	-5.138212	-2.158562	1.083898
H	-8.079587	1.083846	-9.668809
H	-9.771932	0.881221	-9.113209
H	-8.792515	2.276352	-8.559155
C	-4.631372	-0.810063	-6.331176
H	-5.393251	1.046433	-5.566482
H	-6.731463	0.129791	-3.721642
H	-6.273022	-1.508003	-4.133305
H	-5.004832	-0.020048	-2.200303
H	-3.998199	0.431076	-3.563948
H	-4.544086	-2.413564	-2.570301
H	-4.569664	-0.438610	-7.356957
H	-3.640289	-0.697439	-5.881553
H	-4.891103	-1.873527	-6.353587

TS(**VII**$^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$→**VIII**$^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$).

G = -2500.680281 kcal.mol^{-1}

Zn	-0.398379	1.182977	1.121488
C	1.505519	-3.510071	3.624270
C	1.937908	0.576807	2.711565
C	2.719298	1.205193	1.726548
C	2.348966	1.822999	0.518583
N	1.104857	1.864199	0.036850
N	0.617232	0.397163	2.630998
H	2.884677	-0.985842	3.849906
H	3.642330	0.600005	4.031356
H	0.221259	3.679734	5.895761
H	1.053437	2.124033	6.051815
H	3.776896	1.263227	1.956554
H	4.428487	2.071078	0.006999
H	3.514718	3.578622	0.109102
H	3.311326	2.539383	-1.297125
H	1.161693	6.785194	-0.515512

H	2.861088	0.450524	-3.361538	H	0.289690	2.155886	-4.481705	H	-1.045498	-4.014986	2.584184
C	1.614304	6.021389	0.125996	H	2.120611	-4.090058	2.927574	C	0.692706	1.917368	-2.383208
H	2.602144	5.789050	-0.285139	H	-0.007534	2.397399	3.803497	C	3.464960	2.533573	-0.217364
H	1.754211	6.472211	1.114488	C	-0.185733	-1.633143	3.790575	C	-0.773525	0.596714	4.643414
H	2.885038	0.272585	-1.597629	C	-0.637478	2.113496	4.652610	H	1.177986	-1.953800	2.183507
C	2.351127	-0.009519	-2.507041	C	0.072665	2.594678	5.928119	C	0.566979	-2.568198	2.852353
C	0.729730	4.771523	0.234952	H	-0.518010	2.368134	6.822769	H	2.175093	-2.968133	4.299048
H	1.188942	4.111319	0.977506	H	-2.685954	2.559625	5.279544	H	-1.064295	-3.274250	4.863636
H	2.434420	-1.096966	-2.612675	C	-1.987748	2.820111	4.475843	H	-0.999537	-2.740369	1.343403
C	0.635642	4.006092	-1.078304	C	-0.985250	-2.192230	4.793235	H	0.183927	-4.054700	1.313872
C	-0.667023	5.138137	0.759837	H	-2.433129	2.552889	3.513969	C	-0.099685	-0.222912	3.706435
H	-0.588429	5.680199	1.709472	H	-1.849825	3.907127	4.500213	O	-2.112424	1.839309	1.228809
H	-1.191659	5.786419	0.048254	H	-2.078328	0.605123	6.349781	C	-3.282101	1.592522	0.501959
H	0.152838	-1.315318	-3.555554	C	-1.674852	-1.398499	5.701211	H	-3.069681	1.022549	-0.417733
H	-1.278079	4.245203	0.922968	H	-2.290916	-1.855235	6.471316	H	-2.655424	-0.475077	1.980608
H	0.434293	-0.022863	-1.556256	C	-1.556211	-0.016252	5.626472	H	-3.214946	3.475743	-0.566711
C	0.138328	-0.225925	-3.653672	H	0.940302	-4.223933	4.233543	C	-3.907941	2.919707	0.070843
H	-0.907394	0.087544	-3.694855	H	2.101418	0.235952	4.843366	H	-4.128342	3.534168	0.950834
H	0.616539	0.022184	-4.608626	C	2.684078	0.087267	3.931705	H	-4.516275	1.417462	2.231896
C	0.391105	2.662417	-3.527343	C	0.826882	2.608143	-1.154934	H	-4.841130	2.764752	-0.484317
H	0.162216	5.772426	-2.209462	C	0.871442	0.405390	-2.466563	C	-4.280115	0.790552	1.363396
C	0.205668	4.039558	-3.469110	C	0.319822	4.698039	-2.252211	H	-4.136875	-0.785321	2.851332
H	-0.033429	4.595794	-4.371655	C	-0.385721	-3.388550	1.972097	C	-3.737163	-0.554945	1.855744

H	-5.221546	0.652045	0.812882
C	-4.085213	-1.763841	1.000511
H	-3.475001	-2.628287	1.280220
H	-5.139687	-2.029340	1.114667
O	-3.974370	-1.576779	-0.432585
C	-2.759481	-1.393263	-0.952660
O	-2.771381	-1.357750	-2.287429
O	-1.724700	-1.274227	-0.329631
C	-3.993956	-1.546336	-3.050863
C	-4.701208	-0.197335	-3.183428
C	-6.028114	-0.250736	-3.962188
C	-5.880056	0.170470	-5.413483
O	-7.174766	0.054499	-6.024971
C	-7.208306	0.366495	-7.324662
O	-6.266702	0.720301	-7.998168
C	-3.555136	-2.177856	-4.359718
O	-8.467237	0.217074	-7.751607
C	-8.656703	0.519688	-9.135136
H	-8.046599	-0.134739	-9.763127
H	-9.716183	0.351873	-9.328099
H	-8.391144	1.558989	-9.345185
H	-5.166802	-0.451586	-5.962948
H	-5.535984	1.207982	-5.491755
H	-6.761545	0.412216	-3.491770
H	-6.462497	-1.257718	-3.922085
H	-4.889352	0.171238	-2.171286
H	-4.007739	0.515929	-3.647862
H	-4.425159	-2.425340	-4.974405
H	-3.003373	-3.101910	-4.167817
H	-2.906212	-1.502098	-4.924744
H	-4.638259	-2.239163	-2.500800

VIII$^{\alpha\delta,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.701996 kcal.mol^{-1}

C	-1.870864	1.797102	4.956388
C	-1.087017	0.738484	4.444139
C	-1.517908	-0.602687	4.555285
C	-2.748863	-0.857761	5.167099
C	-3.536392	0.174099	5.663927
C	-3.093292	1.487151	5.560098
N	0.117528	1.030189	3.726020
Zn	0.038576	1.162650	1.772351
O	-1.284093	0.887210	0.539284
C	-2.647941	1.088980	0.817467
C	-3.525607	0.726134	-0.379910
C	-3.514400	-0.756781	-0.765325
C	-2.343698	-1.193306	-1.637682
C	-2.293202	-2.698306	-1.847073
C	-0.694111	-1.757877	4.004872
C	-1.310430	-2.299529	2.705821
C	-1.437971	3.252590	4.846324
C	-2.288730	4.006986	3.813849
C	1.277093	1.179177	4.373237
C	1.304349	0.997923	5.872503
C	2.494662	1.503967	3.751797
C	2.790884	1.727557	2.393354
C	4.213488	2.115013	2.064539
N	1.905338	1.617380	1.401188
C	2.315051	1.853032	0.047211
C	2.105039	3.123816	-0.528719
C	2.473386	3.318075	-1.863626
C	3.030513	2.290118	-2.613720
C	3.216491	1.038425	-2.036569
C	2.865445	0.792400	-0.707135
C	1.450976	4.258277	0.244857
C	2.255256	5.563273	0.184501
C	3.018076	-0.602608	-0.118581
C	4.292132	-1.323580	-0.574671
C	1.773864	-1.448244	-0.433878
C	0.009509	4.475518	-0.243057

O	-2.551270	-0.533111	-2.920299	H	-0.855916	0.746866	-7.939461	H	-1.955926	5.047002	3.723337
C	-1.490008	-0.426317	-3.715694	H	-0.492795	5.242142	0.357949	H	1.786098	6.327696	0.813471
O	-0.370759	-0.841265	-3.499332	H	-3.344854	4.016114	4.105196	H	3.282837	5.421860	0.535013
O	-1.880895	0.221497	-4.825546	H	-2.490553	4.076253	6.582898	H	-0.001375	4.808405	-1.287148
C	-0.864252	0.433812	-5.831077	H	2.304407	5.965489	-0.833091	H	-0.572109	3.549508	-0.186940
C	-1.597160	0.508788	-7.165226	H	-0.403472	3.267348	4.489040	H	4.411745	-2.258863	-0.017721
C	-2.341758	-0.776584	-7.525853	H	1.402760	3.956830	1.296630	H	4.257478	-1.586826	-1.637160
C	-3.070469	-0.650262	-8.854129	H	3.078099	-0.501227	0.970628	H	5.186945	-0.714109	-0.409433
O	-3.698413	-1.885265	-9.243640	H	-1.445094	-3.380974	5.273812	H	1.865619	-2.449478	0.002892
C	-4.893904	-2.230672	-8.755244	H	-3.097391	-1.883449	5.254286	H	0.864034	-0.985074	-0.039246
O	-5.431889	-3.271710	-9.037516	H	-2.224092	3.542511	2.825255	H	1.632226	-1.551961	-1.514082
H	-2.367991	-0.444987	-9.667477	H	-1.404810	-0.820910	-1.221949	H	0.172805	-3.649091	4.625544
C	-0.500256	-2.884563	5.028184	H	0.299353	-1.367957	3.759795	H	-0.068475	-2.512209	5.962824
C	-1.469387	3.976652	6.199739	H	4.815270	2.211540	2.969201	H	-0.697044	-3.109914	2.296384
O	-5.410908	-1.290681	-7.938847	H	4.679663	1.371316	1.410643	H	-2.314944	-2.697750	2.888798
C	-6.695190	-1.619218	-7.403197	H	2.323356	1.055150	6.257331	H	-1.393305	-1.517160	1.943963
H	-3.711477	2.290785	5.952039	H	0.872861	0.032718	6.154333	H	-2.856080	2.144100	1.070990
H	4.238072	3.064314	1.520661	H	3.337135	1.606934	4.424845	H	-2.982019	0.493052	1.687028
H	0.701788	1.765275	6.368529	H	3.635609	0.234523	-2.633925	H	-4.554287	1.019356	-0.129614
H	-4.438333	-1.013792	-1.299813	H	3.314767	2.460529	-3.648552	H	-3.230463	1.332538	-1.244515
H	-4.491573	-0.044841	6.133359	H	2.317188	4.291204	-2.321606	H	-3.502611	-1.372209	0.143891
H	-3.231280	-3.060478	-2.281567	H	-1.059031	4.987252	6.099663	H	-2.142168	-3.203515	-0.887923
H	-1.466642	-2.968175	-2.507939	H	-0.883559	3.447807	6.958439	C	-0.082286	1.695815	-5.503600

H	-2.298235	1.353374	-7.130394
H	-3.063507	-1.009718	-6.737609
H	-1.638042	-1.616070	-7.587098
H	-3.812885	0.152339	-8.824858
H	-6.963576	-0.786706	-6.752747
H	-6.647234	-2.550471	-6.833971
H	-7.428909	-1.732006	-8.205155
H	-0.191741	-0.431145	-5.812042
H	0.680829	1.877799	-6.267462
H	-0.748991	2.563353	-5.466823
H	0.418107	1.592801	-4.537954

VIII$^{\delta\alpha,\delta\alpha}{}_{7CC\text{-}\gamma(R)}$

G = -2500.701204 kcal.mol^{-1}

C	1.743727	2.847713	-0.953721
C	2.098125	1.699767	-0.213669
C	2.747377	0.606228	-0.829129
C	3.047235	0.695726	-2.190656
C	2.721097	1.827870	-2.929490
C	2.070280	2.888961	-2.312865
N	1.733988	1.614619	1.170842
C	2.610762	1.965253	2.114031
C	3.976030	2.458954	1.696321
C	3.066281	-0.664028	-0.053859
C	1.926547	-1.682895	-0.210706
C	0.981046	4.005079	-0.327226
C	-0.480688	4.000511	-0.802814
C	2.356369	1.905998	3.497806
C	1.191153	1.534989	4.190157
C	1.251391	1.574449	5.698575
N	0.052598	1.160788	3.599798
Zn	-0.060183	0.999129	1.649276
O	-1.373596	0.412593	0.518591
C	-2.738186	0.430929	0.861600
C	-3.613733	-0.063508	-0.289080
C	-3.478459	-1.550824	-0.629092
C	-2.241948	-1.935352	-1.432464
O	-2.389548	-1.266166	-2.717306
C	-1.281138	-1.107493	-3.435050
O	-1.604224	-0.410783	-4.536999
C	-0.509152	-0.147861	-5.425478
C	-1.058515	0.612532	-6.618997
C	-2.070094	-0.197314	-7.431618
C	-2.742642	0.604062	-8.543913
C	-1.802172	1.054196	-9.648572
C	-1.105335	0.840606	4.379177
C	-1.381263	-0.510968	4.685312
C	-2.574190	-0.812696	5.349373
C	-3.472103	0.184721	5.710876
C	-3.180022	1.511265	5.416589
C	-2.001807	1.867203	4.753643
C	-0.430743	-1.633225	4.293913
C	-0.091050	-2.552391	5.474827
C	-1.733243	3.331764	4.435611
C	-1.855108	4.231974	5.673241
C	-2.127001	-3.435759	-1.650123
C	-2.653427	3.834160	3.313354
C	-0.990210	-2.443050	3.114082
C	4.411084	-1.291452	-0.439575
C	1.640007	5.365402	-0.589586
O	-0.169848	-1.513727	-3.171175
O	-3.726390	-0.233074	-9.205936
C	-4.953300	-0.402628	-8.705901
O	-5.160723	0.311753	-7.581075
C	-6.466332	0.158033	-7.019100
O	-5.772366	-1.116882	-9.228509
H	-3.883812	2.288390	5.703529
H	3.886981	3.314408	1.019766
H	0.556414	2.320145	6.097011
H	-4.359157	-1.883219	-1.194735

H	-4.395553	-0.070731	6.223354
H	-3.019613	-3.823285	-2.153020
H	-1.247291	-3.671270	-2.252782
H	-0.204155	0.904715	-7.241776
H	-1.054365	4.789434	-0.303028
H	-3.706681	3.763891	3.606741
H	-2.884527	4.275654	6.044592
H	1.631168	5.624145	-1.653837
H	-0.703958	3.410714	4.071649
H	0.977370	3.850488	0.756885
H	3.126174	-0.400670	1.007978
H	-0.966720	-3.111098	5.822093
H	-2.804298	-1.848425	5.585405
H	-2.526242	3.247367	2.398568
H	-1.344056	-1.535714	-0.955969
H	0.505573	-1.172901	3.961251
H	4.569972	2.754355	2.562200
H	4.519187	1.683853	1.146514
H	2.256358	1.816061	6.047251
H	0.951788	0.611259	6.122736
H	3.187353	2.200254	4.127291
H	3.538985	-0.137167	-2.683647
H	2.972379	1.879895	-3.985623
H	1.806103	3.767223	-2.896152
H	-1.553748	5.256206	5.428609
H	-1.223660	3.881151	6.495791
H	-2.439288	4.882449	3.077085
H	1.100920	6.157311	-0.058306
H	2.681777	5.381538	-0.253221
H	-0.538212	4.178059	-1.882808
H	-0.962444	3.037972	-0.602157
H	4.648523	-2.115907	0.241023
H	4.394238	-1.707808	-1.452337
H	5.228936	-0.564761	-0.389537
H	2.142047	-2.594270	0.359120
H	0.974053	-1.275604	0.142879
H	1.781801	-1.952761	-1.260993
H	0.666127	-3.285969	5.177972
H	0.300955	-1.987802	6.327010
H	-0.289464	-3.232492	2.820197
H	-1.939422	-2.919887	3.383580
H	-1.170516	-1.807078	2.241148
H	-3.077166	1.450107	1.117927
H	-2.945517	-0.190586	1.752441
H	-4.658344	0.134510	-0.011797
H	-3.406980	0.537763	-1.182224
H	-3.467333	-2.139384	0.298203
H	-2.027795	-3.946066	-0.686699
H	0.251322	0.433292	-4.893758
H	-1.520984	1.540985	-6.259747
H	-2.846036	-0.565386	-6.753909
H	-1.581821	-1.074316	-7.876699
H	-3.257517	1.469195	-8.113299
H	-6.471484	0.770711	-6.117533
H	-6.657360	-0.888734	-6.771449
H	-7.230279	0.500711	-7.721340
H	-0.051747	-1.097534	-5.726382
H	-1.050119	1.745227	-9.257565
H	-1.289382	0.195525	-10.093022
H	-2.359127	1.566774	-10.437260

VIII$^{\delta\alpha,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.701553 kcal.mol^{-1}

C	0.018634	-0.009483	3.860548
C	0.076968	-1.420103	3.809482
C	-0.849066	-2.150903	4.559240
C	-1.809937	-1.516666	5.338514
C	-1.861977	-0.128564	5.368746
C	-0.960541	0.648733	4.635102
C	1.074837	-2.150040	2.922176

C	0.380236	-2.661348	1.649956	C	-3.327485	0.191553	-0.389486	H	3.493621	1.053499	5.193850
C	-1.087057	2.164556	4.655902	C	-3.408045	-1.141132	0.348702	H	-1.100624	3.834257	6.046389
C	-2.342424	2.609941	3.889079	C	-4.818570	-1.642801	0.591801	H	-0.183194	2.436766	6.632765
N	0.919040	0.763984	3.057617	O	-5.535172	-1.907904	-0.639204	H	4.005633	2.014740	3.322714
C	2.118331	1.096791	3.528629	C	-5.336892	-3.126548	-1.170296	H	5.018444	3.114964	1.772928
C	2.510029	0.667526	4.922829	O	-4.609327	-3.980944	-0.728006	H	3.963762	4.207357	0.855167
C	3.072776	1.837896	2.801473	C	1.762182	6.451893	0.623395	H	4.579199	2.754745	0.089719
C	3.000511	2.393537	1.515778	C	-1.077868	2.739477	6.078778	H	1.460845	7.112627	-0.196471
C	4.212915	3.157583	1.038730	C	4.228331	0.628658	-2.323145	H	4.166028	0.792258	-3.404407
N	1.940867	2.298452	0.700836	C	1.799026	-3.293386	3.644108	H	2.851841	6.353755	0.583960
C	1.952950	2.952215	-0.574497	C	-1.860805	2.008322	-1.335591	H	1.502278	6.956417	1.560197
C	1.492985	4.285305	-0.676809	O	-6.061569	-3.328292	-2.280923	H	4.972353	1.326482	-1.925773
C	1.418373	4.867027	-1.945908	C	-6.953335	-2.319793	-2.780154	H	1.348561	4.520286	1.433953
C	1.791962	4.165799	-3.086355	H	-7.711039	-2.883048	-3.331270	H	4.602976	-0.388810	-2.168024
C	2.258899	2.862158	-2.968354	C	-6.232661	-1.326813	-3.682686	H	-0.765541	5.818130	1.477420
C	2.353268	2.233351	-1.723065	C	-7.187773	-0.327571	-4.359498	H	-0.818933	5.816841	-0.293068
C	1.061783	5.088019	0.542984	C	-7.550457	-0.683389	-5.798506	H	2.198715	-1.216148	-2.126695
C	-0.463582	5.262348	0.582719	O	-8.371823	0.418531	-6.262490	H	-0.976809	4.296563	0.592872
C	2.863740	0.802037	-1.641345	C	-8.337684	0.663292	-7.574693	H	2.993925	0.557170	-0.582201
C	1.840600	-0.185202	-2.221641	O	-9.156868	1.693732	-7.819696	H	0.877127	-0.113031	-1.707533
Zn	0.355707	1.305378	1.244946	C	-9.221379	2.078782	-9.193771	H	1.662018	0.011898	-3.284527
O	-1.325929	0.829019	0.732937	O	-7.684772	0.070842	-8.405934	H	1.056820	5.887516	-2.041623
C	-1.888551	0.700801	-0.547043	H	2.527739	-0.423999	5.001989	H	1.722229	4.635034	-4.063874

H	2.555628	2.318490	-3.861445
H	2.569256	-3.722243	2.994080
H	-0.217465	2.577320	4.133749
H	-1.950058	2.412392	6.655093
H	-3.249945	2.244436	4.383258
H	-2.339818	2.221191	2.865925
H	-2.402776	3.703602	3.848134
H	-2.622131	0.365182	5.968636
H	-2.519840	-2.103625	5.915015
H	1.114680	-4.105155	3.912330
H	1.777204	1.019436	5.655152
H	-0.377802	-3.412943	1.896653
H	1.836234	-1.427041	2.612164
H	2.284998	-2.951567	4.563894
H	-0.820841	-3.236704	4.527015
H	-0.125562	-1.848381	1.120052
H	1.104094	-3.125187	0.970229
H	-1.339771	-0.060411	-1.135851
H	-2.850269	-1.916592	-0.190269
H	-0.835014	2.373361	-1.454442
H	-2.438728	2.777538	-0.811044
H	-3.899117	0.953308	0.159999
H	-2.288863	1.881522	-2.337075
H	-2.922463	-1.028120	1.324462
H	-3.785524	0.102622	-1.383055
H	-4.809885	-2.561037	1.184207
H	-5.429464	-0.888183	1.095936
H	-9.577379	1.251586	-9.813373
H	-9.924288	2.911040	-9.230767
H	-8.239286	2.393701	-9.556065
C	-8.315700	-1.983761	-5.978622
H	-6.646394	-0.705550	-6.416961
H	-6.730777	0.666953	-4.378631
H	-8.112789	-0.221688	-3.776808
H	-5.505328	-0.784656	-3.071596
H	-5.656303	-1.883061	-4.432623
H	-7.441708	-1.803770	-1.948962
H	-8.560156	-2.130148	-7.033658
H	-7.708803	-2.836294	-5.659297
H	-9.243305	-1.973737	-5.397051

VIII$^{\alpha\delta,\alpha\delta}{}_{7CC\text{-}\gamma(R)}$

G = -2500.69797 kcal.mol^{-1}

C	-1.895486	1.771246	5.218316
C	-1.065266	0.738993	4.725975
C	-1.383602	-0.619021	4.952535
C	-2.552173	-0.918741	5.659259
C	-3.386067	0.085280	6.136953
C	-3.053163	1.416790	5.918038
N	0.073423	1.070291	3.921828
Zn	-0.124492	1.158484	1.977399
O	-1.383891	0.849229	0.687036
C	-2.745094	1.207788	0.685793
C	-3.339687	0.926350	-0.706881
C	-3.184409	-0.520563	-1.198426
C	-1.912105	-0.775695	-1.983415
H	-1.731934	-1.845325	-2.131613
C	-0.507494	-1.749638	4.431649
C	-1.170511	-2.459607	3.241624
C	-1.578720	3.242277	4.988133
C	-2.544781	3.864411	3.968957
C	1.260143	1.287069	4.503265
C	1.364387	1.170059	6.005518
C	2.435135	1.623368	3.814634
C	2.662504	1.790343	2.434144
C	4.060088	2.185641	2.019760
N	1.730784	1.621459	1.496533
C	2.070342	1.806905	0.115814
C	1.841359	3.060324	-0.491710
C	2.137828	3.204999	-1.850140
C	2.641578	2.145439	-2.594158
C	2.848617	0.912789	-1.985500
C	2.573702	0.717442	-0.629276

C	1.243920	4.228631	0.277572	H	-4.291999	-0.169226	6.680192	H	3.099841	5.383806	0.406565
C	2.051871	5.523316	0.121928	H	-0.551359	0.115544	-8.510144	H	-0.292824	4.739137	-1.183911
C	2.775354	-0.654619	-0.002087	H	-0.684616	5.231405	0.472038	H	-0.801112	3.521466	-0.010426
C	4.080784	-1.332117	-0.437932	H	-3.577822	3.825546	4.331915	H	4.236562	-2.251141	0.137119
C	1.569660	-1.561138	-0.296232	H	-2.577604	4.101234	6.739883	H	4.062495	-1.614964	-1.495681
C	-0.221868	4.442172	-0.131473	H	2.034595	5.893115	-0.909002	H	4.948805	-0.683142	-0.280744
O	-2.073733	-0.159233	-3.282738	H	-0.571019	3.302464	4.564722	H	1.706014	-2.547359	0.162393
C	-1.093241	-0.396353	-4.149746	H	1.255272	3.965386	1.340517	H	0.642082	-1.129040	0.092488
O	-0.095874	-1.056687	-3.947978	H	2.828045	-0.521013	1.083849	H	1.436923	-1.698375	-1.374599
O	-1.411741	0.213523	-5.303209	H	-1.016058	-3.302999	5.892443	H	0.566385	-3.499951	5.138524
C	-0.459313	0.072975	-6.381265	H	-2.815200	-1.958590	5.834912	H	0.327623	-2.268730	6.389780
C	-1.263283	0.133771	-7.674424	H	-2.513746	3.337024	3.010550	H	-0.523199	-3.256059	2.858132
C	-2.271501	-1.006189	-7.817218	H	-1.047484	-0.334510	-1.484403	H	-2.122723	-2.913864	3.538076
C	-3.058124	-0.904149	-9.114328	H	0.425636	-1.305742	4.070016	H	-1.375365	-1.763176	2.422860
O	-3.928500	-2.033859	-9.305932	H	4.708673	2.312379	2.887652	H	-2.857467	2.297910	0.844497
C	-5.126606	-2.085448	-8.715012	H	4.498918	1.431043	1.359766	C	-3.539239	0.513990	1.793771
O	-5.863964	-3.031998	-8.829323	H	2.386068	1.347647	6.343726	H	-4.403013	1.196480	-0.678370
H	-2.389892	-0.938450	-9.980053	H	1.051449	0.176456	6.340508	H	-2.871482	1.600379	-1.433621
C	-0.138601	-2.757902	5.528421	H	3.303670	1.780198	4.442528	H	-3.189584	-1.214122	-0.349943
C	-1.579155	4.052473	6.292318	H	3.224782	0.083823	-2.577141	C	0.587561	1.169760	-6.270338
O	-5.401521	-0.973407	-8.004242	H	2.870823	2.278377	-3.647909	H	-1.778127	1.102686	-7.720473
C	-6.680123	-0.986540	-7.364242	H	1.966638	4.163516	-2.333017	H	-2.964518	-0.985299	-6.971044
H	-3.706396	2.199144	6.295708	H	-1.257712	5.081661	6.099466	H	-1.752896	-1.972747	-7.794818
H	4.043263	3.121023	1.452049	H	-0.903827	3.622577	7.038999	H	-3.635724	0.023654	-9.157237
H	0.702263	1.887131	6.500276	H	-2.292101	4.914822	3.786549	H	-6.746347	-0.043774	-6.821113
H	-4.034706	-0.803849	-1.830269	H	1.631669	6.311442	0.756299	H	-6.756327	-1.831665	-6.676105

H -7.480139 -1.060043 -8.104978

H 0.020388 -0.906279 -6.275397

H -4.589343 0.829230 1.784087

H -3.509333 -0.574863 1.683890

H -3.127916 0.755514 2.778925

H 1.323395 1.079114 -7.075852

H 0.120541 2.157703 -6.335242

H 1.112309 1.090730 -5.315259

3.2. Ring-opening polymerization of γ-substituted trimethylene carbonate

Initiation Step of the ROP of TMC-γMe.

TMC-γ(*R*)

G = -420.776625 kcal.mol^{-1}

H 3.49358 -7.68623 3.46032

C 2.73925 -7.74229 2.67156

H 1.08673 -7.96021 4.03133

H 2.68768 -8.77452 2.31188

C 1.38918 -7.30367 3.20207

H 3.05522 -7.09721 1.84645

O 1.57824 -5.98271 3.75258

C 0.58051 -5.08256 3.88394

O -0.64177 -5.38629 3.39600

C -0.93983 -6.66143 2.81751

C 0.28305 -7.26735 2.16656

H 0.06059 -8.27805 1.80918

H -1.32828 -7.31956 3.60604

H 0.59762 -6.66512 1.30597

H -1.74536 -6.47556 2.10286

O 0.78206 -4.01903 4.40071

TMC-γ(*S)*

G = -420.774799 kcal.mol^{-1}

O 3.59513 -7.87722 3.25234

C 2.69936 -7.68110 2.47895

O 1.50959 -7.21189 2.90877

O 2.85943 -7.93107 1.16095

H 2.07322 -8.07520 -0.69014

H 1.97821 -6.45224 0.01294

C 1.85798 -7.52204 0.22663

C 0.48513 -7.83441 0.77827

H -0.29736 -7.53183 0.07510

H 0.40072 -8.91636 0.92765

C -0.02857 -5.62592 1.96298

C 0.31403 -7.10123 2.10099

H -0.46294 -7.59038 2.69905

H -1.01834 -5.50881 1.51023

H -0.04129 -5.15356 2.94828

H 0.70095 -5.09460 1.34418

$I_{TMC\text{-}\gamma(R,re)}$

G = -2001.370044 kcal.mol^{-1}

C 3.181769 -7.664405 3.352141

C 2.110407 -7.994933 2.332305

O 0.785040 -7.942972 2.904519

C 0.550780 -7.451396 4.114598

O 1.494517 -7.553906 5.045669

C 2.745607 -8.202667 4.701687

O -0.554120 -7.009917 4.402841

Zn -0.805135 -5.101216 3.222621

O 1.073156 -5.070422 3.087548

C 1.881598 -4.169025 3.784743

N -1.972386 -3.816007 4.192411

C -3.231915 -3.626598 3.792517

C -3.807906 -4.209138 2.650938

C -3.245848 -5.039459 1.661273

N -2.040871 -5.600118 1.740637

C -1.586248 -6.476035 0.704049

C -0.818930 -5.962253 -0.364953

C -0.351077 -6.850773 -1.339091

C -0.639726 -8.208256 -1.277450

C -1.393728 -8.701080 -0.217985

C -1.867998 -7.861532 0.794381

C -0.482014 -4.483173 -0.485559

C -0.909089 -3.901735 -1.841013

C -2.672127 -8.448324 1.948631

C -2.079073 -9.759820 2.480563

C -1.423495 -2.996184 5.228740

C	-0.999278	-1.677790	4.927545
C	-0.389793	-0.927006	5.937129
C	-0.212081	-1.440666	7.216461
C	-0.648609	-2.727867	7.503010
C	-1.251907	-3.528353	6.527576
C	-1.166265	-1.056982	3.545417
C	0.175854	-0.952414	2.806274
C	-1.740145	-4.920177	6.900999
C	-0.654528	-5.757978	7.587720
C	-1.847457	0.318633	3.603848
C	-4.128069	-2.678460	4.560529
C	-4.084148	-5.216779	0.413095
C	1.010654	-4.230760	-0.223024
C	-4.145297	-8.673044	1.570505
C	-2.997067	-4.846037	7.782407
H	1.631609	-4.759707	-0.956307
H	-5.148341	-5.123789	0.640513
H	-4.650106	-7.743612	1.297398
H	-4.692020	-9.110942	2.413376
H	0.242667	-5.831288	6.969223
H	-3.353711	-5.852898	8.027020
H	-2.788132	-4.326238	8.724591
H	-3.813543	-4.314605	7.283970
H	2.598016	-4.696300	4.443634
H	-1.021987	-6.774827	7.761235
H	-2.011005	-5.435993	5.975821
H	1.330720	-3.473479	4.435805
H	2.486949	-3.550900	3.097021
H	2.214568	-9.013521	1.947189
H	2.102894	-7.290219	1.499232
C	3.700761	-7.919567	5.840927
H	2.544632	-9.281590	4.635509
H	-0.371611	-5.340151	8.560899
H	-0.520291	-3.123846	8.507065
H	0.260339	-0.837612	7.987376
H	-0.048630	0.081191	5.715878
H	-1.206904	1.068381	4.080863
H	-2.787525	0.287148	4.163708
H	-2.066360	0.676565	2.591885
H	0.035532	-0.495325	1.820054
H	0.886056	-0.332403	3.365085
H	0.629884	-1.935731	2.662619
H	-1.807509	-1.716465	2.953259
H	-4.025585	-1.657613	4.176884
H	-3.876436	-2.651324	5.622082
H	-5.174458	-2.969932	4.446354
H	-4.831953	-3.908035	2.459444
H	1.287787	-4.563467	0.783311
H	1.237792	-3.161532	-0.308553
H	-1.043704	-3.951524	0.289487
H	-0.746941	-2.818367	-1.858339
H	-1.967512	-4.090265	-2.048179
H	-0.330024	-4.330250	-2.666522
H	-3.829092	-4.423490	-0.299995
H	-3.902967	-6.168434	-0.087026
H	0.242073	-6.467041	-2.165538
H	-0.278574	-8.880843	-2.051309
H	-1.613169	-9.764300	-0.170879
H	-2.638365	-7.721239	2.765305
H	-1.015242	-9.654232	2.702495
H	-2.595528	-10.052833	3.400950
H	-2.200873	-10.583925	1.767943
H	-4.230089	-9.362667	0.722321
H	3.306581	-6.581214	3.432047
H	4.136510	-8.105319	3.048150
H	4.645594	-8.445413	5.675227
H	3.903959	-6.847536	5.914125
H	3.276998	-8.258238	6.789790

$I_{TMC\text{-}\gamma(R,si)}$

G = -2001.36957 kcal.mol^{-1}

C	3.269959	-7.821155	3.661117
C	2.310022	-7.715912	2.470822
O	0.922182	-7.852787	2.923716
C	0.558030	-7.490515	4.145208
O	1.386218	-7.784557	5.148122
C	2.564132	-8.532246	4.796341
O	-0.527879	-6.980385	4.377273

Zn	-0.802987	-5.081526	3.184787	C	-1.787326	-4.910475	6.913649	H	-0.534548	-3.113978	8.500142
O	1.061595	-4.894436	3.012979	C	-0.718872	-5.762685	7.609972	H	0.309016	-0.859551	7.943155
C	1.848105	-4.326157	4.020706	C	-1.653969	0.297692	3.507752	H	0.040675	0.025044	5.653420
N	-1.989532	-3.837254	4.191249	C	-4.121883	-2.661525	4.558164	H	-0.941550	1.008822	3.939772
C	-3.246862	-3.634473	3.797575	C	-4.140661	-5.258494	0.444731	H	-2.581368	0.368426	4.085455
C	-3.834513	-4.224767	2.664721	C	0.897794	-4.157130	-0.346137	H	-1.863529	0.632256	2.485920
C	-3.278416	-5.054891	1.672758	C	-4.093511	-8.731029	1.618333	H	0.116680	-0.749082	1.727308
N	-2.060935	-5.594862	1.727542	C	-3.041357	-4.804205	7.795659	H	1.009165	-0.613556	3.251024
C	-1.616543	-6.461564	0.678918	H	1.504499	-4.690007	-1.088215	H	0.588406	-2.212159	2.609585
C	-0.895343	-5.932698	-0.414749	H	-5.200516	-5.172355	0.693697	H	-1.807539	-1.752406	2.937182
C	-0.440007	-6.811819	-1.402966	H	-4.634740	-7.820243	1.352000	H	-3.953689	-1.638458	4.203718
C	-0.697194	-8.175573	-1.332648	H	-4.604064	-9.179695	2.478036	H	-3.901981	-2.669312	5.627297
C	-1.405047	-8.683886	-0.248246	H	0.178131	-5.859741	6.994167	H	-5.177520	-2.896031	4.406176
C	-1.863813	-7.852874	0.778406	H	-3.415979	-5.801632	8.052012	H	-4.860949	-3.927419	2.481193
C	-0.597339	-4.446516	-0.549401	H	-2.821396	-4.278230	8.731849	H	1.221241	-4.453404	0.657087
C	-1.089255	-3.879571	-1.889097	H	-3.849222	-4.263692	7.293218	H	1.096785	-3.085532	-0.463952
C	-2.619271	-8.455597	1.956441	H	1.873221	-4.928934	4.947730	H	-1.140921	-3.926465	0.245999
C	-1.968992	-9.743626	2.479723	H	-1.105446	-6.770479	7.794923	H	-0.952125	-2.792992	-1.915028
C	-1.422846	-3.017939	5.217382	H	-2.068024	-5.428878	5.992431	H	-2.150336	-4.092070	-2.055472
C	-0.957990	-1.719602	4.892343	H	1.528222	-3.315908	4.320847	H	-0.532627	-4.297846	-2.735092
C	-0.331704	-0.968125	5.890758	H	2.892842	-4.231603	3.674766	H	-3.908793	-4.475081	-0.286777
C	-0.176269	-1.463295	7.180790	C	2.507911	-8.781605	1.414285	H	-3.961012	-6.216444	-0.043922
C	-0.649168	-2.732516	7.488755	H	2.339848	-6.710247	2.043568	H	0.117004	-6.415683	-2.248463
C	-1.269313	-3.533609	6.524233	H	3.160175	-8.572154	5.708859	H	-0.349842	-8.840193	-2.119615
C	-1.096980	-1.132949	3.492471	H	2.267664	-9.551495	4.520776	H	-1.601832	-9.751315	-0.194485
C	0.233907	-1.184141	2.726740	H	-0.427579	-5.339746	8.578332	H	-2.589985	-7.720832	2.766355

H	-0.898930	-9.609677	2.652488
H	-2.437768	-10.039979	3.424224
H	-2.097246	-10.579015	1.781568
H	-4.177532	-9.429465	0.777364
H	3.568570	-6.826906	4.004801
H	4.175890	-8.365716	3.375485
H	3.473636	-8.631728	0.921731
H	2.495292	-9.785702	1.852212
H	1.719829	-8.719292	0.660032

TS($I_{TMC\text{-}\gamma(R,re)} \rightarrow II^{\gamma\alpha}_{TM\text{-}\gamma(R,re)}$)

G = -2001.358726 kcal.mol^{-1}

C	3.495322	-7.559994	3.425140
C	2.401513	-7.743443	2.366764
O	1.096683	-7.812566	2.953842
C	0.818378	-6.984222	3.993902
O	1.750577	-6.972670	4.984842
C	2.898754	-7.826419	4.799263
O	-0.398420	-6.893375	4.331275
Zn	-0.986926	-5.276958	3.261419
O	1.023510	-5.347220	3.165934
C	1.884177	-4.385086	3.730654
N	-1.999350	-3.827036	4.161848
C	-3.237594	-3.547756	3.752228
C	-3.854710	-4.111006	2.619447
C	-3.356272	-4.998081	1.647046
N	-2.170100	-5.603295	1.711699
C	-1.754099	-6.487983	0.664933
C	-0.967266	-5.984446	-0.396069
C	-0.512679	-6.873834	-1.374217
C	-0.824861	-8.226855	-1.321205
C	-1.601667	-8.708255	-0.274745
C	-2.077301	-7.863514	0.733158
C	-0.588084	-4.513968	-0.494467
C	-0.989234	-3.896467	-1.841512
C	-2.916775	-8.457161	1.856943
C	-2.120267	-9.481704	2.677791
C	-1.392137	-3.078790	5.219432
C	-0.866899	-1.788374	4.960766
C	-0.192334	-1.124925	5.990774
C	-0.045864	-1.696834	7.248600
C	-0.583600	-2.954183	7.494313
C	-1.256509	-3.668947	6.498644
C	-1.003263	-1.094637	3.609998
C	0.348059	-0.967202	2.891438
C	-1.870145	-5.021150	6.833564
C	-0.900982	-5.951858	7.571514
C	-1.657653	0.289676	3.741252
C	-4.070418	-2.529258	4.500428
C	-4.242134	-5.240770	0.446563
C	0.910918	-4.313013	-0.225798
C	-4.212708	-9.093628	1.330578
C	-3.166383	-4.842620	7.640446
H	1.516774	-4.831653	-0.978153
H	-5.217212	-4.768337	0.573656
H	-4.819449	-8.387619	0.754765
H	-4.823467	-9.455897	2.164850
H	0.018830	-6.097213	7.001542
H	-3.621443	-5.815892	7.855553
H	-2.967661	-4.345777	8.597153
H	-3.903215	-4.240552	7.100004
H	2.594192	-4.870837	4.412370
H	-1.365417	-6.934006	7.708952
H	-2.130064	-5.511156	5.891038
H	1.348004	-3.626434	4.314114
H	2.458198	-3.876008	2.942027
H	2.506829	-8.692869	1.836815
H	2.404087	-6.928256	1.638601
C	3.839940	-7.547778	5.952634
H	2.546338	-8.866458	4.848605
H	-0.644237	-5.571404	8.567048
H	-0.480411	-3.394508	8.482203
H	0.479519	-1.162034	8.035360
H	0.223970	-0.138486	5.801611
H	-1.005738	0.992962	4.270854
H	-2.603606	0.245707	4.289336
H	-1.856615	0.712941	2.750548
H	0.222818	-0.462703	1.926732

H	1.057550	-0.379957	3.485295
H	0.797781	-1.945272	2.704790
H	-1.649059	-1.709272	2.975711
H	-3.976656	-1.543024	4.033549
H	-3.761310	-2.431204	5.542056
H	-5.126165	-2.808093	4.463829
H	-4.862762	-3.756984	2.435976
H	1.182854	-4.700438	0.760948
H	1.171073	-3.248821	-0.266013
H	-1.135698	-3.978538	0.287560
H	-0.782916	-2.820437	-1.844221
H	-2.054668	-4.036558	-2.050958
H	-0.429308	-4.338156	-2.673107
H	-3.774464	-4.831409	-0.455283
H	-4.385703	-6.308227	0.264126
H	0.095503	-6.497198	-2.192975
H	-0.465349	-8.902878	-2.092628
H	-1.844039	-9.767263	-0.233479
H	-3.193985	-7.641809	2.532197
H	-1.220851	-9.031508	3.101065
H	-2.734343	-9.863686	3.501364
H	-1.823720	-10.338595	2.061559
H	-4.001537	-9.950846	0.681312
H	3.892942	-6.540158	3.407729
H	4.333020	-8.241383	3.242812
H	4.700938	-8.221641	5.908691
H	4.203784	-6.516335	5.916726
H	3.328786	-7.699723	6.906772

TS($I_{TMC\text{-}\gamma(R,si)} \rightarrow II^{ay}_{TMC\text{-}\gamma(R,si)}$)

G = -2001.358878 kcal.mol^{-1}

C	3.497420	-7.589330	3.464485
C	2.418649	-7.740200	2.375438
O	1.107798	-7.820552	2.974325
C	0.811174	-6.992095	4.008609
O	1.732660	-6.973601	5.010282
C	2.861873	-7.834012	4.820498
O	-0.409292	-6.902618	4.331319
Zn	-0.987655	-5.275333	3.271564
O	1.020617	-5.347832	3.187284
C	1.889461	-4.393558	3.753353
N	-2.002150	-3.823549	4.165485
C	-3.237839	-3.541622	3.750538
C	-3.851994	-4.105379	2.616197
C	-3.352527	-4.996627	1.648445
N	-2.168082	-5.604783	1.719280
C	-1.751122	-6.495345	0.678352
C	-0.960199	-5.998612	-0.383071
C	-0.502447	-6.893821	-1.354246
C	-0.816341	-8.246543	-1.294983
C	-1.597991	-8.721273	-0.248469
C	-2.076414	-7.870130	0.753017
C	-0.580673	-4.528746	-0.488927
C	-0.971300	-3.920925	-1.843459
C	-2.922981	-8.456295	1.875444
C	-2.135614	-9.482335	2.703129
C	-1.396911	-3.075541	5.224446
C	-0.867655	-1.786727	4.966281
C	-0.196084	-1.123479	5.998358
C	-0.055903	-1.694327	7.257380
C	-0.596757	-2.950519	7.502168
C	-1.267119	-3.664930	6.504535
C	-0.995787	-1.094787	3.613790
C	0.359545	-0.972014	2.901997
C	-1.883840	-5.016096	6.837962
C	-0.918273	-5.947990	7.579165
C	-1.647438	0.291341	3.739412
C	-4.071044	-2.519754	4.493642
C	-4.234461	-5.240496	0.445300
C	0.916000	-4.325049	-0.209627
C	-4.219841	-9.087904	1.345327
C	-3.182463	-4.835236	7.640490
H	1.528168	-4.849665	-0.952672
H	-5.209643	-4.767197	0.568261
H	-4.820115	-8.381009	0.763897
H	-4.836376	-9.443576	2.178160
H	0.003445	-6.094910	7.012596
H	-3.639834	-5.807685	7.854389

H	-2.986077	-4.338451	8.597700	H	1.180135	-4.704078	0.782485	O	1.624080	-5.054150	2.769035
H	-3.916467	-4.232037	7.097422	H	1.175969	-3.261107	-0.256459	C	1.579307	-5.720082	4.029078
H	2.593545	-4.885570	4.436778	H	-1.134698	-3.988193	0.284974	O	2.489491	-6.793877	4.041349
H	-1.384442	-6.929456	7.715495	H	-0.767161	-2.844535	-1.851147	C	2.555464	-7.487112	2.793276
H	-2.141782	-5.506039	5.894794	H	-2.034545	-4.064622	-2.061437	O	0.318289	-6.115678	4.252232
H	1.358774	-3.629894	4.335276	H	-0.402997	-4.366439	-2.667307	Zn	-0.979171	-5.122397	3.346766
H	2.469680	-3.889645	2.965832	H	-3.763430	-4.832530	-0.455469	O	2.054683	-4.778316	4.952216
C	2.565401	-8.996072	1.538361	H	-4.378239	-6.308069	0.263758	C	2.148412	-5.249749	6.285709
H	2.409116	-6.854191	1.733664	H	0.108703	-6.522388	-2.173086	N	-2.031482	-3.610671	4.011763
H	3.542790	-7.606995	5.643436	H	-0.457009	-8.926739	-2.062871	C	-3.212934	-3.323687	3.460268
H	2.533269	-8.876583	4.917176	H	-1.843590	-9.779375	-0.203296	C	-3.781008	-4.024999	2.379986
H	-0.664085	-5.567637	8.575358	H	-3.198958	-7.637409	2.546854	C	-3.294946	-5.120858	1.645316
H	-0.497970	-3.390258	8.490755	H	-1.236424	-9.035278	3.130127	N	-2.106962	-5.697751	1.847013
H	0.467360	-1.159744	8.045686	H	-2.755933	-9.858717	3.524589	C	-1.665393	-6.769963	1.006663
H	0.223129	-0.138159	5.809808	H	-1.840484	-10.342804	2.091208	C	-1.082857	-6.481054	-0.250009
H	-0.996572	0.993847	4.271319	H	-4.010239	-9.948878	0.700510	C	-0.567734	-7.539953	-1.003068
H	-2.596366	0.250612	4.282588	H	3.930029	-6.584774	3.444535	C	-0.626105	-8.851274	-0.544698
H	-1.840195	0.713546	2.747032	H	4.314690	-8.302034	3.306602	C	-1.216701	-9.121548	0.683211
H	0.240502	-0.469662	1.935370	H	3.498244	-8.957321	0.967096	C	-1.746664	-8.099570	1.477933
H	1.067141	-0.384794	3.498119	H	2.584034	-9.888159	2.173345	C	-0.973182	-5.060393	-0.788522
H	0.808217	-1.951515	2.720331	H	1.729986	-9.084689	0.839555	C	-1.469567	-4.935545	-2.235788
H	-1.639878	-1.708853	2.977225					C	-2.405455	-8.456934	2.802779
H	-3.974747	-1.535054	4.024046	$\mathbf{II}^{V\alpha}_{TMC\text{-}\gamma(R,re)}$				C	-1.410275	-9.095428	3.782174
H	-3.764420	-2.419144	5.535746	G = -2001.369986 kcal.mol^{-1}				C	-1.585305	-2.891785	5.170174
H	-5.127093	-2.797234	4.455136	C	3.215750	-6.556513	1.757562	C	-0.707694	-1.796571	5.019103
H	-4.858180	-3.748660	2.427746	C	2.923026	-5.113349	2.174517	C	-0.254861	-1.144101	6.170267

C	-0.640350	-1.561629	7.437541	H	2.910623	-4.424819	1.326697	H	-4.282131	-6.749680	0.633809
C	-1.493291	-2.651246	7.571060	H	3.659512	-4.755545	2.901950	H	-0.109611	-7.332522	-1.966554
C	-1.982606	-3.332947	6.453418	C	3.317219	-8.776119	3.029027	H	-0.217776	-9.659295	-1.145738
C	-0.232959	-1.313671	3.656739	H	1.533021	-7.720364	2.468859	H	-1.271140	-10.148225	1.036233
C	1.293354	-1.424572	3.528480	H	-1.608341	-5.569752	8.086259	H	-2.764106	-7.526545	3.256004
C	-2.886686	-4.542563	6.649305	H	-1.784365	-2.981837	8.564561	H	-0.575915	-8.419943	3.991471
C	-2.073154	-5.761409	7.112360	H	-0.273987	-1.043131	8.319525	H	-1.908168	-9.327857	4.730387
C	-0.700922	0.119091	3.361260	H	0.418899	-0.297167	6.067982	H	-1.008398	-10.034131	3.383883
C	-4.035365	-2.195369	4.037342	H	-0.279010	0.831756	4.078671	H	-3.343908	-10.330074	2.169150
C	-4.198843	-5.661667	0.562202	H	-1.790860	0.212070	3.406210	H	4.300470	-6.717111	1.720320
C	0.463654	-4.535422	-0.663853	H	-0.379151	0.428260	2.360554	H	2.813231	-6.769355	0.761211
C	-3.629558	-9.361502	2.594084	H	1.610375	-1.153420	2.514897	H	3.423405	-9.332263	2.091919
C	-4.047096	-4.266481	7.614893	H	1.798771	-0.744331	4.223457	H	4.317458	-8.561092	3.419044
H	1.154825	-5.140980	-1.261281	H	1.635911	-2.440152	3.741662	H	2.793508	-9.407620	3.751823
H	-5.195685	-5.223463	0.629380	H	-0.677654	-1.968468	2.900047				
H	-4.360975	-8.907009	1.917804	H	-3.436470	-1.287269	4.144038	**II**$^{\alpha\gamma}_{\text{TMC-}\gamma(R,si)}$			
H	-4.128495	-9.554950	3.550006	H	-4.389430	-2.453905	5.040778	G = -2001.372900 kcal.mol^{-1}			
H	-1.276276	-6.004735	6.402950	H	-4.901810	-1.979345	3.410663	O	1.004325	-4.561453	3.387206
H	-4.725120	-5.126180	7.646543	H	-4.758361	-3.671498	2.074542	O	2.532459	-5.216430	4.964426
H	-3.694190	-4.094944	8.637467	H	0.797125	-4.566172	0.376163	C	2.102170	-4.242567	5.899833
H	-4.628573	-3.388357	7.314956	H	0.530568	-3.500540	-1.018375	O	2.229780	-6.422149	3.105587
H	2.923934	-6.018046	6.382463	H	-1.601869	-4.414499	-0.168036	O	0.484083	-6.335393	4.659413
H	-2.720442	-6.639622	7.218083	H	-1.479858	-3.884058	-2.542285	C	0.687742	-7.759519	4.774972
H	-3.325509	-4.793965	5.678248	H	-2.482212	-5.333542	-2.358895	C	2.176858	-8.058958	4.917170
H	1.191066	-5.655827	6.628923	H	-0.819638	-5.470510	-2.936527	C	2.933663	-7.511184	3.705696
H	2.412508	-4.385403	6.898731	H	-3.794019	-5.442947	-0.430759	H	-0.774068	-4.556630	0.325800

C	-2.779283	-4.251029	6.869082	C	-1.225260	0.203971	3.001329	H	1.276059	-2.212449	3.186155
N	-2.112190	-3.612547	4.078111	C	-3.986868	-3.889060	7.745681	H	-2.478555	-7.719504	3.563808
N	-1.992555	-5.819607	2.002251	C	-1.895578	-5.288839	7.574857	H	-1.123005	-1.906468	2.685226
Zn	-0.858051	-4.967320	3.369771	C	1.594329	-5.568880	3.996445	H	-4.628577	-3.141247	7.269008
C	-1.497522	-6.915403	1.221050	C	-3.894770	-5.682801	0.435192	H	-3.676125	-3.484471	8.715114
C	-1.818128	-8.238589	1.615623	C	1.241847	-5.046290	-0.195645	H	-4.594439	-4.779128	7.942611
C	-1.325883	-9.295922	0.844751	C	-2.339034	-9.857228	3.521606	H	-1.670640	-2.417220	8.505972
C	-0.524461	-9.069276	-0.269329	C	0.866913	-1.210502	3.032598	H	-0.327222	-0.421822	7.937622
C	-0.195291	-7.768735	-0.624059	H	0.321496	-8.226556	3.849404	H	-2.474013	-6.185623	7.825344
C	-0.669160	-6.671876	0.103767	H	-1.567097	-10.317145	1.122896	H	-1.485643	-4.886622	8.508341
C	-2.677871	-8.523321	2.843562	H	-1.057203	-5.588285	6.940547	H	-3.161648	-4.711725	5.952260
C	-4.184402	-8.493648	2.535892	H	-4.523458	-7.506494	2.217772	H	-3.711218	-6.726597	0.179851
C	-0.271601	-5.270280	-0.335741	H	1.046000	-0.922769	1.990237	H	-3.553262	-5.074488	-0.410214
C	-0.729198	-4.971213	-1.771726	H	0.130684	0.118624	5.569873	H	-4.969527	-5.521064	0.542345
C	-3.157070	-5.246472	1.683464	H	-4.431838	-9.211784	1.745848	H	-2.301141	0.253087	3.198112
C	-3.759999	-4.193726	2.397382	H	2.965104	-4.029100	6.534563	H	-0.746761	0.997697	3.585600
C	-3.297424	-3.439380	3.490299	H	1.777151	-3.326632	5.399452	H	-1.066357	0.434840	1.942235
C	-4.221869	-2.359975	4.002606	H	1.281802	-4.619764	6.521568	H	-4.726897	-3.889575	2.014127
C	-0.120913	-8.256545	5.958575	H	0.256728	-7.823185	6.889759	H	-5.110403	-2.270552	3.376219
C	-1.686094	-2.721765	5.116554	H	-1.174697	-7.983684	5.855657	H	-4.539942	-2.584769	5.025569
C	-1.966847	-3.029122	6.466895	H	-0.057242	-9.346974	6.032968	H	-3.715107	-1.392044	4.039791
C	-1.465462	-2.186376	7.463648	H	2.542241	-7.598069	5.839302	H	-0.507488	-3.930631	-2.032710
C	-0.710508	-1.063321	7.148635	H	2.320520	-9.141958	5.001129	H	-1.803609	-5.133209	-1.903750
C	-0.454374	-0.763868	5.815960	H	3.004167	-8.262565	2.913151	H	-0.210074	-5.607954	-2.496675
C	-0.932643	-1.572213	4.779803	H	3.947586	-7.198881	3.980705	H	1.499084	-4.020087	-0.481226
C	-0.637509	-1.175298	3.339292	H	1.416534	-0.504977	3.666506	H	1.579302	-5.210732	0.830222

H	1.799875	-5.722128	-0.854055
H	0.443856	-7.593982	-1.485740
H	-0.151703	-9.907192	-0.852354
H	-4.758306	-8.766505	3.428687
H	-1.264823	-9.976675	3.688723
H	-2.682627	-10.712133	2.928446
H	-2.843304	-9.920229	4.491309

TS($\mathbf{II}^{\gamma\alpha}_{\text{TMC-}\gamma(R,re)} \rightarrow \mathbf{III}^{\gamma\alpha}_{\text{TMC-}\gamma(R,re)}$)

G = -2001.361025 kcal.mol^{-1}

O	1.255567	-4.787590	3.359648
C	1.206349	-6.016105	4.745574
O	2.372845	-6.674575	4.552911
C	2.438626	-7.506175	3.371323
C	2.211540	-6.651116	2.108348
C	2.243457	-5.154978	2.424318
O	0.079463	-6.556224	4.497112
Zn	-0.732471	-5.141100	3.273556
N	-1.894057	-3.726346	4.043075
C	-1.452147	-2.988544	5.189133
C	-0.646112	-1.841822	5.004633
C	-0.158143	-1.179365	6.135097
C	-0.450761	-1.626671	7.417943
C	-1.253736	-2.748650	7.583880
C	-1.771728	-3.445702	6.488069
C	-0.309682	-1.295038	3.624002
C	-0.860409	0.125212	3.425585
C	-2.657244	-4.659292	6.738278
C	-1.874848	-5.813171	7.382743
O	1.258523	-5.214658	5.822989
C	2.481839	-4.538788	6.095588
C	3.804952	-8.163893	3.422342
C	1.200318	-1.335722	3.352759
C	-3.091668	-3.487553	3.513550
C	-3.631730	-4.181267	2.412803
C	-3.108166	-5.228766	1.637373
N	-1.882367	-5.745986	1.773012
C	-1.451554	-6.789773	0.895122
C	-0.687305	-6.448403	-0.249484
C	-0.251522	-7.476973	-1.089749
C	-0.534523	-8.809465	-0.808525
C	-1.263798	-9.130377	0.328509
C	-1.739880	-8.140350	1.195230
C	-0.345630	-4.998187	-0.571665
C	-1.434466	-4.319239	-1.418562
C	-2.542813	-8.555375	2.420165
C	-1.666882	-9.297050	3.441087
C	-3.980056	-2.427872	4.125380
C	1.012403	-4.836352	-1.266158
C	-4.059836	-5.810547	0.613048
C	-3.882522	-4.304072	7.594967
C	-3.765579	-9.406927	2.045690
H	-3.543146	-6.200026	-0.265081
H	-4.791598	-5.063756	0.298185
H	-0.397310	0.834796	4.120274
H	-0.793049	-1.942020	2.885150
H	1.749366	-0.702524	4.059143
H	-2.906755	-7.643878	2.904979
H	0.985461	-5.192040	-2.302140
H	-4.611369	-6.644530	1.061414
H	-4.394916	-8.916731	1.296325
H	-4.379209	-9.598164	2.932611
H	-1.041382	-6.127656	6.751855
H	-4.554364	-5.165934	7.672607
H	-3.591620	-4.024195	8.613527
H	-4.451151	-3.467356	7.176613
H	2.794030	-3.960405	5.221872
H	-2.534275	-6.674381	7.541978
H	-3.021028	-5.012691	5.768085
H	3.268386	-5.243323	6.379417
H	2.263385	-3.863691	6.923229
H	2.112580	-4.574716	1.501667
H	3.232552	-4.889602	2.829843
H	1.654972	-8.264917	3.459068
H	-1.473990	-5.517710	8.359264
H	-1.486213	-3.094633	8.587863
H	-0.061364	-1.098727	8.284592
H	0.460877	-0.294836	6.004720

H	-1.942888	0.168953	3.582153				H	-0.251182	-2.457063	3.492911
H	-0.653528	0.476583	2.408489	TS($\mathbf{II}^{\alpha\gamma}_{\text{TMC-}\gamma(R,si)} \rightarrow \mathbf{III}^{\alpha\gamma}_{\text{TMC-}\gamma(R,si)}$)			C	-3.098024	-5.115935	1.783741
H	1.417306	-0.967167	2.343235	G = -2001.361338 kcal.mol^{-1}			C	-3.639230	-4.131561	2.624936
H	1.573532	-2.359505	3.438811	Zn	-0.891564	-5.359237	3.631840	H	-4.612705	-3.763795	2.315497
H	-3.408782	-1.543492	4.415050	O	-0.669311	-6.626237	5.252644	H	-4.880246	-2.791487	4.785519
H	-4.453716	-2.810980	5.035537	O	1.048537	-5.644765	3.908082	C	-3.975481	-2.382777	4.323727
H	-4.770141	-2.133712	3.432302	C	2.305109	-5.824875	3.292340	H	-4.296943	-1.728362	3.508599
H	-4.633716	-3.874841	2.135804	H	3.075754	-5.523142	4.024854	C	-3.119811	-3.504915	3.773472
H	1.806971	-5.380249	-0.746973	C	2.452273	-4.960059	2.052004	C	-3.287950	-8.748366	2.182127
H	1.289507	-3.777497	-1.300838	H	2.265144	-3.908960	2.289034	H	-3.801365	-7.790603	2.075796
H	-0.299110	-4.461544	0.384182	H	1.741892	-5.283888	1.285395	H	-3.451542	-1.788742	5.072594
H	-1.144661	-3.289719	-1.657060	H	3.463021	-5.041428	1.636110	H	-3.700198	-9.249794	3.064695
H	-2.394480	-4.279658	-0.899719	H	1.865611	-7.597698	2.137845	C	-1.583813	-3.237153	5.599355
H	-1.579632	-4.855261	-2.363513	C	2.528251	-7.305505	2.961950	C	-1.131128	-9.929831	2.651598
H	0.327659	-7.233150	-1.975257	H	3.562726	-7.454433	2.626369	C	-0.116185	-1.734758	6.803253
H	-0.182063	-9.594125	-1.472655	H	2.925089	-7.980066	4.995251	C	-0.678413	-2.133706	8.010024
H	-1.475263	-10.173208	0.550640	H	2.376425	-9.261334	3.894269	C	-1.699455	-3.076367	8.008411
H	-0.851017	-8.662362	3.795449	C	2.261206	-8.206026	4.154202	C	-2.176124	-3.641794	6.820918
H	-2.264946	-9.592281	4.310728	H	1.916908	-5.458830	7.735910	H	-3.583237	-4.940317	5.880688
H	-1.242072	-10.209366	3.006085	H	0.151428	-5.614144	7.487741	C	-3.316666	-4.649566	6.901127
H	-3.469451	-10.380260	1.638984	C	1.119352	-5.515933	6.993741	C	-4.563205	-4.037072	7.560608
H	2.983882	-6.879213	1.363198	H	1.119507	-4.617830	6.371860	H	-4.866347	-3.101567	7.081338
H	1.249270	-6.901199	1.650608	O	1.410346	-6.667997	6.206195	H	-5.404422	-4.736876	7.506664
H	3.906457	-8.876137	2.598008	O	0.892197	-8.074544	4.565397	H	-4.386967	-3.820297	8.620056
H	4.599987	-7.416251	3.332649	C	0.062733	-1.772132	4.287662	H	-3.747356	-6.628680	7.685546
H	3.940909	-8.701691	4.364801	C	-0.478940	-0.378423	3.932974	C	-2.903904	-5.930063	7.641860

H	-2.143327	-3.381953	8.952612	C	0.554800	-6.931547	5.198646	C	2.033036	-6.838767	2.269175
H	-2.605268	-5.711642	8.673976	H	-2.086867	-3.180471	-2.090002	C	2.167775	-5.307712	2.229283
H	-2.075854	-6.426195	7.131056	H	0.545133	-8.622105	-1.746941	O	0.078317	-6.622912	4.573643
H	-1.593857	-7.932206	3.202956	H	0.213518	-6.202969	-2.115653	Zn	-0.608619	-4.983192	3.086472
C	-1.767378	-8.574670	2.332032	H	-1.203378	-4.541486	-2.783541	N	-1.840665	-3.715595	4.004056
C	-1.169277	-7.882940	1.112808	H	-0.364173	-9.692352	0.280402	C	-1.392064	-2.994591	5.157250
C	-1.819147	-4.231223	-1.932281	H	-2.736711	-4.825391	-1.959372	C	-0.538072	-1.880045	4.985830
H	-1.669433	-3.952144	0.186880	H	-0.042844	-9.861735	2.719044	C	-0.033053	-1.243005	6.123690
C	-3.986040	-5.499971	0.615731	H	-1.388198	-10.690359	1.904605	C	-0.358261	-1.679302	7.402519
H	-3.605376	-6.360446	0.065743	H	-3.523677	-9.361696	1.304615	C	-1.217234	-2.761303	7.556318
H	-4.089771	-4.661847	-0.079925	H	-1.499124	-10.286930	3.618113	C	-1.754176	-3.432846	6.453520
H	-4.988396	-5.734083	0.986922	H	0.670477	-0.984862	6.802659	C	-0.191648	-1.319623	3.613008
N	-1.903696	-5.693865	1.947506	H	-0.328873	-1.705906	8.945883	C	-0.772118	0.091601	3.429798
N	-1.979951	-3.846182	4.368653	H	-0.202418	0.355097	4.698889	C	-2.710281	-4.593792	6.700228
C	-1.059968	-4.397393	-0.604461	H	-1.570215	-0.379494	3.853383	C	-2.009206	-5.793201	7.353827
C	-1.325562	-6.487751	0.909539	H	-0.070250	-0.034954	2.975917	O	1.125228	-5.277558	5.990512
C	-0.845025	-5.872460	-0.274228	H	1.989031	-2.756641	4.562228	C	2.345425	-4.604906	6.325477
C	0.249671	-3.598591	-0.659756	H	1.991884	-1.474030	3.337702	C	3.951606	-7.896276	3.579822
H	0.047799	-2.561113	-0.949211	H	1.989989	-1.052533	5.048157	C	1.319327	-1.330818	3.347670
H	0.753606	-3.584852	0.308443					C	-3.063360	-3.509495	3.518519
H	0.944718	-4.019041	-1.395067	**III**$^{\gamma\alpha}_{TMC\text{-}\gamma(R,re)}$				C	-3.630151	-4.224126	2.446161
C	-0.493432	-8.624312	0.139665	G = -2001.36872 kcal.mol^{-1}				C	-3.114992	-5.269310	1.661514
C	0.016383	-8.025786	-1.008170	O	1.238846	-4.619067	3.006249	N	-1.868648	-5.743368	1.741633
C	-0.169534	-6.665698	-1.209433	C	1.134014	-6.187153	5.031221	C	-1.437435	-6.771645	0.845694
C	-0.547854	-2.273995	5.587430	O	2.345842	-6.612161	4.719355	C	-0.703815	-6.403657	-0.312106
C	1.595624	-1.766267	4.316534	C	2.484051	-7.507336	3.575307	C	-0.256010	-7.416285	-1.164655

C	-0.502515	-8.757713	-0.890228
C	-1.207332	-9.103993	0.253914
C	-1.689858	-8.131598	1.137528
C	-0.414873	-4.942106	-0.637720
C	-1.596763	-4.263088	-1.349168
C	-2.462154	-8.580564	2.370568
C	-1.563715	-9.353400	3.347463
C	-3.953911	-2.458959	4.144437
C	0.856677	-4.740827	-1.470786
C	-4.098069	-5.881264	0.684900
C	-3.915510	-4.164113	7.553011
C	-3.691205	-9.425915	2.001525
H	-3.607531	-6.309287	-0.190285
H	-4.827505	-5.136647	0.358713
H	-0.328138	0.800830	4.137491
H	-0.658963	-1.966143	2.863598
H	1.860750	-0.722895	4.081966
H	-2.812724	-7.683761	2.890730
H	0.721881	-5.069652	-2.507715
H	-4.651929	-6.686991	1.179459
H	-4.336944	-8.919905	1.277622
H	-4.285785	-9.642137	2.895822
H	-1.207067	-6.173102	6.719986
H	-4.649945	-4.975087	7.609955
H	-3.614205	-3.925170	8.578975
H	-4.416094	-3.279290	7.147643
H	2.765588	-4.144291	5.429727
H	-2.728070	-6.602793	7.525717
H	-3.088533	-4.931064	5.730186
H	3.063919	-5.298246	6.769538
H	2.055272	-3.839987	7.044345
H	2.115233	-5.008498	1.168412
H	3.185390	-5.034387	2.564270
H	1.863411	-8.385244	3.783484
H	-1.580218	-5.518357	8.324274
H	-1.481519	-3.093781	8.557068
H	0.043036	-1.169705	8.274864
H	0.620964	-0.382948	6.001300
H	-1.856394	0.109730	3.580249
H	-0.566145	0.460283	2.418710
H	1.530664	-0.912274	2.356571
H	1.697246	-2.356564	3.373382
H	-3.377447	-1.604867	4.505017
H	-4.488121	-2.874747	5.004942
H	-4.699643	-2.111588	3.426604
H	-4.648336	-3.940364	2.205098
H	1.712411	-5.280411	-1.054186
H	1.112348	-3.676904	-1.503847
H	-0.267838	-4.422269	0.317489
H	-1.346243	-3.225006	-1.594926
H	-2.495558	-4.246764	-0.729976
H	-1.834754	-4.782290	-2.284667
H	0.301852	-7.152798	-2.057748
H	-0.142034	-9.528410	-1.566376
H	-1.393661	-10.153003	0.469945
H	-0.733837	-8.732957	3.692605
H	-2.138425	-9.664718	4.227171
H	-1.157566	-10.257710	2.879488
H	-3.399730	-10.387190	1.563747
H	2.629592	-7.274175	1.456873
H	0.992480	-7.101944	2.054308
H	4.131709	-8.661593	2.819631
H	4.583744	-7.031631	3.354372
H	4.247370	-8.298614	4.552794

III$^{\alpha\gamma}{}_{TMC\text{-}\gamma(R,si)}$

G = -2001.366476 kcal.mol^{-1}

C	-1.828673	-4.160752	6.484944
C	-1.408043	-3.401547	5.365028
C	-0.582613	-2.267914	5.531474
C	-0.193749	-1.909721	6.826916
C	-0.609136	-2.636224	7.935405
C	-1.422104	-3.750874	7.757906
N	-1.803952	-3.829823	4.057267
C	-2.927422	-3.364889	3.516070
C	-3.675945	-2.223095	4.171188
C	-0.108123	-1.421287	4.359958
C	-0.555991	0.042241	4.491659

C	-2.732271	-5.378057	6.334385	C	-4.179244	-5.316592	0.480946	H	-1.637959	0.129938	4.631726
C	-4.209981	-5.009575	6.544116	C	-1.561985	-4.442094	-1.749655	H	-0.282497	0.607061	3.593417
Zn	-0.656703	-5.077974	2.989989	C	-2.381488	-9.321773	3.294865	H	1.738703	-0.909986	3.333156
N	-1.981657	-5.613152	1.591219	C	1.414790	-1.510174	4.191810	H	1.934477	-1.126346	5.077787
C	-1.768903	-6.746779	0.739340	C	-2.347276	-6.534656	7.264547	H	1.711336	-2.548736	4.023231
C	-1.051143	-6.580674	-0.472585	H	0.630245	-5.724759	-2.705489	H	-0.560363	-1.831174	3.450972
C	-0.845082	-7.698703	-1.286818	H	-4.988802	-5.855126	0.984415	H	-3.307023	-1.273464	3.766279
C	-1.316827	-8.955539	-0.926772	H	-4.997337	-7.976330	1.430496	H	-3.529424	-2.195553	5.251435
C	-2.006416	-9.107969	0.267878	H	-5.068603	-8.778907	3.008026	H	-4.744583	-2.280086	3.953350
C	-2.247948	-8.023756	1.118860	H	-1.288875	-6.784420	7.166956	H	-4.424910	-3.369045	2.039053
C	-0.528954	-5.219272	-0.917173	H	-4.846156	-5.894673	6.429325	H	1.529813	-5.924558	-1.193102
C	0.785079	-5.307919	-1.704073	H	-4.371290	-4.609241	7.551881	H	1.208553	-4.307354	-1.838894
C	-3.042778	-8.268249	2.394676	H	-4.552794	-4.259007	5.827445	H	-0.340917	-4.635534	-0.007718
C	-4.488174	-8.690503	2.083024	H	2.494139	-5.053772	5.743174	H	-1.138090	-3.489635	-2.087148
O	-0.210478	-7.008550	4.060715	H	-2.934469	-7.424415	7.012753	H	-2.465990	-4.217872	-1.181018
C	0.830011	-6.813968	4.686731	H	-2.620820	-5.736557	5.306260	H	-1.852685	-5.014611	-2.637972
O	1.193428	-4.737445	3.219032	H	2.715137	-6.577052	6.667466	H	-4.621410	-4.420822	0.036363
C	2.274075	-5.171042	2.448660	H	1.735601	-5.239395	7.352936	H	-3.792326	-5.955486	-0.312226
C	2.064348	-6.596812	1.903582	H	3.164580	-5.205878	3.106176	H	-0.304471	-7.583264	-2.220987
C	2.183022	-7.701630	2.960695	H	3.188216	-8.127318	2.975200	H	-1.146239	-9.810685	-1.575369
O	2.033078	-7.222280	4.318983	H	1.460607	-8.504442	2.793402	H	-2.374840	-10.091107	0.549693
C	2.593984	-4.184718	1.324602	H	-2.553994	-6.303796	8.315916	H	-3.074392	-7.328432	2.954369
O	0.807380	-6.244169	5.878098	H	-1.747573	-4.316085	8.626778	H	-1.365234	-9.027965	3.561327
C	2.032589	-5.754792	6.440607	H	-0.304802	-2.334179	8.934329	H	-2.955011	-9.438496	4.221195
C	-3.493581	-3.847843	2.321269	H	0.442289	-1.038846	6.965728	H	-2.348165	-10.302028	2.805806
C	-3.125994	-4.926717	1.499760	H	-0.074323	0.532838	5.344857	H	-4.513984	-9.665594	1.583206

H	2.802370	-6.817856	1.121965
H	1.080217	-6.636778	1.421726
H	3.496815	-4.469907	0.770995
H	1.761934	-4.122402	0.617266
H	2.748328	-3.188277	1.747258

TS(**III**$^{\gamma\alpha}_{TMC\text{-}\gamma(R,re)}$→ **IV**$^{\gamma\alpha}_{TMC\text{-}\gamma(R)}$)

G = -2001.366852 kcal.mol^{-1}

C	-1.696560	-8.144276	1.153402
C	-1.413120	-6.787584	0.877152
C	-0.626510	-6.423003	-0.245540
C	-0.152349	-7.437750	-1.080963
C	-0.426861	-8.776809	-0.822011
C	-1.187118	-9.118674	0.287401
N	-1.864074	-5.756883	1.762712
C	-3.108026	-5.277669	1.668227
C	-4.075747	-5.873371	0.668467
C	-0.317119	-4.962912	-0.558337
C	0.987737	-4.763186	-1.338257
C	-2.526087	-8.588357	2.350661
C	-3.738025	-9.432208	1.924530
C	-3.625996	-4.237680	2.458520
C	-3.063393	-3.538865	3.542620
C	-3.939203	-2.478559	4.169733
N	-1.845682	-3.764782	4.036980
C	-1.385460	-3.053028	5.193392
C	-0.499680	-1.964222	5.021320
C	0.016410	-1.336490	6.159006
C	-0.327627	-1.760256	7.437057
C	-1.214186	-2.819508	7.590291
C	-1.764597	-3.480484	6.487730
C	-0.121996	-1.427760	3.647340
C	1.386131	-1.533239	3.383036
C	-2.749280	-4.617160	6.733430
C	-3.940143	-4.158653	7.591758
Zn	-0.629900	-5.006196	3.109451
O	0.292466	-7.147779	5.141906
C	1.301171	-6.533752	5.432707
O	1.279034	-5.550188	6.328506
C	2.423805	-4.700413	6.452453
O	2.529209	-6.790327	4.981151
C	2.638341	-7.739508	3.889553
C	4.128081	-8.002444	3.752565
C	1.994756	-7.194803	2.607621
C	2.083429	-5.673481	2.429714
O	1.209368	-4.949056	3.250113
C	-0.616487	0.014547	3.457765
C	-2.075997	-5.836759	7.378735
C	-1.468807	-4.280848	-1.314857
C	-1.677770	-9.359666	3.373004
H	-3.569227	-6.303536	-0.196601
H	-4.788497	-5.118429	0.329330
H	-0.131383	0.699300	4.162222
H	-0.629667	-2.045311	2.898980
H	1.960858	-0.950058	4.111740
H	-2.902328	-7.690497	2.851046
H	0.895623	-5.096870	-2.378074
H	-4.649959	-6.674441	1.146910
H	-4.345608	-8.929019	1.166136
H	-4.376614	-9.641748	2.789466
H	-1.285252	-6.242462	6.745140
H	-4.695971	-4.949812	7.645769
H	-3.629731	-3.935645	8.618479
H	-4.418328	-3.257521	7.194470
H	2.673851	-4.274941	5.479042
H	-2.817562	-6.625172	7.553412
H	-3.141757	-4.940159	5.763882
H	3.278611	-5.249946	6.855948
H	2.118801	-3.913013	7.141196
H	1.915756	-5.456764	1.362442
H	3.113342	-5.341940	2.647015
H	2.123097	-8.654567	4.201556
H	-1.636010	-5.574990	8.347804
H	-1.488449	-3.144332	8.590567
H	0.083944	-1.260127	8.309951
H	0.696021	-0.496449	6.037704
H	-1.697706	0.096379	3.609019
H	-0.389472	0.366400	2.445187

H	1.624239	-1.140523	2.387528
H	1.709509	-2.577125	3.428612
H	-3.351363	-1.621028	4.503950
H	-4.454044	-2.878030	5.049299
H	-4.698998	-2.139828	3.462903
H	-4.638725	-3.942844	2.208397
H	1.826684	-5.299304	-0.884769
H	1.242828	-3.698982	-1.365692
H	-0.207843	-4.442504	0.402322
H	-1.210579	-3.241041	-1.544693
H	-2.393388	-4.270616	-0.734452
H	-1.666066	-4.796003	-2.261856
H	0.446847	-7.178031	-1.947878
H	-0.045285	-9.549684	-1.483842
H	-1.394602	-10.165998	0.491136
H	-0.868995	-8.745857	3.776215
H	-2.300774	-9.680090	4.215708
H	-1.242167	-10.259416	2.922965
H	-3.428094	-10.396983	1.507850
H	2.480571	-7.689948	1.756684
H	0.939516	-7.482337	2.568126
H	4.299587	-8.793138	3.016440
H	4.655862	-7.102866	3.420463
H	4.555796	-8.319848	4.707709

TS($\mathbf{III}^{\alpha\gamma}{}_{\text{TMC-}\gamma(R,si)} \rightarrow \mathbf{IV}^{\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$)

G = -2001.365718 kcal.mol^{-1}

C	-1.895072	-7.966287	0.691950
C	-1.642318	-6.581996	0.562668
C	-0.973739	-6.068662	-0.580354
C	-0.560129	-6.970137	-1.565274
C	-0.784499	-8.337173	-1.439540
C	-1.445658	-8.822380	-0.320669
N	-2.022617	-5.670207	1.602622
C	-3.247940	-5.128237	1.591254
C	-4.280517	-5.622055	0.600561
C	-0.721825	-4.573135	-0.762700
C	-1.950377	-3.836021	-1.323534
C	-2.672201	-8.562108	1.858983
C	-1.816062	-9.514465	2.705562
Zn	-0.754824	-5.194351	3.043643
O	1.049559	-5.298471	3.432880
C	2.059372	-5.982437	2.739390
C	2.254618	-5.444878	1.325340
N	-1.888428	-3.920026	4.074127
C	-3.072441	-3.548483	3.591507
C	-3.689730	-4.125437	2.465102
C	-1.417019	-3.373036	5.312085
C	-1.946017	-3.836665	6.541302
C	-1.402087	-3.332800	7.727127
C	-0.383813	-2.386920	7.719062
C	0.107307	-1.923187	6.504585

C	-0.390853	-2.400646	5.288774
C	-3.091846	-4.838450	6.636362
C	-2.642775	-6.191084	7.207339
C	0.145796	-1.813261	3.991368
C	1.666276	-1.971221	3.867879
C	-3.867005	-2.454867	4.270215
C	-0.273462	-0.342876	3.838868
C	-4.258054	-4.282624	7.471442
O	-0.277239	-7.548566	4.986757
C	0.724493	-7.078383	5.489326
O	0.660790	-6.207394	6.491679
C	1.851347	-5.525640	6.898881
C	0.486121	-4.256579	-1.654102
C	-3.935878	-9.290858	1.371314
O	1.979896	-7.406521	5.177565
C	2.155770	-8.223485	4.006271
C	1.812488	-7.502071	2.705359
H	0.280274	-4.479077	-2.707282
H	-4.826357	-6.461532	1.045212
H	-4.552820	-8.661177	0.723311
H	-4.546584	-9.603971	2.225116
H	-1.893422	-6.666944	6.573011
H	-5.121880	-4.953532	7.409056
H	-3.987169	-4.202050	8.529900
H	-4.573032	-3.288028	7.140430
H	2.291886	-5.004186	6.047349

H	-3.503947	-6.864381	7.292219	H	-2.800968	-3.863535	-0.640975	N	-0.588793	0.536330	2.069820
H	-3.464971	-5.025452	5.624847	H	-2.261045	-4.274757	-2.278527	C	-0.767732	0.963839	0.819583
H	2.575258	-6.222900	7.329087	H	-5.008538	-4.839710	0.376146	C	-1.980578	0.493584	0.052680
H	1.522831	-4.806235	7.648179	H	-3.837820	-5.976842	-0.330634	C	-0.150067	-2.342507	1.837648
H	2.998142	-5.806696	3.295054	H	-0.046566	-6.597822	-2.445750	C	-0.549652	-3.450518	0.854649
H	3.219518	-8.471739	4.042233	H	-0.447487	-9.018925	-2.215785	C	-2.791410	1.678281	3.607413
H	1.575795	-9.144342	4.122549	H	-1.629150	-9.889934	-0.229409	C	-4.225351	2.143738	3.322630
H	-2.214644	-6.071185	8.208963	H	-2.988054	-7.739059	2.508271	Zn	0.971410	1.106453	3.106811
H	-1.792287	-3.687381	8.677681	H	-0.990736	-8.991125	3.192056	O	1.337699	0.498765	4.786189
H	0.015074	-2.003282	8.654651	H	-2.425525	-9.964527	3.496957	C	2.336435	1.021581	5.624957
H	0.888990	-1.167622	6.495971	H	-1.410464	-10.329367	2.095032	C	2.721422	0.042643	6.736726
H	0.158002	0.276823	4.632956	H	-3.681319	-10.192778	0.803441	C	1.613798	-0.232372	7.751643
H	-1.361057	-0.225986	3.881943	H	2.412811	-7.968017	1.913048	O	2.190877	-0.875715	8.926880
H	0.071716	0.058069	2.879182	H	0.763120	-7.663553	2.435999	C	2.741425	-0.069435	9.830184
H	2.013230	-1.561336	2.912203	H	3.154607	-5.859944	0.855705	O	2.806396	1.141017	9.789883
H	2.195245	-1.434264	4.663475	H	1.395984	-5.711259	0.700281	N	1.832587	2.269461	1.799473
H	1.938128	-3.029100	3.909225	H	2.347073	-4.355091	1.347880	C	1.302571	2.438673	0.583795
H	-0.307849	-2.367503	3.163071					C	0.109846	1.837442	0.147436
H	-4.575364	-2.883701	4.986038	**IV**$^{\gamma\alpha}_{\text{TMC-}\gamma(R)}$				C	3.060835	2.912870	2.161320
H	-4.445250	-1.898444	3.528895	G = -2001.384996 kcal.mol^{-1}				C	3.028467	4.188131	2.768714
H	-3.223660	-1.764179	4.817336	C	-2.606771	0.179104	3.425030	C	4.232941	4.746403	3.207087
H	-4.685010	-3.748858	2.256581	C	-1.535784	-0.353736	2.674530	C	5.440002	4.075241	3.051703
H	1.380710	-4.811155	-1.359423	C	-1.339968	-1.748735	2.576747	C	5.457378	2.825541	2.443751
H	0.716520	-3.187990	-1.594118	C	-2.245212	-2.593778	3.225483	C	4.281472	2.222627	1.987292
H	-0.519337	-4.156746	0.232419	C	-3.312255	-2.084819	3.955974	C	1.726291	4.946703	2.981505
H	-1.707264	-2.782586	-1.501889	C	-3.483176	-0.709219	4.055092	C	1.326481	4.947052	4.464776

C	4.343681	0.842976	1.347571	H	-4.309918	-0.315100	4.640072	H	2.005591	1.962726	6.100845
C	5.366722	0.772382	0.205333	H	-2.137555	2.183916	2.889204	H	3.258193	1.268690	5.072352
C	2.020155	3.329146	-0.402003	H	3.359728	0.631910	0.916153	C	0.528344	-1.171951	7.267745
C	4.627471	-0.239974	2.399571	H	-2.979274	1.638740	5.780037	H	3.060080	-0.903326	6.295598
C	1.786742	6.380549	2.437615	H	-1.313614	1.799713	5.215974	H	3.569457	0.482826	7.274846
O	3.222916	-0.833274	10.824741	H	-2.418344	3.190245	5.134826	H	3.130817	0.584411	12.350565
C	3.842541	-0.098463	11.878585	H	3.032460	2.958834	-0.591944	H	4.690043	0.482500	11.504572
C	0.901367	-2.849836	2.837912	H	2.129707	4.341771	-0.002030	H	-0.241845	-1.304024	8.033605
C	-2.346174	2.103235	5.015768	H	1.483195	3.382960	-1.349931	H	0.084712	-0.765337	6.357331
H	4.182652	-0.845671	12.596169	H	6.403046	2.303449	2.323936	H	0.953543	-2.152932	7.032763
H	-1.987666	-0.597844	-0.027584	H	6.364449	4.524781	3.403609				
H	-2.900900	0.771612	0.575457	H	2.079048	5.458855	5.074676	**IV**$^{qy}_{TMC\text{-}\gamma(R)}$			
H	-2.003947	0.919870	-0.951070	H	4.222988	5.722806	3.684382	G = -2001.382776 kcal.mol^{-1}			
H	-4.938250	1.740924	4.050085	H	1.225737	3.929101	4.853668	C	-2.122299	-0.001357	3.853601
H	-4.287500	3.235880	3.379223	H	0.940817	4.419386	2.430347	C	-1.120105	-0.448696	2.965466
H	-4.560795	1.838079	2.326135	H	0.370104	5.461736	4.608937	C	-0.812032	-1.821316	2.849834
H	-0.180217	2.083788	-0.866711	H	0.807655	6.863007	2.529519	C	-1.541337	-2.733404	3.618114
H	-1.310493	-3.109835	0.144656	H	2.076448	6.402751	1.382066	C	-2.543187	-2.310286	4.483154
H	0.323147	-3.781263	0.281318	H	2.505626	6.994925	2.990203	C	-2.821823	-0.953732	4.600102
H	-0.948871	-4.329474	1.371941	H	5.316052	-0.203740	-0.289012	N	-0.356210	0.509524	2.221547
H	0.312170	-1.540479	1.252915	H	5.184522	1.543517	-0.550218	C	-0.771601	0.904464	1.020574
H	-4.004048	-2.758557	4.454170	H	6.392305	0.900633	0.567849	C	-2.050832	0.331992	0.457634
H	-2.106363	-3.669816	3.163198	H	5.598178	-0.075084	2.880238	C	0.322922	-2.316404	1.966181
H	1.786850	-3.224079	2.311494	H	4.646699	-1.232885	1.936750	C	-0.089860	-3.477505	1.052894
H	0.498030	-3.671231	3.440911	H	3.865281	-0.247821	3.185141	C	-2.406963	1.478632	4.061067
H	1.214399	-2.058132	3.525894	H	1.188371	0.721779	8.082357	C	-3.901289	1.819383	4.000706

Zn	1.298527	1.239814	3.011825	C	1.536090	-2.699094	2.829572	H	1.718591	4.474410	-0.246992
O	1.722687	0.663307	4.686040	C	-1.787491	1.954354	5.385140	H	0.867833	3.498205	-1.462359
C	2.677332	1.124199	5.603895	H	3.508094	-3.332162	11.761576	H	6.430015	2.745755	1.054219
C	2.563427	0.229124	6.848177	H	-1.988780	-0.758482	0.390324	H	6.496525	4.890211	2.276466
C	3.394465	0.700178	8.030149	H	-2.896342	0.553323	1.116254	H	2.628596	5.554276	4.825854
O	3.073860	-0.048162	9.220954	H	-2.262502	0.734879	-0.533714	H	4.399573	5.917162	3.082957
C	3.769670	-1.172589	9.399000	H	-4.457584	1.366700	4.828511	H	1.830883	3.977969	4.781876
O	4.656292	-1.599080	8.692078	H	-4.044924	2.903157	4.069132	H	1.008342	4.431587	2.483507
N	1.866060	2.395225	1.549868	H	-4.359504	1.476537	3.067136	H	0.862344	5.460954	4.740270
C	1.115781	2.522856	0.447113	H	-0.564918	2.063796	-0.729670	H	0.738224	6.862159	2.629147
C	-0.088404	1.841734	0.217359	H	-0.955412	-3.219508	0.433731	H	1.751709	6.476957	1.228218
C	3.103957	3.107060	1.669405	H	0.735477	-3.745419	0.384248	H	2.484509	7.108267	2.706307
C	3.128660	4.346485	2.347434	H	-0.347397	-4.375262	1.624972	H	4.937211	0.363262	-1.475427
C	4.364049	4.967649	2.554822	H	0.626016	-1.486514	1.319128	H	4.666519	2.112885	-1.536584
C	5.545729	4.394537	2.100703	H	-3.098540	-3.034929	5.072452	H	6.118930	1.465358	-0.768062
C	5.503942	3.186610	1.413927	H	-1.313643	-3.793393	3.543093	H	5.915888	0.273427	1.560079
C	4.295347	2.523503	1.179781	H	2.385951	-2.986569	2.199938	H	4.858125	-0.880596	0.731546
C	1.858115	5.013342	2.855320	H	1.296536	-3.549598	3.477952	H	4.308422	-0.067352	2.206856
C	1.791391	4.998610	4.389090	H	1.841723	-1.869891	3.475630	H	4.466678	0.608312	7.840148
C	4.298520	1.201282	0.424051	H	-3.593007	-0.625015	5.291767	H	2.441788	2.159055	5.922144
C	5.046533	1.296919	-0.913397	H	-1.915262	2.028607	3.251720	C	4.090950	1.129869	5.025871
C	1.583043	3.462017	-0.639700	H	3.258567	0.943284	0.199734	H	3.161235	1.736750	8.291777
C	4.876473	0.066459	1.282123	H	-2.263521	1.454101	6.236197	H	2.854948	-0.791884	6.576374
C	1.702908	6.444530	2.321298	H	-0.717717	1.726026	5.424433	H	1.509278	0.201626	7.143762
O	3.321134	-1.757132	10.518816	H	-1.923313	3.034764	5.511804	H	5.050514	-2.811814	11.011604
C	3.982738	-2.978639	10.845998	H	2.554142	3.149078	-1.035181	H	3.861481	-3.713836	10.046041

H	4.827497	1.515993	5.740087
H	4.387492	0.112510	4.747515
H	4.141084	1.763209	4.133497

TS($\mathbf{II}^{\gamma\alpha}_{\text{TMC-}\gamma(R,re)} \rightarrow \mathbf{II}^{\alpha\gamma}_{\text{TMC-}\gamma(R,re)}$)

G = -2001.364298 kcal.mol^{-1}

C	-0.365967	3.412883	-7.005610
C	0.877279	3.242663	-6.354872
C	2.055170	2.990815	-7.093033
C	1.961590	2.898340	-8.485375
C	0.745832	3.060860	-9.139502
C	-0.402778	3.323459	-8.400500
N	0.942908	3.345334	-4.924899
Zn	1.377945	5.017417	-4.047695
O	1.877236	6.832344	-6.468790
C	1.709037	7.575462	-5.257955
O	0.425077	8.136231	-5.234495
C	0.213882	9.149536	-6.223403
C	0.932056	8.806829	-7.533427
C	1.116491	7.295714	-7.596970
O	1.900275	6.773481	-4.211234
O	2.599275	8.665598	-5.237419
C	3.966210	8.319075	-5.156085
C	1.819010	6.785240	-8.841736
C	3.413895	2.832540	-6.426284
C	4.079173	1.490835	-6.764499
C	-1.647317	3.690355	-6.230252
C	-2.812515	2.794452	-6.673057
N	1.341774	4.445588	-2.152279
C	1.016264	3.196792	-1.834940
C	0.980388	2.779293	-0.383743
C	1.696557	5.380951	-1.125735
C	0.725260	6.280138	-0.636577
C	1.111339	7.212339	0.331413
C	2.416808	7.268681	0.802105
C	3.365244	6.384443	0.301148
C	3.030801	5.430362	-0.663304
C	-0.713770	6.273010	-1.130399
C	-1.706126	5.976366	0.004029
C	4.111691	4.516005	-1.222297
C	4.957688	3.849666	-0.129257
C	0.717683	2.197271	-2.785711
C	0.700851	2.248578	-4.186040
C	0.377001	0.955411	-4.898073
C	5.005254	5.280458	-2.211178
C	-1.068530	7.588815	-1.838444
C	4.341170	4.003961	-6.784467
C	-2.047599	5.170983	-6.317875
H	-0.397654	7.785475	-2.678817
H	-2.095740	7.549663	-2.219051
H	0.534133	10.122410	-5.834058
H	-0.871326	9.173191	-6.367595
H	-0.808390	5.466189	-1.864979
H	0.241653	0.140706	-4.185759
H	2.696731	8.003187	1.552394
H	1.174362	0.684182	-5.596270
H	5.290446	3.922464	-6.243149
H	4.412766	5.731854	-3.012339
H	5.544190	6.088581	-1.703823
H	4.258741	7.645235	-5.970943
H	4.526790	9.253102	-5.246030
H	4.200797	7.848475	-4.195697
H	0.120411	6.830711	-7.547846
H	1.910267	9.293497	-7.578510
H	0.342840	9.142969	-8.394107
H	3.617881	3.715685	-1.782934
H	0.478827	1.228378	-2.364195
H	3.255221	2.853887	-5.343184
H	0.482559	3.533091	0.230905
H	-2.728325	5.923025	-0.386798
H	-1.486157	5.025957	0.501433
H	-1.686426	6.761699	0.767617
H	1.998210	2.676478	0.008362
H	0.470386	1.822195	-0.263199
H	-1.005375	8.437671	-1.148072
H	0.372972	7.910743	0.716724
H	4.335885	3.320723	0.600407
H	4.388803	6.439024	0.662191

H	5.562634	4.578771	0.420393
H	5.648951	3.125542	-0.573783
H	5.747823	4.611886	-2.661892
H	-1.262972	5.832275	-5.937527
H	-1.450596	3.469805	-5.176481
H	-2.956239	5.358060	-5.734458
H	-0.535570	1.054137	-5.493884
H	-2.253332	5.456977	-7.355947
H	-3.147109	3.031390	-7.688707
H	-2.542445	1.733520	-6.653127
H	-3.671225	2.937050	-6.008422
H	-1.350099	3.453188	-8.916890
H	0.693141	2.986972	-10.222360
H	2.859717	2.700357	-9.064592
H	4.312766	1.413201	-7.831956
H	5.020890	1.385014	-6.215015
H	3.440040	0.641298	-6.502894
H	3.880722	4.964232	-6.540481
H	4.569346	4.009240	-7.856474
H	1.811714	5.693652	-8.810187
H	1.291627	7.109801	-9.744851
H	2.851533	7.144707	-8.884792

$TS(\mathbf{II}^{\alpha\gamma}_{TMC\text{-}\gamma(R,si)} \rightarrow \mathbf{II}^{\gamma\alpha}_{TMC\text{-}\gamma(R,si)})$

G = -2001.363507 kcal.mol^{-1}

C	1.844966	1.399878	-2.223510
C	0.943722	4.161644	0.844678
C	0.619529	6.202151	-0.614119
H	0.385785	4.163017	-1.213891
H	-1.883158	0.664615	-4.985636
C	0.048455	1.876406	-3.879591
C	2.469660	4.589971	-1.149416
C	3.567178	5.048445	-0.415138
C	2.698574	4.054972	-2.436193
H	5.697144	5.350831	-0.343509
C	5.062553	4.480121	-2.206443
C	3.998961	4.010374	-2.982884
C	4.856718	4.990557	-0.930721
C	4.683929	4.677776	-5.308887
C	4.267235	3.513714	-4.395733
C	5.308752	2.386819	-4.434734
N	1.584830	3.623208	-3.227365
N	-0.711870	3.811021	-5.154448
C	-0.803688	2.521617	-4.786418
H	-1.802683	1.625254	-6.476178
C	-0.339413	2.699066	-9.160493
C	-0.104773	3.682899	-8.006786
C	-1.903778	1.678220	-5.387703
C	-1.395142	4.284095	-7.468678
C	-1.668324	4.340370	-6.084117
C	-2.333583	4.823827	-8.353299
C	-2.853635	4.935376	-5.599857
C	-3.151449	5.051684	-4.111884
C	-3.512969	5.398293	-7.893205
C	-3.763508	5.453157	-6.527198
C	-4.511218	4.448089	-3.733873
C	-3.058021	6.514393	-3.650400
H	1.820239	4.356075	-8.777955
Zn	0.693734	4.917505	-4.426917
O	1.548281	6.534182	-4.313960
C	1.298751	7.676158	-4.955280
O	2.267315	7.833030	-5.986548
O	1.359679	8.780114	-4.078135
H	3.937471	5.477109	-5.306185
C	2.603316	8.930372	-3.417117
H	5.636321	5.108946	-4.979567
H	3.417503	9.090674	-4.133962
H	2.506129	9.809330	-2.774874
H	2.835437	8.052966	-2.804665
O	0.007771	7.687699	-5.503090
C	-0.401956	8.949134	-6.074302
H	-0.770476	9.584943	-5.260660
C	-1.534536	8.634261	-7.034008
H	-1.176499	8.039411	-7.879991
H	-2.318462	8.061961	-6.532771
H	-1.970422	9.562416	-7.418352
C	1.822102	8.561494	-7.123934
H	2.714208	9.007780	-7.575892

H	1.389829	7.866440	-7.859415
C	0.797512	9.625758	-6.760316
H	1.256522	10.356508	-6.089809
H	0.473717	10.151373	-7.666123
C	1.148979	2.370677	-3.147266
C	0.875698	4.788212	-8.429013
C	1.068211	4.732215	-0.574213
H	3.330097	3.104958	-4.788252
H	-0.179428	0.831637	-3.707375
H	0.364901	3.122643	-7.191974
H	-0.415056	6.301077	-0.265729
H	1.765634	1.734833	-1.184441
H	-0.097405	4.208081	1.182123
H	1.267983	3.116844	0.893196
H	1.543595	4.727578	1.565533
H	2.913596	1.346371	-2.450723
H	1.415560	0.400165	-2.302347
H	1.250806	6.817481	0.037162
H	3.406709	5.464762	0.575862
H	5.022661	1.543913	-3.796848
H	6.069361	4.452126	-2.615157
H	6.292662	2.734451	-4.101435
H	5.424775	2.011060	-5.457271
H	4.817271	4.328063	-6.339245
H	-2.087865	6.952409	-3.902596
H	-2.382829	4.486405	-3.575146
H	-3.200912	6.586625	-2.566361
H	-2.886421	2.115866	-5.189674
H	-3.833749	7.123852	-4.128491
H	-5.339875	4.995624	-4.195919
H	-4.593825	3.400939	-4.042690
H	-4.656590	4.490732	-2.649009
H	-4.682901	5.910138	-6.169940
H	-4.232983	5.805793	-8.597736
H	-2.138149	4.790331	-9.421780
H	-0.725435	3.201027	-10.054218
H	0.602676	2.216700	-9.442115
H	-1.052390	1.914491	-8.887127
H	1.099746	5.469950	-7.602896
H	0.456703	5.384378	-9.247774
H	0.687456	6.615324	-1.625099

$\mathbf{II}^{\alpha\gamma}_{\text{TMC-}\gamma(R,re)}$

G = -2001.365638 kcal.mol^{-1}

O	1.004325	-4.561453	3.387206
O	2.532459	-5.216430	4.964426
C	2.102170	-4.242567	5.899833
O	2.229780	-6.422149	3.105587
O	0.484083	-6.335393	4.659413
C	0.687742	-7.759519	4.774972
C	2.176858	-8.058958	4.917170
C	2.933663	-7.511184	3.705696
H	-0.774068	-4.556630	0.325800
C	-2.779283	-4.251029	6.869082
N	-2.112190	-3.612547	4.078111
N	-1.992555	-5.819607	2.002251
Zn	-0.858051	-4.967320	3.369771
C	-1.497522	-6.915403	1.221050
C	-1.818128	-8.238589	1.615623
C	-1.325883	-9.295922	0.844751
C	-0.524461	-9.069276	-0.269329
C	-0.195291	-7.768735	-0.624059
C	-0.669160	-6.671876	0.103767
C	-2.677871	-8.523321	2.843562
C	-4.184402	-8.493648	2.535892
C	-0.271601	-5.270280	-0.335741
C	-0.729198	-4.971213	-1.771726
C	-3.157070	-5.246472	1.683464
C	-3.759999	-4.193726	2.397382
C	-3.297424	-3.439380	3.490299
C	-4.221869	-2.359975	4.002606
C	-0.120913	-8.256545	5.958575
C	-1.686094	-2.721765	5.116554
C	-1.966847	-3.029122	6.466895
C	-1.465462	-2.186376	7.463648
C	-0.710508	-1.063321	7.148635
C	-0.454374	-0.763868	5.815960
C	-0.932643	-1.572213	4.779803

C	-0.637509	-1.175298	3.339292
C	-1.225260	0.203971	3.001329
C	-3.986868	-3.889060	7.745681
C	-1.895578	-5.288839	7.574857
C	1.594329	-5.568880	3.996445
C	-3.894770	-5.682801	0.435192
C	1.241847	-5.046290	-0.195645
C	-2.339034	-9.857228	3.521606
C	0.866913	-1.210502	3.032598
H	0.321496	-8.226556	3.849404
H	-1.567097	-10.317145	1.122896
H	-1.057203	-5.588285	6.940547
H	-4.523458	-7.506494	2.217772
H	1.046000	-0.922769	1.990237
H	0.130684	0.118624	5.569873
H	-4.431838	-9.211784	1.745848
H	2.965104	-4.029100	6.534563
H	1.777151	-3.326632	5.399452
H	1.281802	-4.619764	6.521568
H	0.256728	-7.823185	6.889759
H	-1.174697	-7.983684	5.855657
H	-0.057242	-9.346974	6.032968
H	2.542241	-7.598069	5.839302
H	2.320520	-9.141958	5.001129
H	3.004167	-8.262565	2.913151
H	3.947586	-7.198881	3.980705
H	1.416534	-0.504977	3.666506
H	1.276059	-2.212449	3.186155
H	-2.478555	-7.719504	3.563808
H	-1.123005	-1.906468	2.685226
H	-4.628577	-3.141247	7.269008
H	-3.676125	-3.484471	8.715114
H	-4.594439	-4.779128	7.942611
H	-1.670640	-2.417220	8.505972
H	-0.327222	-0.421822	7.937622
H	-2.474013	-6.185623	7.825344
H	-1.485643	-4.886622	8.508341
H	-3.161648	-4.711725	5.952260
H	-3.711218	-6.726597	0.179851
H	-3.553262	-5.074488	-0.410214
H	-4.969527	-5.521064	0.542345
H	-2.301141	0.253087	3.198112
H	-0.746761	0.997697	3.585600
H	-1.066357	0.434840	1.942235
H	-4.726897	-3.889575	2.014127
H	-5.110403	-2.270552	3.376219
H	-4.539942	-2.584769	5.025569
H	-3.715107	-1.392044	4.039791
H	-0.507488	-3.930631	-2.032710
H	-1.803609	-5.133209	-1.903750
H	-0.210074	-5.607954	-2.496675
H	1.499084	-4.020087	-0.481226
H	1.579302	-5.210732	0.830222
H	1.799875	-5.722128	-0.854055
H	0.443856	-7.593982	-1.485740
H	-0.151703	-9.907192	-0.852354
H	-4.758306	-8.766505	3.428687
H	-1.264823	-9.976675	3.688723
H	-2.682627	-10.712133	2.928446
H	-2.843304	-9.920229	4.491309

II$^{\gamma\alpha}{}_{\text{TMC-}\gamma(R,si)}$

G = -2001.367173 kcal.mol^{-1}

C	-1.801346	-3.697726	6.618060
C	-1.634079	-3.096284	5.349900
C	-0.980834	-1.848172	5.221611
C	-0.486032	-1.235813	6.377359
C	-0.631895	-1.822349	7.629229
C	-1.290271	-3.040919	7.742001
N	-2.062423	-3.795495	4.176520
C	-3.273928	-3.577439	3.660498
C	-4.196489	-2.599439	4.349094
C	-0.800794	-1.155336	3.877526
C	-1.382843	0.266321	3.881880
C	-2.509865	-5.033383	6.793901
C	-3.711659	-4.929624	7.744201
C	-3.765329	-4.198209	2.499572
C	-3.203962	-5.204535	1.689585

C	-4.073859	-5.658306	0.536875
N	-2.009354	-5.761418	1.889835
Zn	-0.800617	-5.002410	3.259680
O	0.558761	-6.403353	4.367775
C	0.768023	-7.820943	4.342958
C	2.239368	-8.148258	4.542401
C	3.060951	-7.516084	3.404796
C	3.334864	-8.469870	2.255164
C	-1.562650	-6.873022	1.107373
C	-2.064750	-8.170940	1.370044
C	-1.520259	-9.248970	0.664192
C	-0.524256	-9.064229	-0.286944
C	-0.061992	-7.780845	-0.554296
C	-0.560607	-6.668283	0.129255
C	-3.181500	-8.441375	2.372121
C	-4.364413	-9.173851	1.719594
C	-0.072666	-5.275375	-0.242720
C	-0.778343	-4.783556	-1.517338
O	1.068639	-4.576502	3.164434
C	1.674165	-5.592799	3.740064
O	2.593264	-5.275413	4.734790
C	2.154481	-4.334742	5.699634
O	2.327845	-6.415941	2.834107
C	1.449418	-5.184915	-0.393651
C	-2.685025	-9.228343	3.593033
C	0.673128	-1.131374	3.444155
C	-1.537996	-6.123254	7.269398
H	-4.423476	-4.164251	7.418961
H	-4.243599	-5.886225	7.792121
H	-3.399180	-4.676532	8.763253
H	-1.410562	-3.494988	8.722528
H	-1.123669	-5.881493	8.254870
H	-2.053151	-7.087108	7.354801
H	-0.704362	-6.237485	6.570541
H	-2.889812	-5.336855	5.813096
H	-0.238266	-1.328910	8.513832
H	0.024157	-0.279776	6.292523
H	-5.146113	-2.510908	3.819663
H	-4.396805	-2.919333	5.376284
H	-3.737027	-1.609225	4.416388
H	-4.752012	-3.872335	2.190084
H	-2.431473	0.281241	4.196761
H	-0.827894	0.927494	4.556387
H	-1.325644	0.701973	2.878435
H	-4.542097	-4.791254	0.063536
H	-3.509396	-6.213363	-0.213115
H	0.774206	-0.638549	2.470347
H	1.283265	-0.570390	4.161907
H	1.081106	-2.142426	3.358016
H	-0.355246	-4.597021	0.568394
H	-0.538474	-5.429272	-2.370001
H	-0.456533	-3.766036	-1.765752
H	-1.866839	-4.773755	-1.403634
H	1.741133	-4.143482	-0.566434
H	1.810939	-5.766030	-1.249995
H	0.703358	-7.636490	-1.311268
H	1.954241	-5.532481	0.509972
H	-4.880552	-6.303595	0.900456
H	-1.890454	-10.252060	0.861312
H	-0.118045	-9.915721	-0.826329
H	-5.198751	-9.254791	2.425023
H	-3.548843	-7.479022	2.740500
H	-4.722111	-8.654876	0.825523
H	-4.090740	-10.191366	1.420302
H	-1.914836	-8.675587	4.135622
H	-3.511235	-9.423790	4.285875
H	-2.261145	-10.194965	3.298562
H	1.887108	-3.382739	5.234780
H	2.995282	-4.186453	6.380911
H	1.294712	-4.709949	6.265852
H	0.411271	-8.228098	3.388590
H	0.158713	-8.242999	5.148398
H	2.369472	-9.236351	4.553641
H	2.565228	-7.759785	5.510949
H	4.008003	-7.132255	3.801495
H	2.402579	-8.884757	1.858921
H	3.844557	-7.945536	1.442164
H	3.973289	-9.293738	2.589994

H	-1.351967	-1.733791	3.129251

$TS(\mathbf{II}^{\alpha\gamma}{}_{TMC\text{-}\gamma(R,re)} \rightarrow \mathbf{III}^{\alpha\gamma}{}_{TMC\text{-}\gamma(R,re)})$

G = -2001.360682 kcal.mol^{-1}

C	-0.730738	-6.421555	-0.173346
C	-1.503075	-6.687974	0.985025
C	-1.917381	-8.005223	1.287185
C	-1.561229	-9.034611	0.409201
C	-0.821198	-8.785685	-0.738152
C	-0.411890	-7.487410	-1.020473
N	-1.832801	-5.609635	1.871927
Zn	-0.734153	-5.237674	3.484183
O	-0.310379	-6.702571	4.869185
C	0.933513	-6.847436	4.707042
O	1.806750	-6.744240	5.726604
C	1.414438	-5.871178	6.785406
C	-2.746320	-8.348185	2.516704
C	-4.124650	-8.906304	2.129080
C	-0.268347	-5.013169	-0.528315
C	-1.256220	-4.291166	-1.459764
C	-2.977730	-4.940048	1.705629
C	-3.949479	-5.347266	0.616703
C	-3.421109	-3.879644	2.516060
C	-2.948208	-3.398681	3.751849
C	-3.827946	-2.353973	4.405777
N	-1.845675	-3.831780	4.359732
C	-1.548785	-3.433648	5.700712
C	-0.551515	-2.455638	5.930213
C	-0.239440	-2.115299	7.250104
C	-0.873586	-2.727678	8.325034
C	-1.842391	-3.693682	8.086544
C	-2.202451	-4.064349	6.786643
C	0.144232	-1.743098	4.779378
C	-0.551335	-0.413922	4.445710
C	-3.279124	-5.126081	6.603952
C	-4.602744	-4.714742	7.268359
C	-2.822760	-6.494028	7.132879
C	1.636843	-1.508064	5.035894
C	-2.012886	-9.332648	3.438663
C	1.128075	-4.982352	-1.164074
O	1.229867	-5.237949	3.763484
C	2.474018	-5.127707	3.111738
C	2.510715	-3.922936	2.183351
C	2.806546	-6.435780	2.385753
C	2.688408	-7.636099	3.310147
O	1.342649	-7.754818	3.794019
H	3.239868	-4.980798	3.895089
H	1.760927	-4.025681	1.393875
H	3.493717	-3.821681	1.709564
H	2.302330	-3.005887	2.738938
H	2.122384	-6.572602	1.539415
H	3.828541	-6.392564	1.987381
H	3.381994	-7.566173	4.155224
H	2.877765	-8.571851	2.778965
H	2.245732	-5.874089	7.491791
H	0.505570	-6.233256	7.269993
H	1.244546	-4.861820	6.403686
H	0.057829	-2.390964	3.900367
H	-4.346225	-3.420093	2.184085
H	-4.706985	-2.830367	4.852600
H	-4.190937	-1.648304	3.653633
H	-4.673216	-8.227756	1.468945
H	-3.309925	-1.805016	5.192676
H	-4.733456	-9.075818	3.024026
H	-3.464810	-5.237865	5.531425
H	-4.942392	-3.728909	6.936589
H	-5.387824	-5.442119	7.034219
H	-4.508008	-4.677697	8.359344
H	-3.609916	-7.241169	6.979133
H	-2.335817	-4.173497	8.928056
H	-2.616821	-6.451800	8.208943
H	-1.921578	-6.832820	6.616797
H	-2.905064	-7.424608	3.082214
H	-0.230272	-4.443979	0.408189
H	-3.478004	-5.911208	-0.187529
H	-4.446923	-4.468317	0.199056
H	-4.728753	-5.981669	1.053746
H	1.487062	-3.949786	-1.230263

H	1.857259	-5.559093	-0.588492
H	1.116930	-5.380577	-2.184569
H	-0.876427	-3.296660	-1.719923
H	-0.560678	-9.599061	-1.410173
H	0.169856	-7.299340	-1.918164
H	-1.390585	-4.853502	-2.390944
H	-1.875782	-10.050949	0.632442
H	-2.237509	-4.160293	-1.000407
H	-1.047047	-8.932603	3.751713
H	-1.847425	-10.295048	2.940791
H	-4.030790	-9.865746	1.608169
H	-2.610453	-9.524715	4.336746
H	0.513547	-1.356206	7.440902
H	-0.614501	-2.450511	9.343458
H	-0.522854	0.267044	5.304175
H	-1.599064	-0.562536	4.171692
H	-0.053084	0.082846	3.605379
H	2.150210	-2.441122	5.285468
H	2.110180	-1.085571	4.142932
H	1.809141	-0.795616	5.850087

TS($\mathbf{II}^{\gamma\alpha}_{\text{TMC-}\gamma(R,si)} \rightarrow \mathbf{III}^{\gamma\alpha}_{\text{TMC-}\gamma(R,si)}$)

G = -2001.364187 kcal.mol^{-1}

C	-1.679648	-3.724494	6.650848
C	-1.583949	-3.136517	5.367881
C	-0.972800	-1.870945	5.198391
C	-0.445841	-1.231075	6.324751
C	-0.520850	-1.804292	7.588956
C	-1.140460	-3.038476	7.744132
N	-2.038406	-3.868665	4.227088
C	-3.235605	-3.626152	3.691974
C	-4.140133	-2.600294	4.335910
C	-0.866359	-1.183756	3.842806
C	-1.479686	0.225025	3.865064
C	-2.365327	-5.063984	6.879621
C	-3.606373	-4.916444	7.773039
C	-3.728440	-4.248494	2.532176
C	-3.168545	-5.245598	1.710250
C	-4.025108	-5.645207	0.526961
N	-1.993605	-5.837991	1.923002
Zn	-0.833897	-5.210870	3.409549
O	0.380652	-6.377440	4.491461
C	0.568936	-7.775357	4.410586
C	2.041907	-8.099562	4.646158
C	2.923965	-7.531254	3.522236
C	3.188561	-8.519887	2.400999
C	-1.542692	-6.916488	1.097182
C	-2.053158	-8.223207	1.291307
C	-1.508952	-9.268819	0.537729
C	-0.502800	-9.044494	-0.393402
C	-0.030436	-7.752256	-0.593046
C	-0.530236	-6.671146	0.138451
C	-3.183868	-8.536116	2.264639
C	-4.387985	-9.166514	1.546186
C	-0.036162	-5.262616	-0.161129
C	-0.780007	-4.681007	-1.374613
O	1.067868	-4.525689	3.145874
C	1.755452	-5.446501	3.687588
O	2.594953	-5.184989	4.714498
C	2.206603	-4.129462	5.589362
O	2.264124	-6.408515	2.885210
C	1.479425	-5.178936	-0.369003
C	-2.728202	-9.447805	3.412577
C	0.585938	-1.122362	3.346112
C	-1.398614	-6.107836	7.455882
H	-4.323055	-4.200567	7.358090
H	-4.117072	-5.879866	7.880794
H	-3.337666	-4.570596	8.777427
H	-1.210535	-3.481271	8.734642
H	-1.023354	-5.805508	8.440275
H	-1.908148	-7.070303	7.580910
H	-0.544549	-6.252704	6.788061
H	-2.703398	-5.430174	5.904955
H	-0.104877	-1.287814	8.449954
H	0.032793	-0.262169	6.206945
H	-5.164626	-2.700917	3.973771
H	-4.134923	-2.695679	5.424399
H	-3.796658	-1.586731	4.105004

H	-4.707330	-3.906197	2.214362	H	-2.366929	-10.411425	3.036351	O	1.723696	-6.843407	5.815367
H	-2.504991	0.223521	4.248691	H	2.127615	-3.184238	5.049685	C	1.312033	-5.994688	6.898660
H	-0.897030	0.907194	4.493869	H	2.994015	-4.067507	6.342018	C	-2.594848	-8.308535	2.655614
H	-1.495508	0.647778	2.854595	H	1.251602	-4.356995	6.069785	C	-4.048546	-8.716177	2.368648
H	-4.427277	-4.751466	0.042200	H	0.252836	-8.168684	3.432559	C	-0.297937	-5.090441	-0.653951
H	-3.472176	-6.230650	-0.207969	H	-0.043661	-8.269166	5.178883	C	-1.276805	-4.464840	-1.661442
H	0.632348	-0.624323	2.370757	H	2.178695	-9.185536	4.703558	C	-2.912672	-4.929142	1.684518
H	1.213652	-0.548638	4.038415	H	2.336553	-7.676175	5.610816	C	-3.888914	-5.335544	0.597442
H	1.009406	-2.124008	3.238590	H	3.874310	-7.173724	3.933812	C	-3.356828	-3.859137	2.480408
H	-0.275059	-4.636345	0.703658	H	2.250423	-8.895995	1.981580	C	-2.905094	-3.386513	3.727511
H	-0.585226	-5.277866	-2.273207	H	3.754886	-8.043047	1.596258	C	-3.783897	-2.327297	4.360205
H	-0.448171	-3.655730	-1.573165	H	3.769864	-9.366703	2.778538	N	-1.814661	-3.826937	4.347651
H	-1.862559	-4.659280	-1.217900	H	-1.429613	-1.781456	3.119481	C	-1.546151	-3.465225	5.704278
H	1.780014	-4.130518	-0.467712					C	-0.572804	-2.478411	5.987095
H	1.798827	-5.691962	-1.283651	**III**$^{oy}_{TMC\text{-}\gamma(R,re)}$)				C	-0.278471	-2.190172	7.323942
H	0.743155	-7.576699	-1.334763	G = -2001.371466 kcal.mol^{-1}				C	-0.914043	-2.854167	8.366269
H	2.016411	-5.605621	0.480508	C	-0.739215	-6.479938	-0.209693	C	-1.873172	-3.816751	8.076159
H	-4.879335	-6.241016	0.864944	C	-1.451436	-6.701233	0.996119	C	-2.211902	-4.139430	6.758096
H	-1.887997	-10.277705	0.681657	C	-1.836876	-8.010442	1.369982	C	0.116186	-1.684206	4.887665
H	-0.096193	-9.871161	-0.969933	C	-1.528458	-9.070351	0.510952	C	-0.437519	-0.252417	4.817007
H	-5.227646	-9.285622	2.239986	C	-0.852788	-8.863779	-0.683837	C	-3.297809	-5.181131	6.521367
H	-3.516122	-7.594377	2.711929	C	-0.460778	-7.577015	-1.031801	C	-4.646194	-4.725970	7.102725
H	-4.726530	-8.558527	0.702548	N	-1.763643	-5.593034	1.853507	C	-2.916301	-6.554412	7.092544
H	-4.142872	-10.160292	1.155651	Zn	-0.584590	-5.077360	3.376605	C	1.640481	-1.672154	5.047157
H	-1.921821	-8.990784	3.989941	O	-0.351744	-6.706230	4.924292	C	-1.902411	-9.391497	3.494491
H	-3.561853	-9.649323	4.094604	C	0.839762	-7.000820	4.843806	C	1.112206	-5.081225	-1.261155

O	1.257469	-4.847771	3.724773	H	-5.435273	-5.440443	6.843033	H	-0.239821	0.293387	5.746806
C	2.427744	-4.896278	2.970122	H	-4.605849	-4.664254	8.196086	H	-1.519223	-0.243654	4.652049
C	2.495391	-3.784509	1.924002	H	-3.711269	-7.281858	6.892014	H	0.032610	0.302555	3.997254
C	2.661177	-6.276811	2.334179	H	-2.379103	-4.328291	8.891427	H	2.029165	-2.693291	5.038434
C	2.651745	-7.426253	3.328490	H	-2.781207	-6.510591	8.179610	H	2.102085	-1.120847	4.220192
O	1.302349	-7.663418	3.793483	H	-1.993334	-6.921593	6.639542	H	1.953693	-1.180168	5.974901
H	3.272644	-4.731787	3.668986	H	-2.611004	-7.391967	3.252404				
H	1.683260	-3.891405	1.198075	H	-0.290166	-4.453185	0.237899	**III**$^{\gamma\alpha}{}_{TMC\text{-}\gamma(R,si)}$)			
H	3.445854	-3.791678	1.376896	H	-3.456224	-6.012853	-0.137590	G = -2001.371737 kcal.mol^{-1}			
H	2.386481	-2.811946	2.410631	H	-4.273268	-4.448324	0.086531	C	-1.621247	-3.769123	6.659334
H	1.892702	-6.474094	1.574828	H	-4.749755	-5.835778	1.053491	C	-1.553755	-3.197153	5.365878
H	3.634068	-6.286990	1.823055	H	1.452290	-4.050349	-1.405674	C	-0.947580	-1.930800	5.171452
H	3.307999	-7.241210	4.183112	H	1.839148	-5.591385	-0.624035	C	-0.386885	-1.283995	6.277786
H	2.944205	-8.365847	2.854152	H	1.131169	-5.564337	-2.244233	C	-0.422836	-1.847949	7.547666
H	2.166436	-5.957764	7.574017	H	-0.923855	-3.474642	-1.970899	C	-1.045886	-3.076654	7.730079
H	0.441673	-6.415136	7.404388	H	-0.629048	-9.700718	-1.339991	N	-2.034203	-3.944895	4.246434
H	1.075968	-5.000430	6.515850	H	0.071892	-7.419253	-1.965171	C	-3.208932	-3.660861	3.684785
H	-0.107714	-2.178204	3.937311	H	-1.356239	-5.088192	-2.559606	C	-4.098112	-2.601663	4.297715
H	-4.275718	-3.396151	2.134478	H	-1.829913	-10.077547	0.786698	C	-0.890908	-1.233452	3.817008
H	-4.750337	-2.754853	4.645658	H	-2.279301	-4.346205	-1.246942	C	-1.560279	0.150172	3.865156
H	-3.986132	-1.537924	3.629866	H	-0.858046	-9.136946	3.683265	C	-2.344472	-5.080737	6.931956
H	-4.583128	-7.954541	1.794572	H	-1.933380	-10.367872	2.997468	C	-3.605535	-4.843320	7.777704
H	-3.329905	-1.883469	5.246169	H	-4.088514	-9.649179	1.794656	C	-3.702882	-4.268781	2.516674
H	-4.593635	-8.878885	3.305153	H	-2.408831	-9.500446	4.459492	C	-3.150386	-5.264423	1.689982
H	-3.419569	-5.300470	5.440786	H	0.458293	-1.423789	7.550086	C	-3.993455	-5.633646	0.486450
H	-4.942586	-3.741175	6.730586	H	-0.670904	-2.615157	9.398297	N	-1.996003	-5.890160	1.920547

Zn	-0.940573	-5.456544	3.552061	H	-4.151006	-5.782433	7.923058	H	1.725512	-5.686644	-1.420525
O	0.052316	-6.597635	4.665751	H	-3.351406	-4.450197	8.768580	H	0.782247	-7.619309	-1.306144
C	0.488622	-7.899155	4.415582	H	-1.096258	-3.508557	8.726468	H	2.129347	-5.844348	0.303363
C	2.000041	-8.019432	4.668591	H	-1.048061	-5.781004	8.552708	H	-4.824229	-6.277555	0.794860
C	2.882313	-7.441845	3.554580	H	-1.990510	-7.051061	7.766872	H	-1.976704	-10.296131	0.566128
C	3.145707	-8.414551	2.419646	H	-0.592197	-6.358423	6.923598	H	-0.137703	-9.894378	-1.033180
C	-1.552570	-6.958578	1.079813	H	-2.665651	-5.486869	5.967677	H	-5.284579	-9.329202	2.138204
C	-2.102419	-8.254365	1.226496	H	0.019441	-1.326030	8.392247	H	-3.604326	-7.613284	2.598674
C	-1.569262	-9.294132	0.456882	H	0.085695	-0.314636	6.139052	H	-4.760836	-8.637181	0.591696
C	-0.535416	-9.072572	-0.443551	H	-5.145605	-2.797546	4.059205	H	-4.175562	-10.223697	1.097404
C	-0.018432	-7.789848	-0.592995	H	-3.980053	-2.555115	5.382080	H	-2.023329	-8.931731	3.948440
C	-0.505507	-6.715973	0.157120	H	-3.846861	-1.613417	3.899317	H	-3.643810	-9.641253	4.026953
C	-3.250374	-8.560379	2.180872	H	-4.669059	-3.899815	2.189134	H	-2.396869	-10.390296	3.018298
C	-4.433400	-9.221525	1.456835	H	-2.572476	0.108006	4.278630	H	2.374206	-3.009607	5.011213
C	0.044966	-5.312833	-0.058550	H	-0.986146	0.849101	4.483469	H	3.046119	-3.986739	6.354578
C	-0.769963	-4.561624	-1.124127	H	-1.620492	0.579222	2.858915	H	1.311513	-4.120669	5.919512
O	1.073056	-4.430032	3.218920	H	-4.428711	-4.734512	0.042740	H	0.262382	-8.244079	3.392024
C	1.926390	-5.225057	3.608810	H	-3.421664	-6.166737	-0.273775	H	-0.010603	-8.613826	5.095147
O	2.696357	-5.042413	4.671713	H	0.548945	-0.593451	2.320172	H	2.277454	-9.073835	4.795945
C	2.322459	-3.961887	5.540352	H	1.159381	-0.495444	3.975255	H	2.210803	-7.514176	5.616371
O	2.221177	-6.307202	2.913098	H	1.013348	-2.076502	3.174187	H	3.831687	-7.082661	3.965216
C	1.533296	-5.282679	-0.419706	H	-0.065224	-4.770739	0.885825	H	2.207144	-8.771708	1.986148
C	-2.798337	-9.430350	3.362322	H	-0.718581	-5.078830	-2.089365	H	3.731624	-7.938514	1.628449
C	0.546254	-1.097217	3.293715	H	-0.376504	-3.548357	-1.263440	H	3.707712	-9.274605	2.795210
C	-1.431234	-6.125995	7.585276	H	-1.823387	-4.474029	-0.846147	H	-1.438745	-1.849354	3.097567
H	-4.285881	-4.128833	7.302978	H	1.889699	-4.247243	-0.420146				

TS(**III**$^{\alpha\gamma}_{\text{TMC-}\gamma(R,re)}$→ **IV**$^{\alpha\gamma}_{\text{TMC-}\gamma(R,re)}$)

G = -2001.367776 kcal.mol^{-1}

C	-1.777505	-7.710913	0.870904
C	-1.577123	-6.329048	0.660775
C	-0.936459	-5.853089	-0.510186
C	-0.531772	-6.788974	-1.467089
C	-0.726800	-8.152587	-1.275485
C	-1.336300	-8.603099	-0.111918
N	-1.974061	-5.391055	1.669389
Zn	-0.778568	-5.032229	3.190328
O	0.852921	-5.589308	3.808025
C	2.071339	-5.691512	3.130080
C	2.029104	-5.106366	1.721254
C	-0.687922	-4.366005	-0.744495
C	-1.853988	-3.686579	-1.481583
C	-2.436368	-8.253184	2.131121
C	-3.605615	-9.197008	1.815260
C	-3.205726	-4.870190	1.646099
C	-4.212969	-5.373364	0.636173
C	-3.675988	-3.898544	2.545305
C	-3.102253	-3.400374	3.729123
C	-3.907617	-2.359534	4.471932
N	-1.935842	-3.811563	4.229483
C	-1.521458	-3.370263	5.528072
C	-2.066268	-3.978860	6.683614
C	-1.592283	-3.571043	7.934223
C	-0.617151	-2.588116	8.057208
C	-0.095603	-1.996293	6.914069
C	-0.528882	-2.371774	5.638945
C	-3.121264	-5.075830	6.616299
C	-4.340181	-4.772286	7.500559
C	0.080608	-1.694437	4.421488
C	-0.202135	-0.185501	4.402733
C	1.586390	-1.977054	4.328939
C	-2.526303	-6.441191	6.987085
C	2.582511	-7.139750	3.079728
C	2.837440	-7.776261	4.435647
O	1.608137	-8.301112	4.969958
C	1.228314	-8.087310	6.225771
O	0.171125	-8.487265	6.654687
O	2.144272	-7.419415	6.952632
C	1.737598	-7.122959	8.289144
C	0.617459	-4.082932	-1.499585
C	-1.410523	-8.944097	3.041523
H	2.827180	-5.115142	3.701053
H	1.329409	-5.675656	1.098070
H	3.012319	-5.131085	1.236136
H	1.701634	-4.060845	1.754501
H	1.883827	-7.764967	2.510261
H	3.536263	-7.149191	2.533907
H	3.275181	-7.058852	5.131718
H	3.519589	-8.629079	4.341197
H	2.614171	-6.691973	8.774015
H	1.418416	-8.030944	8.805847
H	0.915597	-6.402864	8.287392
H	-0.393126	-2.124551	3.532252
H	-4.664053	-3.512546	2.322300
H	-3.260242	-1.584608	4.889303
H	-4.447548	-2.809024	5.311264
H	-4.340479	-8.729019	1.151962
H	-4.640783	-1.896284	3.809165
H	-4.116658	-9.487427	2.739289
H	-3.473787	-5.144090	5.582427
H	-4.771651	-3.788335	7.289660
H	-5.119105	-5.525574	7.340777
H	-4.082448	-4.794644	8.564954
H	-3.283385	-7.228149	6.896182
H	-1.998075	-4.034481	8.829684
H	-2.170465	-6.445373	8.023310
H	-1.680521	-6.715176	6.353002
H	-2.846413	-7.402197	2.685384
H	-0.609394	-3.896063	0.243206
H	-3.755271	-5.666344	-0.309161
H	-4.985461	-4.624911	0.448234
H	-4.706933	-6.263318	1.043992
H	0.832731	-3.009447	-1.478081
H	1.469138	-4.608766	-1.060344
H	0.548462	-4.372370	-2.554145

H	-1.619052	-2.633843	-1.674538
H	-0.397620	-8.861578	-2.030365
H	-0.044798	-6.444890	-2.374425
H	-2.037539	-4.171771	-2.447052
H	-1.477012	-9.669865	0.040108
H	-2.781164	-3.716074	-0.906010
H	-0.598175	-8.272259	3.330773
H	-0.963693	-9.810426	2.540156
H	-3.263042	-10.118096	1.331112
H	-1.883839	-9.298857	3.962767
H	0.665244	-1.225714	7.009693
H	-0.267059	-2.284215	9.040133
H	0.254229	0.317947	5.262144
H	-1.276179	0.024774	4.428350
H	0.209105	0.270872	3.495458
H	1.774686	-3.054056	4.331919
H	2.004349	-1.549092	3.410481
H	2.126932	-1.535943	5.173948

TS(**III**$^{\gamma\alpha}_{\text{TMC-}\gamma(R,si)}$ → **IV**$^{\gamma\alpha}_{\text{TMC-}\gamma(R,si)}$)

G = -2001.371402 kcal.mol^{-1}

C	-2.379654	-8.240434	1.233208
C	-1.826218	-6.953804	1.031751
C	-0.835430	-6.737390	0.046860
C	-0.405115	-7.829302	-0.714021
C	-0.927716	-9.101281	-0.516543
C	-1.908186	-9.297198	0.449097
N	-2.218183	-5.871784	1.885471
Zn	-1.116998	-5.451746	3.454167
O	0.316058	-6.263852	4.254528
C	0.715915	-7.584842	3.995630
C	2.093859	-7.842434	4.616902
C	3.289809	-7.398837	3.766768
O	3.013456	-6.166860	3.054298
C	2.865048	-5.011695	3.701523
O	2.491592	-4.007645	3.140154
C	-0.249526	-5.360079	-0.230783
C	1.278952	-5.338211	-0.099541
C	-3.450595	-8.514110	2.281638
C	-2.879147	-9.293834	3.474737
C	-3.337455	-5.184538	1.642012
C	-4.164197	-5.527119	0.424746
C	-3.837477	-4.164884	2.469559
C	-3.309325	-3.600123	3.645997
C	-4.155179	-2.540238	4.312088
N	-2.132677	-3.932794	4.180924
C	-1.641493	-3.247462	5.340677
C	-1.000521	-1.992560	5.206039
C	-0.468452	-1.393869	6.352858
C	-0.561849	-1.999037	7.600486
C	-1.199758	-3.227625	7.717846
C	-1.747020	-3.872560	6.604668
C	-0.855163	-1.273399	3.871025
C	0.612617	-1.203400	3.423818
C	-2.441143	-5.213111	6.796147
C	-1.463200	-6.285742	7.296778
C	-3.658179	-5.095238	7.725598
C	-1.456485	0.140681	3.909461
C	3.656766	-8.394757	2.678514
C	-0.677924	-4.843569	-1.613538
C	-4.665639	-9.250019	1.698365
O	3.240020	-5.083838	4.988070
C	3.033529	-3.884420	5.737494
H	-4.377531	-4.355588	7.359399
H	-4.174104	-6.058668	7.803144
H	-3.362936	-4.796997	8.737631
H	-1.277439	-3.699444	8.694061
H	-1.065574	-6.029906	8.285598
H	-1.971405	-7.252828	7.386583
H	-0.624219	-6.395956	6.603299
H	-2.813043	-5.536426	5.818093
H	-0.142387	-1.513254	8.477522
H	0.030298	-0.432367	6.262572
H	-5.186971	-2.591480	3.960516
H	-4.141031	-2.650391	5.399164
H	-3.770722	-1.540686	4.088091
H	-4.784896	-3.745768	2.151323
H	-2.492023	0.146034	4.264056

H	-0.883341	0.799635	4.570877
H	-1.437510	0.587669	2.909580
H	-4.873727	-4.729323	0.199291
H	-3.530697	-5.700366	-0.448144
H	0.685304	-0.725938	2.439938
H	1.203498	-0.600595	4.123756
H	1.076388	-2.190133	3.358758
H	-0.655579	-4.669950	0.516115
H	-0.294816	-5.488138	-2.412664
H	-0.284086	-3.835361	-1.782224
H	-1.766875	-4.800511	-1.716612
H	1.655034	-4.321704	-0.254373
H	1.753582	-5.982505	-0.848620
H	0.354364	-7.675681	-1.476074
H	1.610508	-5.662017	0.889279
H	-4.731547	-6.448831	0.591494
H	-2.317405	-10.293001	0.598997
H	-0.575913	-9.936781	-1.115787
H	-5.458503	-9.328551	2.450088
H	-3.802706	-7.550707	2.663550
H	-5.076316	-8.733156	0.825188
H	-4.411838	-10.268857	1.386581
H	-2.057419	-8.751044	3.950165
H	-3.653659	-9.468052	4.230200
H	-2.492835	-10.269230	3.158482
H	3.530901	-3.039342	5.256043
H	3.466686	-4.074752	6.719943
H	1.966019	-3.672659	5.829572
H	0.741625	-7.813884	2.917099
H	0.014703	-8.308360	4.446698
H	2.217579	-8.914860	4.817374
H	2.110910	-7.329510	5.582910
H	4.157403	-7.228570	4.413884
H	2.801595	-8.596335	2.026331
H	4.473370	-8.007944	2.062828
H	3.977936	-9.338522	3.129332
H	-1.400668	-1.849403	3.116719

Propagation Step of the ROP of TMC-γ(*R*).

$\mathbf{V}^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.144485 kcal.mol^{-1}

C	0.743442	-8.247871	2.440485
C	2.086141	-7.802406	2.380308
C	2.780423	-7.465785	3.564564
C	2.118289	-7.590738	4.790209
C	0.799462	-8.020244	4.861225
C	0.123300	-8.340382	3.689890
N	2.716717	-7.640892	1.106199
C	3.245570	-8.698083	0.492116
C	3.322902	-10.023012	1.219836
C	4.222679	-6.984186	3.546335
C	5.176147	-8.009611	4.178022
C	-0.053333	-8.595417	1.190553
C	-0.750131	-9.959174	1.297173
C	3.698765	-8.708324	-0.840664
C	3.572876	-7.744270	-1.859433
C	3.884428	-8.236673	-3.256466
N	3.151007	-6.492208	-1.678665
C	2.991533	-5.627268	-2.809072
C	1.742445	-5.555607	-3.467461
C	1.605702	-4.684469	-4.552829
C	2.665872	-3.904787	-4.996943
C	3.886453	-3.976977	-4.337352
C	4.071756	-4.818637	-3.236341
C	0.539871	-6.377920	-3.029553
C	-0.565633	-5.475113	-2.461628
C	5.423795	-4.832305	-2.537023
C	6.525956	-5.458552	-3.404782
Zn	2.587511	-5.894417	0.137221
O	1.251616	-4.621948	0.423914
C	0.901897	-4.222075	1.712696
C	0.043845	-2.950464	1.704569
C	0.792845	-1.745135	1.151792
C	0.788230	-1.629962	-0.358608

O	4.486621	-4.930247	0.877218	H	4.933887	-8.182846	5.232910	H	-1.431260	-6.076100	-2.160719
C	4.946135	-3.830654	1.137231	H	5.131681	-8.975257	3.665537	H	0.866624	-7.043564	-2.224153
O	6.194443	-3.754455	1.597706	H	5.395715	-5.251011	4.124021	H	-0.810025	-7.899040	-3.798686
C	6.847417	-2.495089	1.927987	H	4.513935	-6.850962	2.501026	H	0.776897	-7.904243	-4.587152
C	5.803519	-1.464829	2.306250	H	5.199178	-1.074260	0.264294	H	-0.407461	-6.655957	-4.985583
C	4.765215	-1.414505	1.211569	H	3.908071	-0.784555	1.456330	H	2.957412	-8.558700	-3.744935
O	4.214618	-2.735313	0.984918	H	7.364986	-2.174633	1.014131	H	4.319157	-7.459133	-3.885562
C	7.857565	-2.810890	3.010508	H	4.165726	-5.691278	5.315544	H	0.646680	-4.620564	-5.060870
O	0.161346	-0.545068	1.713229	H	2.649212	-7.343058	5.706129	H	2.540637	-3.241701	-5.848817
C	0.962266	0.474716	2.014583	H	0.300745	-8.105364	5.823072	H	4.715656	-3.363319	-4.680731
O	2.170113	0.509650	1.910569	H	-0.910579	-8.671337	3.744344	H	5.320089	-5.437954	-1.632190
O	0.286900	1.533439	2.483348	H	-1.541250	-9.954817	2.054944	H	5.045751	-2.929725	-1.538048
C	-1.136540	1.461013	2.585242	H	-0.047353	-10.756955	1.559145	H	6.745565	-3.463960	-1.485640
C	-0.000576	-7.258519	-4.165855	H	-1.218366	-10.220276	0.341879	H	6.071065	-2.783173	-2.967990
C	5.842334	-3.418978	-2.105625	H	-1.646749	-7.750954	-0.028843	H	6.661090	-4.899247	-4.337753
C	4.372526	-5.623810	4.241377	H	-1.775976	-7.352479	1.691151	H	5.337479	-1.728366	3.262910
C	-1.068580	-7.489607	0.864911	H	-0.567097	-6.535127	0.678953	H	6.269462	-0.481390	2.422257
H	-0.908422	-4.753096	-3.212069	H	0.646321	-8.650131	0.350831	H	8.450348	-1.919202	3.235412
H	4.558538	-9.094891	-3.224447	H	2.355970	-10.536705	1.175665	H	7.355157	-3.136065	3.925962
H	6.299685	-6.495138	-3.668732	H	3.564578	-9.892255	2.276381	H	8.534979	-3.604092	2.684583
H	7.483433	-5.453918	-2.871383	H	4.068021	-10.674320	0.758739	H	1.789071	-4.011225	2.342734
H	3.684923	-4.885485	3.817730	H	4.107965	-9.657171	-1.168595	H	0.332334	-5.002236	2.249917
H	6.211374	-7.653428	4.127482	H	-0.208390	-4.927683	-1.584397	H	-0.874990	-3.126458	1.131231

H	-0.250627	-2.730238	2.738744
H	1.818649	-1.759839	1.526720
H	1.383083	-0.772782	-0.689163
H	-0.235936	-1.512638	-0.728026
H	1.203665	-2.551443	-0.772042
H	-1.446951	2.432335	2.972197
H	-1.444218	0.669150	3.273120
H	-1.594492	1.283439	1.608852

$\mathbf{V}^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.141061 kcal.mol^{-1}

O	4.110194	-2.787738	1.281435
C	4.894384	-3.851205	1.212546
O	6.155297	-3.794294	1.646903
C	6.706071	-2.562632	2.148469
C	5.642929	-1.774562	2.878194
C	4.474325	-1.529338	1.939021
O	4.485996	-4.905559	0.754848
Zn	2.600941	-5.928686	0.048491
O	1.215438	-4.707814	0.325177
C	0.931638	-4.228622	1.604407
C	-0.049350	-3.050260	1.570263
C	0.465273	-1.869904	0.749564
O	-0.171262	-0.637155	1.227543
C	0.489616	0.081998	2.132431
O	-0.195448	1.168364	2.518412
C	-1.489032	1.409408	1.961576
C	4.718004	-0.480491	0.869608
N	3.189636	-6.503701	-1.765562
C	3.675346	-7.732160	-1.944883
C	3.823985	-8.696249	-0.929578
C	3.358211	-8.708404	0.399159
N	2.796043	-7.670859	1.017868
C	2.186003	-7.856882	2.299009
C	2.894737	-7.529026	3.477564
C	2.257712	-7.689865	4.712255
C	0.948366	-8.144811	4.798843
C	0.256169	-8.451239	3.633617
C	0.851669	-8.323321	2.375255
C	4.325967	-7.016110	3.444495
C	4.456898	-5.671262	4.173334
C	0.034213	-8.655121	1.135032
C	-1.020685	-7.569002	0.876224
C	2.991189	-5.644574	-2.893866
C	4.015456	-4.753490	-3.292161
C	3.783267	-3.905772	-4.379728
C	2.569820	-3.910209	-5.056040
C	1.565786	-4.778362	-4.646253
C	1.752295	-5.658503	-3.575796
C	5.357854	-4.687505	-2.578187
C	5.653175	-3.266982	-2.076236
C	0.613599	-6.585506	-3.176941
C	0.136644	-7.452918	-4.350848
C	4.044660	-8.192692	-3.338411
C	-0.555021	-5.793279	-2.572191
C	6.512055	-5.179952	-3.464418
C	3.465248	-10.037587	1.115472
C	5.314715	-8.033706	4.033057
C	-0.619360	-10.042004	1.214811
C	0.161707	-1.958956	-0.730365
O	1.586588	-0.152291	2.592074
H	-0.952225	-5.069321	-3.293352
H	4.724687	-9.045702	-3.298983
H	6.367072	-6.214778	-3.787369
H	7.461616	-5.132249	-2.919228
H	3.743761	-4.938778	3.781946
H	6.339742	-7.649863	3.977602
H	5.092173	-8.241886	5.085976
H	5.287214	-8.985393	3.494261
H	5.470360	-5.273705	4.051851

H	4.594335	-6.850393	2.397375
H	3.569853	-1.262744	2.489928
H	7.526625	-2.866694	2.800927
H	7.125275	-2.005523	1.303534
H	4.268717	-5.771436	5.248192
H	2.800455	-7.450148	5.623335
H	0.469288	-8.258091	5.767717
H	-0.771419	-8.799375	3.699408
H	-1.388070	-10.085590	1.994152
H	0.113165	-10.826807	1.430321
H	-1.107140	-10.285483	0.264628
H	-1.617621	-7.816457	-0.008923
H	-1.706055	-7.480806	1.727182
H	-0.548992	-6.596132	0.708595
H	0.713531	-8.661542	0.277090
H	2.512404	-10.575545	1.055123
H	3.691843	-9.912868	2.175881
H	4.231661	-10.664319	0.655307
H	4.272737	-9.627273	-1.256517
H	-0.240049	-5.253469	-1.674243
H	-1.372788	-6.468970	-2.297181
H	0.990171	-7.259809	-2.401108
H	-0.614782	-8.173855	-4.010346
H	0.960684	-8.012189	-4.805659
H	-0.325510	-6.848575	-5.139301
H	3.141949	-8.507669	-3.874355
H	4.499540	-7.396123	-3.929142
H	0.613467	-4.778280	-5.170643
H	2.407049	-3.240429	-5.896305
H	4.570260	-3.226813	-4.698977
H	5.299295	-5.339736	-1.702498
H	4.822544	-2.878301	-1.480804
H	6.560620	-3.264350	-1.460881
H	5.819508	-2.571274	-2.906361
H	6.612694	-4.562302	-4.364201
H	5.310348	-2.337073	3.757106
H	6.047287	-0.819884	3.228005
H	4.832024	0.498715	1.343948
H	5.609898	-0.688226	0.270792
H	3.858707	-0.428613	0.197829
H	1.840856	-3.876352	2.126804
H	0.488612	-5.007118	2.252696
H	-1.020427	-3.378380	1.177735
H	-0.208767	-2.718327	2.604134
H	1.538716	-1.755217	0.916759
H	0.572568	-1.101708	-1.273103
H	-0.919333	-1.994620	-0.901312
H	0.605928	-2.882171	-1.107650
H	-1.837921	2.329557	2.431952
H	-2.176209	0.590074	2.187761
H	-1.435104	1.540743	0.877721

$\mathbf{V}^{\gamma\alpha,\alpha\gamma}{}_{\mathrm{TMC}\text{-}\gamma(R)}$

G = -2422.142892 kcal.mol^{-1}

O	3.192595	-3.268512	1.355591
C	4.206766	-4.112261	1.494078
O	5.355552	-3.704527	2.032424
C	5.581282	-2.333156	2.468377
C	4.261678	-1.709333	2.874774
C	3.288914	-1.874006	1.732364
O	4.099329	-5.275602	1.146410
Zn	2.618667	-6.806914	0.366000
N	3.447235	-8.446733	1.150456
C	2.983089	-8.971506	2.398220
C	3.524558	-8.503177	3.616778
C	3.017313	-9.010714	4.817929
C	1.993765	-9.949048	4.833114
C	1.462091	-10.396363	3.629285
C	1.939874	-9.929500	2.401776
C	4.639850	-7.470642	3.664239

C	5.931957	-8.046499	4.262019	C	0.508266	-5.440522	1.844239	H	5.987874	-1.799606	1.598956
C	1.298276	-10.435460	1.117050	C	-0.008549	-6.368682	2.944657	H	4.025756	-6.443611	5.498813
C	1.212198	-11.967268	1.062101	C	-0.574472	-4.419573	1.452584	H	3.435107	-8.660741	5.758905
C	6.623046	-2.402713	3.564656	C	-0.127666	-3.573968	0.275282	H	1.610271	-10.328356	5.776577
N	3.271105	-7.002997	-1.519989	O	-1.051571	-2.478294	0.033657	H	0.654578	-11.123693	3.641094
C	4.128770	-7.974330	-1.825207	C	-0.819491	-1.347356	0.699237	H	0.518808	-12.364978	1.811303
C	4.524551	-8.221382	-3.266319	O	0.103248	-1.124676	1.452610	H	2.186245	-12.437934	1.231583
C	2.739004	-6.163994	-2.550128	O	-1.743170	-0.409770	0.446847	H	0.847010	-12.289387	0.080801
C	3.438799	-4.995482	-2.936765	C	-2.820905	-0.717036	-0.439859	H	-0.542840	-10.164741	-0.012039
C	2.889803	-4.183220	-3.933697	C	4.205730	-6.219805	4.441173	H	-0.759535	-10.074102	1.743061
C	1.671763	-4.488664	-4.528148	C	-0.088558	-9.805576	0.918621	H	-0.024958	-8.714460	0.873307
C	0.984410	-5.626642	-4.125499	H	-1.257299	-6.756244	-2.806857	H	1.924797	-10.114133	0.279417
C	1.496600	-6.482300	-3.144651	H	5.553816	-8.583521	-3.325290	H	4.273889	-11.219987	1.041614
C	4.768841	-4.598890	-2.310584	H	6.047327	-5.796152	-3.631968	H	5.244810	-10.204156	2.094046
C	5.943066	-4.763988	-3.287733	H	6.885676	-4.475829	-2.808401	H	5.861131	-10.667372	0.490269
C	0.703101	-7.723094	-2.763772	H	3.282428	-5.799577	4.031110	H	5.411570	-9.562297	-1.317927
C	-0.642116	-7.352554	-2.122865	H	6.727106	-7.292381	4.254662	H	-0.483701	-6.785810	-1.200540
C	4.680254	-8.880995	-0.897422	H	5.785710	-8.366459	5.299992	H	-1.207382	-8.258160	-1.875651
C	4.328112	-9.150406	0.436470	H	6.289201	-8.912502	3.696558	H	1.282380	-8.270231	-2.013219
C	4.971089	-10.375139	1.050721	H	4.986809	-5.453602	4.391229	H	0.004040	-9.581694	-3.651855
C	0.504148	-8.658687	-3.965652	H	4.851914	-7.161960	2.637133	H	1.457193	-8.930354	-4.430871
C	4.733830	-3.157426	-1.782451	H	3.617750	-1.319422	0.845984	H	-0.119290	-8.194501	-4.738144
O	0.909482	-6.144330	0.704203	H	2.265215	-1.577951	1.965403	H	3.879768	-9.001017	-3.688563

H	4.416569	-7.335578	-3.891735
H	0.029283	-5.864841	-4.587100
H	1.260541	-3.843134	-5.299739
H	3.428003	-3.292388	-4.248258
H	4.941184	-5.261388	-1.457393
H	3.866793	-2.996512	-1.136356
H	5.646162	-2.939912	-1.214063
H	4.679983	-2.427876	-2.598146
H	5.810405	-4.129803	-4.171798
H	3.877604	-2.192954	3.780623
H	4.400087	-0.646343	3.095557
H	6.907253	-1.391479	3.870619
H	6.233265	-2.935110	4.436827
H	7.517422	-2.921758	3.211283
H	1.346478	-4.855336	2.267936
H	-0.313271	-5.806487	3.836296
H	-0.872988	-6.936796	2.584051
H	0.765600	-7.084450	3.236909
H	-1.503103	-4.945460	1.195954
H	-0.785508	-3.767000	2.309071
H	0.866584	-3.158999	0.440930
H	-0.124449	-4.148643	-0.649371
H	-3.413074	-1.556323	-0.066327
H	-2.453173	-0.957133	-1.440870
H	-3.432301	0.185584	-0.473450

$\mathbf{V}^{\alpha\gamma,\alpha\gamma}{}_{\mathrm{TMC}\text{-}\gamma(R)}$

G = -2422.141127 kcal.mol^{-1}

C	3.510167	-4.572815	-3.177874
C	2.538765	-5.450892	-2.639821
C	1.204016	-5.409298	-3.103511
C	0.871402	-4.495989	-4.109071
C	1.820160	-3.643434	-4.658954
C	3.127342	-3.687516	-4.190194
N	2.899164	-6.358293	-1.592451
C	3.399981	-7.553853	-1.898409
C	3.561175	-7.955578	-3.348779
C	0.116707	-6.314810	-2.544789
C	-0.943977	-5.499669	-1.790215
C	4.952012	-4.552961	-2.689776
C	5.947512	-4.981932	-3.778156
C	3.744361	-8.545158	-0.957892
C	3.458971	-8.639562	0.415630
C	3.757406	-9.978426	1.055606
N	2.904632	-7.672490	1.149439
C	2.424098	-7.987528	2.460624
C	3.192652	-7.662918	3.601280
C	2.675187	-7.958029	4.867410
C	1.426152	-8.544993	5.020853
C	0.672921	-8.848651	3.892939
C	1.148619	-8.586768	2.605230
C	4.562497	-7.011096	3.497532
C	5.680082	-7.938515	3.997297
C	0.265243	-8.912598	1.408922
C	-0.299912	-10.338897	1.457817
Zn	2.536631	-5.890143	0.318931
O	1.167895	-4.708321	0.769725
C	1.134182	-3.899018	1.910240
C	0.440616	-4.588459	3.086250
O	4.484577	-4.827731	0.840104
C	5.033423	-3.824725	1.261292
O	6.290811	-3.920520	1.699351
C	6.999608	-2.768049	2.193138
C	6.043158	-1.800856	2.851546
C	4.951641	-1.432810	1.861456
O	4.398990	-2.661524	1.288015
C	5.384431	-0.514683	0.733340
C	0.427280	-2.576345	1.570210
C	1.040014	-1.933371	0.340520
O	0.526282	-0.588161	0.141422

C	1.190165	0.394968	0.748664	H	1.039736	-8.762368	6.013053	H	3.870297	-3.017767	-4.616912
O	2.200756	0.287164	1.409230	H	-0.308924	-9.298556	4.013694	H	5.031422	-5.259920	-1.859046
O	0.621658	1.592078	0.549770	H	-1.010195	-10.470247	2.281459	H	4.618797	-2.829167	-1.395580
C	-0.575260	1.673106	-0.226951	H	0.489680	-11.087605	1.580570	H	6.332773	-3.192439	-1.706375
C	4.600432	-5.676432	4.255071	H	-0.836955	-10.563090	0.529766	H	5.348850	-2.415852	-2.950807
C	-0.866270	-7.882413	1.277371	H	-1.494386	-8.112283	0.409087	H	5.915263	-4.303022	-4.637962
C	-0.526679	-7.180614	-3.638227	H	-1.507906	-7.892838	2.166265	H	5.604759	-2.265512	3.741390
C	5.331123	-3.166246	-2.152384	H	-0.468564	-6.870347	1.158154	H	6.576032	-0.901043	3.173515
H	-1.418626	-4.764194	-2.450395	H	0.880034	-8.837449	0.506886	H	5.697114	0.447261	1.150826
H	4.285987	-8.765732	-3.450068	H	2.839154	-10.566521	1.160506	H	6.209758	-0.929094	0.147047
H	5.744390	-5.991494	-4.146038	H	4.171320	-9.861160	2.059401	H	4.539038	-0.326772	0.069865
H	6.970791	-4.971567	-3.385774	H	4.456467	-10.552501	0.444593	H	2.156004	-3.626686	2.237081
H	3.811203	-5.002337	3.907450	H	4.197109	-9.432176	-1.385756	H	0.427906	-3.950074	3.978618
H	6.658303	-7.458365	3.880863	H	-0.494463	-4.976603	-0.940349	H	-0.594434	-4.832661	2.823365
H	5.552735	-8.183812	5.057874	H	-1.732046	-6.158789	-1.408846	H	0.952614	-5.521814	3.338534
H	5.704111	-8.880362	3.440933	H	0.586828	-6.991507	-1.824023	H	-0.640754	-2.760995	1.397613
H	5.568785	-5.185860	4.108550	H	-1.245654	-7.879377	-3.196604	H	0.514755	-1.888413	2.420719
H	4.750243	-6.796546	2.441771	H	0.219063	-7.764786	-4.187489	H	2.126254	-1.881458	0.423901
H	4.089910	-0.985795	2.360703	H	-1.069963	-6.570283	-4.368156	H	0.774097	-2.474251	-0.566337
H	7.737356	-3.169073	2.890734	H	2.600422	-8.316935	-3.733939	H	-1.379944	1.087622	0.225002
H	7.532982	-2.310908	1.352979	H	3.861288	-7.121343	-3.983529	H	-0.408443	1.321555	-1.248442
H	4.461262	-5.817893	5.332709	H	-0.153403	-4.458388	-4.469807	H	-0.842083	2.730633	-0.235019
H	3.265783	-7.721642	5.749293	H	1.542505	-2.947262	-5.446012				

TS($\mathbf{V}^{\gamma\alpha,\gamma\alpha}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VI}^{\gamma\alpha,\gamma\alpha}_{\text{TMC-}\gamma(R)}$)

G = -2422.115567 kcal.mol^{-1}

C	0.844378	-7.527078	2.629115
C	2.238640	-7.486962	2.378925
C	3.158672	-7.319300	3.441518
C	2.656209	-7.149924	4.735816
C	1.289898	-7.139268	4.988686
C	0.398557	-7.335233	3.940521
N	2.715508	-7.540380	1.031310
C	2.729718	-8.700172	0.369080
C	2.433221	-9.988994	1.105381
C	4.665081	-7.376666	3.225951
C	5.228856	-8.719942	3.718465
C	-0.183643	-7.788330	1.532616
C	-1.142823	-8.927965	1.910585
C	2.970396	-8.834141	-1.008691
C	3.172330	-7.858403	-2.004076
C	3.129111	-8.363260	-3.429859
N	3.351094	-6.558533	-1.768041
C	3.578938	-5.665435	-2.864770
C	2.479797	-5.087493	-3.537418
C	2.729564	-4.183648	-4.574786
C	4.027498	-3.867833	-4.956885
C	5.100078	-4.449979	-4.290633
C	4.907145	-5.344075	-3.233052
C	1.042886	-5.403041	-3.147996
C	0.421649	-4.234024	-2.371035
C	6.111750	-5.965364	-2.537754
C	6.680517	-7.144715	-3.343793
Zn	3.353632	-5.897464	0.111174
O	2.936088	-3.953908	0.797334
C	2.463677	-3.815501	2.134648
C	1.007120	-3.367946	2.263648
C	0.725145	-1.906604	1.919853
C	0.557915	-1.627838	0.440968
O	5.067372	-5.046619	0.684653
C	4.728748	-3.819560	0.645446
O	5.133976	-3.048251	1.691448
C	5.519700	-1.689932	1.402270
C	4.459744	-1.061414	0.512389
C	4.336435	-1.893357	-0.762099
O	4.820412	-3.228812	-0.581967
C	5.708641	-0.995842	2.735276
O	-0.531409	-1.506072	2.537989
C	-0.453347	-1.072281	3.806634
O	0.554156	-0.966235	4.462559
O	-1.655714	-0.745804	4.301155
C	-2.815624	-0.894906	3.481606
C	0.170116	-5.778550	-4.353096
C	7.222736	-4.949661	-2.245865
C	5.412617	-6.211498	3.884936
C	-0.982326	-6.530863	1.164714
H	0.386457	-3.328565	-2.987930
H	3.346137	-9.432354	-3.470918
H	5.949164	-7.946381	-3.477120
H	7.550073	-7.572115	-2.831915
H	5.061581	-5.247862	3.510617
H	6.306252	-8.775062	3.527281
H	5.073051	-8.840827	4.796740
H	4.756351	-9.570518	3.217548
H	6.480904	-6.281524	3.655418
H	4.852264	-7.312035	2.150312
H	4.960710	-1.486944	-1.562530
H	3.305825	-1.942592	-1.124106
H	6.477569	-1.727059	0.863116
H	5.310742	-6.223723	4.976125
H	3.352282	-7.022671	5.560337
H	0.921304	-6.992489	6.000270
H	-0.669026	-7.346315	4.144959
H	-1.812496	-8.638516	2.727743

H	-0.604838	-9.825316	2.231538
H	-1.772333	-9.194536	1.054553
H	-1.745913	-6.767489	0.414961
H	-1.489909	-6.109991	2.039751
H	-0.332016	-5.758893	0.745463
H	0.352253	-8.094172	0.629702
H	1.362773	-10.217555	1.072244
H	2.721598	-9.932375	2.156239
H	2.961117	-10.820755	0.633595
H	2.923237	-9.852905	-1.376269
H	1.003602	-4.005199	-1.473796
H	-0.603708	-4.471259	-2.064440
H	1.063383	-6.265187	-2.473676
H	-0.820258	-6.105735	-4.018043
H	0.615779	-6.588811	-4.938769
H	0.019551	-4.928637	-5.027398
H	2.123766	-8.211128	-3.839788
H	3.822127	-7.829300	-4.081413
H	1.892067	-3.725740	-5.094842
H	4.203599	-3.171730	-5.772890
H	6.112989	-4.201405	-4.594923
H	5.768379	-6.348558	-1.572640
H	6.829529	-4.088546	-1.702488
H	7.997594	-5.417876	-1.629572
H	7.709863	-4.597215	-3.162582
H	7.004832	-6.817995	-4.338891
H	3.515479	-1.038147	1.065112
H	4.725770	-0.027003	0.271062
H	6.091800	0.017467	2.581246
H	4.761994	-0.930115	3.280138
H	6.423803	-1.546397	3.351905
H	3.100664	-3.085395	2.650506
H	2.568998	-4.759996	2.683370
H	0.347713	-4.019492	1.682034
H	0.748280	-3.512056	3.319027
H	1.506124	-1.277127	2.359821
H	0.428785	-0.558622	0.248601
H	-0.315726	-2.158653	0.050639
H	1.437279	-1.992125	-0.092686
H	-3.651516	-0.573519	4.104137
H	-2.955626	-1.935893	3.178407
H	-2.753712	-0.267551	2.588411

TS($\mathbf{V}^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VI}^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.115648 kcal.mol^{-1}

O	4.615611	-2.960605	-0.354785
C	4.460213	-3.657846	0.807661
O	4.722457	-2.951330	1.943436
C	5.041878	-1.568235	1.768075
C	4.034053	-0.909311	0.847432
C	4.052767	-1.640681	-0.501386
O	4.880877	-4.859050	0.781035
Zn	3.259730	-5.820985	0.129463
O	2.673782	-3.925229	0.812886
C	2.072617	-3.841968	2.102627
C	0.584827	-3.484688	2.101952
C	0.246815	-2.025242	1.800309
O	-1.080203	-1.723171	2.319136
C	-1.141041	-1.367066	3.612826
O	-2.398174	-1.121337	4.007857
C	-3.467291	-1.255618	3.070641
C	4.896718	-0.944804	-1.554236
N	3.394750	-6.473773	-1.745822
C	3.324194	-7.783467	-1.990289
C	3.139675	-8.772893	-1.008359
C	2.834783	-8.665532	0.360056
N	2.716264	-7.517159	1.028706
C	2.197710	-7.501401	2.362433
C	3.074141	-7.262264	3.448215
C	2.526459	-7.125877	4.727624

C	1.156793	-7.219058	4.945243	C	0.191619	-1.683474	0.326386	H	-1.729484	-6.582344	2.034350
C	0.311631	-7.489496	3.876135	O	-0.204982	-1.262134	4.367144	H	-0.627437	-5.985303	0.785627
C	0.805123	-7.649756	2.577187	H	0.320890	-3.394893	-3.036893	H	0.403111	-8.191944	0.550519
C	4.585010	-7.221063	3.267435	H	3.714658	-9.331065	-3.442465	H	1.673917	-10.443215	0.738287
C	5.255293	-6.058865	4.008216	H	6.247527	-7.637174	-3.569039	H	2.583331	-9.881953	2.148965
C	-0.172395	-8.008814	1.462534	H	7.756720	-7.198783	-2.760714	H	3.417451	-10.681609	0.797342
C	-1.152969	-6.871652	1.148854	H	4.847197	-5.095923	3.694354	H	3.176518	-9.791710	-1.378512
C	3.624377	-5.564007	-2.827798	H	6.291690	-8.548984	3.523993	H	0.923276	-4.066822	-1.514601
C	4.948409	-5.182191	-3.148950	H	5.037105	-8.752761	4.758102	H	-0.637009	-4.606096	-2.167936
C	5.137579	-4.268487	-4.191236	H	4.790819	-9.402088	3.131821	H	1.134534	-6.301066	-2.549853
C	4.063694	-3.726543	-4.888659	H	6.327058	-6.049797	3.784565	H	-0.697556	-6.208872	-4.160824
C	2.768664	-4.106549	-4.556485	H	4.789862	-7.082048	2.202390	H	0.795069	-6.604232	-5.031539
C	2.524711	-5.032513	-3.537962	H	3.033785	-1.771172	-0.878076	H	0.118656	-4.974475	-5.119664
C	6.161141	-5.757831	-2.428747	H	5.029780	-1.136039	2.770778	H	2.406018	-8.227690	-3.877561
C	7.144761	-4.673529	-1.971233	H	6.060157	-1.485252	1.365935	H	4.072580	-7.690426	-4.032116
C	1.092745	-5.428208	-3.208987	H	5.150648	-6.147686	5.095673	H	1.930240	-3.683605	-5.103840
C	0.286855	-5.826650	-4.452439	H	3.188764	-6.943197	5.569044	H	4.236265	-3.015783	-5.692685
C	3.398729	-8.286454	-3.415562	H	0.751855	-7.096243	5.946041	H	6.149116	-3.976380	-4.460737
C	0.383866	-4.308739	-2.434679	H	-0.756855	-7.586402	4.052342	H	5.799879	-6.264201	-1.529286
C	6.890988	-6.795460	-3.297705	H	-1.627098	-9.148225	2.637828	H	6.640839	-3.925661	-1.357145
C	2.614846	-9.988393	1.064581	H	-0.275726	-10.118865	2.051571	H	7.943815	-5.126333	-1.374243
C	5.209160	-8.560680	3.692659	H	-1.554142	-9.605815	0.934292	H	7.620778	-4.169420	-2.820447
C	-0.947074	-9.295244	1.791857	H	-1.863059	-7.181378	0.373752	H	7.256455	-6.342209	-4.226540

H	3.044717	-0.964984	1.310016
H	4.276347	0.150619	0.714783
H	4.449747	0.020279	-1.813086
H	5.914065	-0.769739	-1.188883
H	4.954306	-1.556948	-2.457468
H	2.614033	-3.088674	2.689147
H	2.185585	-4.789941	2.643131
H	0.029762	-4.140096	1.423095
H	0.230220	-3.699745	3.116335
H	0.948220	-1.377063	2.336811
H	0.028126	-0.613092	0.170215
H	-0.619491	-2.233335	-0.160435
H	1.128641	-1.982805	-0.145719
H	-4.372038	-1.011838	3.628787
H	-3.530957	-2.276528	2.684906
H	-3.349064	-0.563483	2.232651

TS($\mathbf{V}^{\gamma\alpha,\alpha\gamma}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VI}^{\gamma\alpha,\alpha\gamma}_{\text{TMC-}\gamma(R)}$)

G = -2422.114922 kcal.mol^{-1}

O	4.178656	-3.273261	0.508871
C	4.082398	-4.252228	1.443320
O	4.036126	-3.800658	2.730809
C	4.407642	-2.419764	2.925814
C	3.477934	-1.534161	2.107682
C	3.383503	-2.095136	0.679518
O	4.711130	-5.320305	1.198501
Zn	3.280006	-6.538974	0.435203
N	3.392369	-8.428423	1.067788
C	3.059286	-8.789968	2.413052
C	3.976216	-8.520448	3.456920
C	3.592201	-8.809155	4.770300
C	2.344878	-9.347210	5.062454
C	1.463032	-9.628778	4.026633
C	1.797588	-9.368778	2.693684
C	5.380893	-7.996068	3.190636
C	6.419031	-9.117647	3.361051
C	0.794515	-9.729672	1.603934
C	0.412464	-11.217574	1.651323
C	4.354175	-2.160281	4.416565
N	3.422492	-6.852675	-1.543478
C	3.780392	-8.059856	-1.981472
C	3.889313	-8.332860	-3.467820
C	3.120271	-5.818160	-2.486860
C	4.092651	-4.824052	-2.762946
C	3.745735	-3.790445	-3.638144
C	2.486984	-3.721799	-4.225958
C	1.551442	-4.711343	-3.958452
C	1.847751	-5.777433	-3.101778
C	5.494082	-4.885665	-2.164590
C	6.402779	-5.861651	-2.931139
C	0.791117	-6.849849	-2.868234
C	-0.357575	-6.324590	-1.999418
C	4.039091	-9.169935	-1.156149
C	3.818783	-9.365755	0.217037
C	4.060286	-10.779532	0.703220
C	0.245156	-7.424950	-4.183823
C	6.186221	-3.521106	-2.084162
O	2.355750	-4.885653	1.175327
C	1.378160	-4.647103	2.175851
C	1.454036	-5.637554	3.330651
C	-0.028389	-4.595453	1.570756
C	-0.179744	-3.514932	0.515591
O	-1.524484	-3.476300	-0.007104
C	-2.400666	-2.750450	0.709655
O	-2.150990	-2.126174	1.711627
O	-3.630014	-2.779507	0.180261
C	-3.865389	-3.532434	-1.010636
C	5.748437	-6.795301	4.069854
C	-0.471452	-8.864905	1.678130
H	-0.857470	-5.472812	-2.472945

H	4.653991	-9.088980	-3.660308
H	6.047391	-6.892089	-2.873616
H	7.414487	-5.841444	-2.510672
H	5.048616	-5.969733	3.926195
H	7.424482	-8.744540	3.136444
H	6.424214	-9.496085	4.389864
H	6.221140	-9.964391	2.696953
H	6.745869	-6.432371	3.799521
H	5.420404	-7.656592	2.152398
H	3.776872	-1.396219	-0.061022
H	2.354056	-2.338610	0.407351
H	5.437363	-2.300194	2.562143
H	5.773691	-7.057539	5.133881
H	4.289462	-8.611946	5.580081
H	2.065948	-9.557158	6.091558
H	0.493132	-10.063964	4.254790
H	-0.151653	-11.457275	2.559218
H	1.292714	-11.866806	1.633511
H	-0.220203	-11.477094	0.795274
H	-1.171549	-9.138409	0.880801
H	-0.988173	-8.996768	2.635234
H	-0.238202	-7.802501	1.571640
H	1.265413	-9.536481	0.635210
H	3.182480	-11.403349	0.503375
H	4.258724	-10.822687	1.774339
H	4.901951	-11.220800	0.163971
H	4.383837	-10.052209	-1.684212
H	0.010749	-5.993569	-1.026051
H	-1.107874	-7.105801	-1.831608
H	1.260126	-7.670934	-2.317635
H	-0.416439	-8.274625	-3.982063
H	1.047867	-7.768185	-4.843700
H	-0.339697	-6.682794	-4.737857
H	2.937871	-8.729473	-3.839467
H	4.119010	-7.436388	-4.044296
H	0.572267	-4.662554	-4.428209
H	2.241565	-2.902666	-4.896842
H	4.475672	-3.019578	-3.863319
H	5.394631	-5.254870	-1.138731
H	5.553792	-2.777916	-1.594051
H	7.106837	-3.614310	-1.499080
H	6.471534	-3.143372	-3.073404
H	6.473735	-5.582407	-3.989076
H	2.491697	-1.513468	2.583812
H	3.858151	-0.507253	2.105412
H	4.661680	-1.132378	4.631493
H	3.338265	-2.305597	4.795776
H	5.023457	-2.841455	4.948046
H	1.592204	-3.649611	2.590887
H	0.738771	-5.372669	4.117517
H	1.229245	-6.656080	3.000790
H	2.456160	-5.633882	3.763264
H	-0.282318	-5.570343	1.137948
H	-0.744910	-4.398225	2.376290
H	0.052263	-2.531100	0.934493
H	0.454156	-3.710009	-0.350427
H	-3.647881	-4.592687	-0.858304
H	-3.261259	-3.158064	-1.841234
H	-4.924913	-3.397758	-1.231399

TS($\mathbf{V}^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VI}^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.112944 kcal.mol^{-1}

C	4.464644	-4.675547	-2.862498
C	3.189339	-5.177153	-2.503558
C	2.012232	-4.637121	-3.069000
C	2.128678	-3.561570	-3.955602
C	3.370632	-3.046176	-4.303434
C	4.523435	-3.611493	-3.767797
N	3.100619	-6.222361	-1.528238
C	2.982420	-7.488518	-1.924116

C	2.868963	-7.823592	-3.397029	O	4.958261	-4.991844	0.958217	H	5.328561	-5.652979	3.705228
C	0.630936	-5.196452	-2.755624	C	4.677818	-3.789632	1.216282	H	6.724444	-9.025483	2.908202
C	-0.168327	-4.246390	-1.856753	O	4.886076	-3.321627	2.483965	H	5.685547	-9.407491	4.290208
C	5.748283	-5.304229	-2.333924	C	5.692045	-2.138755	2.554231	H	5.187675	-9.864212	2.656341
C	6.227306	-6.445870	-3.245984	C	5.037763	-0.991392	1.800614	H	6.799800	-6.601182	3.491196
C	2.910294	-8.595923	-1.058045	C	4.483018	-1.525459	0.464574	H	5.026534	-7.447445	2.027417
C	2.788079	-8.666309	0.337991	O	4.926117	-2.879929	0.241011	H	3.391951	-1.567339	0.507510
C	2.632985	-10.064384	0.897805	C	4.916147	-0.726108	-0.747125	H	5.803037	-1.925783	3.618988
N	2.766373	-7.614963	1.164349	C	0.666184	-2.973035	1.819908	H	6.682743	-2.360849	2.139848
C	2.476326	-7.824585	2.551573	C	0.690368	-1.823851	0.828750	H	5.806118	-6.852845	4.928328
C	3.528376	-7.806445	3.497592	O	-0.643121	-1.451651	0.422646	H	4.008755	-7.927426	5.587547
C	3.207968	-7.935392	4.852894	C	-1.272595	-0.583269	1.234352	H	1.667152	-8.167514	6.338315
C	1.893358	-8.077202	5.279296	O	-0.810514	-0.081434	2.229408	H	-0.155788	-8.240637	4.673022
C	0.871288	-8.116479	4.339005	O	-2.512978	-0.309033	0.811801	H	-1.406356	-9.337641	3.146722
C	1.134391	-8.003381	2.970199	C	-3.006010	-0.932289	-0.375277	H	-0.251598	-10.257036	2.181975
C	4.992061	-7.719373	3.085749	C	5.766982	-6.641887	3.853526	H	-1.619384	-9.445730	1.398746
C	5.682750	-9.084282	3.242747	C	-0.942749	-6.845794	2.087680	H	-1.767616	-6.919698	1.370052
C	-0.033863	-8.079347	1.992988	C	-0.162360	-5.530240	-4.027402	H	-1.378067	-6.749133	3.088497
C	-0.869409	-9.354058	2.192076	C	6.886672	-4.299154	-2.131949	H	-0.392688	-5.925916	1.875291
Zn	3.170088	-5.800911	0.437369	H	-0.319811	-3.275042	-2.340130	H	0.374392	-8.103684	0.978016
O	2.810788	-3.931532	1.165492	H	3.305665	-8.803637	-3.602206	H	1.573957	-10.332633	0.970476
C	2.066283	-3.416725	2.260163	H	5.495269	-7.253311	-3.319071	H	3.057814	-10.153887	1.898690
C	2.000090	-4.377180	3.440159	H	7.156411	-6.877243	-2.856601	H	3.112708	-10.790711	0.238534

H	2.886975	-9.556764	-1.559812
H	0.356234	-4.072731	-0.914736
H	-1.154605	-4.665088	-1.626123
H	0.767819	-6.127591	-2.197134
H	-1.100122	-6.034736	-3.769351
H	0.402809	-6.184129	-4.698651
H	-0.423531	-4.627738	-4.590517
H	1.810432	-7.872842	-3.677435
H	3.342740	-7.078493	-4.036461
H	1.230148	-3.129043	-4.388472
H	3.442520	-2.215297	-5.000518
H	5.492151	-3.216981	-4.059372
H	5.520020	-5.727402	-1.351680
H	6.562706	-3.456325	-1.518916
H	7.720506	-4.790842	-1.619737
H	7.277072	-3.917812	-3.082950
H	6.427011	-6.078241	-4.259516
H	4.228912	-0.557752	2.397194
H	5.778513	-0.201130	1.632299
H	4.548578	0.301625	-0.664745
H	6.008226	-0.695750	-0.819423
H	4.517740	-1.170728	-1.662486
H	2.601679	-2.518695	2.607511
H	1.503951	-3.905889	4.295936
H	1.445573	-5.285596	3.188175
H	3.007120	-4.666799	3.745937
H	0.129149	-3.823004	1.382798
H	0.107532	-2.652698	2.706714
H	1.173786	-0.945146	1.266396
H	1.196369	-2.105404	-0.095738
H	-3.018281	-2.020609	-0.275509
H	-2.403391	-0.659050	-1.245483
H	-4.023238	-0.557794	-0.495478

VI$^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.137523 kcal.mol^{-1}

C	0.629552	-7.498389	2.199477
C	2.001566	-7.790204	2.038074
C	2.846998	-7.947008	3.158907
C	2.287512	-7.826835	4.434371
C	0.935748	-7.555216	4.609446
C	0.120034	-7.389072	3.496910
N	2.558097	-7.850670	0.719225
C	2.644899	-9.012672	0.074131
C	2.140860	-10.267421	0.746106
C	4.342456	-8.190791	3.016461
C	4.825915	-9.399319	3.829586
C	-0.291929	-7.262361	1.011808
C	-1.522908	-8.179318	1.032123
C	3.190852	-9.158769	-1.217124
C	3.681049	-8.193554	-2.112040
C	4.179898	-8.701301	-3.444692
N	3.722097	-6.878022	-1.867111
C	4.155948	-5.957959	-2.876026
C	3.241571	-5.517120	-3.860921
C	3.661205	-4.534467	-4.762478
C	4.945385	-4.003248	-4.709794
C	5.838979	-4.463358	-3.750309
C	5.469457	-5.441732	-2.821558
C	1.824055	-6.066926	-3.959102
C	0.787285	-5.051962	-3.456623
C	6.493702	-5.929960	-1.806666
C	7.694540	-6.594075	-2.498320
Zn	3.225531	-6.198793	-0.116207
O	2.175865	-2.931587	1.376917
C	2.524084	-2.776511	2.749349
C	1.284492	-2.504011	3.588213
C	0.589042	-1.172325	3.308713
C	-0.284563	-1.157063	2.069890
O	3.499930	-4.759939	1.020932

C	3.189526	-3.537667	0.590168	H	4.268340	-10.308681	3.581975	H	1.758264	-6.941561	-3.304596
O	4.351632	-2.727902	0.615770	H	6.207628	-7.088107	3.243475	H	0.496287	-7.021441	-5.390180
C	4.482506	-1.753262	-0.423529	H	4.546465	-8.404704	1.962221	H	2.212625	-7.232597	-5.777802
C	3.112955	-1.217396	-0.820911	H	2.381140	-2.537576	-2.382008	H	1.418288	-5.685199	-6.078829
C	2.250842	-2.381006	-1.307516	H	1.187074	-2.206501	-1.106885	H	3.484125	-8.436988	-4.247498
O	2.658914	-3.619665	-0.711100	H	4.933094	-2.244370	-1.300893	H	5.141416	-8.248572	-3.700392
C	5.426816	-0.682240	0.090980	H	4.978593	-6.673624	4.447751	H	2.968995	-4.179884	-5.521895
O	-0.306596	-0.863555	4.416678	H	2.926095	-7.940638	5.306407	H	5.250737	-3.240568	-5.421171
C	0.255025	-0.285293	5.489607	H	0.521256	-7.466047	5.609997	H	6.847546	-4.058946	-3.719967
O	1.418984	0.007197	5.615538	H	-0.934539	-7.164620	3.636081	H	6.010073	-6.695544	-1.190837
O	-0.641685	-0.045489	6.458190	H	-2.163496	-7.975308	1.896842	H	6.126804	-4.356060	-0.324694
C	-2.007152	-0.408927	6.254594	H	-1.242072	-9.236754	1.071374	H	7.674572	-5.196596	-0.136958
C	1.474162	-6.528086	-5.381485	H	-2.128096	-8.024123	0.132298	H	7.469302	-4.012810	-1.431254
C	6.960767	-4.805892	-0.870982	H	-1.327341	-5.608749	0.042328	H	8.247095	-5.876605	-3.115028
C	5.133672	-6.927561	3.392811	H	-1.315540	-5.508839	1.808645	H	2.659784	-0.732016	0.048770
C	-0.716011	-5.787207	0.934330	H	0.147368	-5.115843	0.900572	H	3.214452	-0.467400	-1.613107
H	0.795687	-4.145590	-4.072850	H	0.272289	-7.492845	0.102172	H	5.650437	0.045342	-0.696043
H	4.289014	-9.786731	-3.432203	H	1.082005	-10.166534	1.003153	H	4.983913	-0.153984	0.941104
H	7.386070	-7.419339	-3.148275	H	2.671929	-10.445855	1.685974	H	6.365907	-1.134096	0.422128
H	8.390564	-6.993761	-1.752895	H	2.264469	-11.138908	0.101824	H	3.248881	-1.958224	2.860115
H	4.824227	-6.067542	2.791637	H	3.223385	-10.177036	-1.585451	H	2.998706	-3.697617	3.103948
H	5.886287	-9.589251	3.631045	H	0.987234	-4.759004	-2.422831	H	0.571815	-3.329838	3.478327
H	4.722550	-9.231346	4.906988	H	-0.221554	-5.477352	-3.505033	H	1.618020	-2.490000	4.631769

H	1.339685	-0.375389	3.273940
H	-0.740208	-0.172788	1.926973
H	-1.082876	-1.900946	2.156798
H	0.319985	-1.410788	1.197825
H	-2.522495	-0.119414	7.171319
H	-2.111807	-1.485086	6.092598
H	-2.436780	0.123788	5.401992

VI$^{\alpha_{\Gamma},\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.133331 kcal.mol^{-1}

O	3.035267	-3.158039	-0.678162
C	3.224590	-3.367666	0.695818
O	4.320409	-2.612605	1.180493
C	4.649865	-1.461933	0.416409
C	3.410296	-0.800565	-0.162597
C	2.694968	-1.811726	-1.073302
O	3.464829	-4.653324	0.952084
Zn	3.289413	-6.076243	-0.199195
O	2.028972	-2.916672	1.324320
C	2.053634	-3.017047	2.745171
C	0.659586	-2.822049	3.322528
C	0.069836	-1.422705	3.154216
O	-1.071911	-1.280348	4.049895
C	-0.792876	-0.949343	5.319954
O	-1.902319	-0.848263	6.067947
C	-3.175594	-1.087411	5.468520
C	3.105321	-1.678471	-2.528980
N	3.799125	-6.790753	-1.924110
C	3.811404	-8.119033	-2.116482
C	3.379380	-9.072854	-1.182813
C	2.826258	-8.905840	0.103892
N	2.678016	-7.724838	0.697463
C	2.084478	-7.633205	1.998325
C	2.907656	-7.663949	3.145532
C	2.305683	-7.508165	4.397914
C	0.933907	-7.324181	4.524790
C	0.138734	-7.286040	3.385610
C	0.690435	-7.434516	2.109621
C	4.418265	-7.825488	3.056987
C	5.130557	-6.516312	3.431829
C	-0.212103	-7.338575	0.888107
C	-0.741554	-5.907146	0.710234
C	4.182992	-5.917672	-2.995285
C	5.495718	-5.401008	-3.036090
C	5.828891	-4.514685	-4.065699
C	4.901886	-4.149551	-5.033783
C	3.612501	-4.668230	-4.980987
C	3.226039	-5.552580	-3.969882
C	6.548457	-5.779211	-2.004036
C	6.918587	-4.583397	-1.113794
C	1.792660	-6.064743	-3.922704
C	1.307448	-6.610474	-5.272350
C	4.321283	-8.652355	-3.434966
C	0.840740	-4.973897	-3.408269
C	7.802827	-6.380120	-2.654841
C	2.384220	-10.157131	0.823862
C	4.932945	-8.992380	3.911545
C	-1.372703	-8.342466	0.934189
C	-0.466556	-1.118756	1.769399
O	0.304110	-0.752004	5.782319
H	0.803909	-4.128839	-4.105415
H	4.366529	-9.742060	-3.424517
H	7.561747	-7.244818	-3.281607
H	8.509542	-6.707683	-1.884766
H	4.796279	-5.687302	2.801504
H	6.008776	-9.129504	3.757630
H	4.777648	-8.809980	4.980396
H	4.433804	-9.934486	3.661451
H	6.215467	-6.625081	3.318998
H	4.667761	-8.049917	2.014588

H	1.607536	-1.694765	-0.984998
H	5.183972	-0.786898	1.092398
H	5.340910	-1.739973	-0.393611
H	4.931449	-6.250556	4.476416
H	2.926022	-7.524811	5.290172
H	0.487088	-7.204982	5.508104
H	-0.932629	-7.131719	3.486841
H	-2.054562	-8.132702	1.765300
H	-1.016511	-9.370996	1.051738
H	-1.958345	-8.292125	0.009687
H	-1.326591	-5.822536	-0.212584
H	-1.396435	-5.629184	1.544035
H	0.071106	-5.175197	0.671964
H	0.392837	-7.578202	0.007759
H	1.309800	-10.122785	1.029099
H	2.882034	-10.243743	1.793986
H	2.599394	-11.049935	0.235244
H	3.462758	-10.101231	-1.512463
H	1.161540	-4.587573	-2.436285
H	-0.177605	-5.365358	-3.305681
H	1.756606	-6.890443	-3.205225
H	0.313404	-7.057467	-5.163825
H	1.980271	-7.377820	-5.668862
H	1.226344	-5.820777	-6.026856
H	3.675741	-8.339228	-4.261094
H	5.318099	-8.258191	-3.653133
H	2.889427	-4.376993	-5.738245
H	5.182248	-3.463051	-5.828082
H	6.836225	-4.108529	-4.109546
H	6.116382	-6.551067	-1.358285
H	6.048859	-4.189458	-0.580847
H	7.664285	-4.879722	-0.367785
H	7.350179	-3.770674	-1.709353
H	8.320659	-5.649050	-3.285152
H	2.757810	-0.486044	0.656428
H	3.690620	0.092466	-0.732574
H	2.769605	-0.715110	-2.926782
H	4.192667	-1.741605	-2.634425
H	2.666905	-2.476872	-3.131269
H	2.747564	-2.272626	3.159017
H	2.418828	-4.010242	3.028760
H	-0.025592	-3.567509	2.903052
H	0.743475	-3.017732	4.397158
H	0.812368	-0.679386	3.463766
H	-0.860972	-0.099566	1.719113
H	-1.269467	-1.815952	1.509338
H	0.333671	-1.238443	1.037519
H	-3.902401	-0.949585	6.270136
H	-3.244378	-2.104924	5.074462
H	-3.373755	-0.377925	4.660603

VI$^{\gamma\alpha,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$

G = -2422.135955 kcal.mol^{-1}

C	4.141658	-5.044612	-4.948606
C	4.648042	-5.430422	-3.684196
C	5.868994	-4.905259	-3.203104
C	6.547898	-3.969186	-3.990465
C	6.049443	-3.560288	-5.220818
C	4.859232	-4.103201	-5.692402
N	3.881212	-6.304418	-2.848561
C	3.885071	-7.623810	-3.059557
C	3.103229	-8.546154	-2.342105
C	2.212838	-8.350512	-1.270024
C	1.538118	-9.585445	-0.720996
C	6.485857	-5.348504	-1.883820
C	7.827375	-6.062676	-2.111825
C	2.841461	-5.604591	-5.512406
C	1.701129	-4.583315	-5.405227
Zn	2.873229	-5.552970	-1.337688
O	3.216396	-3.986119	-0.365407

C	2.366298	-2.987494	-0.627385	O	1.361771	-2.819789	0.341323	H	7.316192	-3.411957	-1.300643
O	3.005731	-1.744241	-0.782386	C	1.630280	-1.993418	1.483415	H	1.748717	-10.457858	-1.341008
C	3.529011	-1.533980	-2.097218	C	2.726344	-2.558113	2.376898	H	8.571075	-5.385940	-2.546825
C	4.441595	-0.325992	-2.034333	C	0.302791	-1.877327	2.227793	H	7.723361	-6.917724	-2.787593
N	1.958444	-7.168475	-0.703966	C	-0.791947	-1.256528	1.377414	H	1.882211	-9.791234	0.297573
C	1.113962	-7.095120	0.453354	O	-2.038010	-1.179163	2.103027	H	8.230169	-6.430252	-1.161722
C	1.681151	-7.281322	1.735317	C	-2.178942	-0.108546	2.902458	H	0.455528	-9.445622	-0.660167
C	0.856661	-7.133102	2.853973	O	-1.380545	0.784770	3.041983	H	4.876005	-9.276246	-4.027067
C	-0.492066	-6.821897	2.722734	O	-3.348841	-0.122589	3.556827	H	5.768881	-7.740146	-4.108909
C	-1.035985	-6.650876	1.456221	C	-4.253983	-1.207419	3.350418	H	4.364614	-7.993716	-5.133069
C	-0.253292	-6.777608	0.304097	H	-1.657257	-8.616429	-1.250656	H	3.214054	-9.576518	-2.657951
C	3.156026	-7.607368	1.928167	H	-2.091155	-6.409419	1.355957	H	-0.122276	-6.718229	-1.817687
C	3.380714	-8.802641	2.864644	H	-1.116377	-6.714629	3.605708	H	-2.841209	-7.467842	-0.618826
C	-0.896750	-6.566937	-1.058546	H	1.279131	-7.264947	3.846564	H	2.552956	-6.466972	-4.903998
C	-1.423282	-5.132539	-1.212847	H	3.812708	-5.526738	1.746497	H	4.478466	-3.790225	-6.661012
O	1.669227	-3.331270	-1.834718	H	3.575815	-6.067650	3.413315	H	2.076149	-6.600747	-7.284413
C	1.169917	-2.179627	-2.517778	H	4.999902	-6.605591	2.510942	H	3.825979	-6.790725	-7.073759
C	2.345966	-1.368181	-3.067308	H	3.568293	-7.880427	0.951451	H	0.765612	-5.005577	-5.789294
C	-2.014892	-7.584769	-1.328626	H	3.076219	-8.577717	3.892336	H	1.541576	-4.287084	-4.365817
C	3.931368	-6.377306	2.423873	H	4.443748	-9.065318	2.892411	H	-1.826910	-4.981690	-2.220792
C	4.775655	-8.195494	-4.138606	H	2.822389	-9.687307	2.540977	H	-2.231471	-4.929563	-0.501000
C	6.647993	-4.182128	-0.898860	H	7.086969	-4.539272	0.039588	H	-0.629384	-4.400990	-1.043146
C	2.990578	-6.092193	-6.960693	H	5.682678	-3.722965	-0.668774	H	-2.423361	-7.445878	-2.335739

H	1.925976	-3.681511	-5.986048
H	0.503910	-2.543589	-3.303030
H	0.577517	-1.585701	-1.813005
H	4.112219	-2.418074	-2.384584
H	3.161238	-5.261617	-7.653965
H	6.590647	-2.829622	-5.815806
H	7.487680	-3.558103	-3.630793
H	5.806163	-6.075487	-1.426716
H	2.057390	-0.313388	-3.154223
H	2.638303	-1.716550	-4.063577
H	4.846548	-0.105867	-3.027162
H	3.889988	0.551931	-1.682684
H	5.275129	-0.506817	-1.350442
H	1.933586	-1.000585	1.126789
H	2.884866	-1.894487	3.233943
H	2.447161	-3.548883	2.746662
H	3.664495	-2.647353	1.826544
H	-0.012159	-2.873571	2.559691
H	0.456690	-1.254684	3.115504
H	-0.514578	-0.249527	1.052634
H	-1.013207	-1.878346	0.509825
H	-3.804001	-2.160159	3.641892
H	-4.570666	-1.266495	2.305644
H	-5.112812	-0.991519	3.987240

VI$^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma\text{®}}$

G = -2422.134868 kcal.mol^{-1}

C	5.282450	-5.472834	-3.149371
C	3.904636	-5.593581	-2.858131
C	2.954597	-4.765106	-3.492751
C	3.406470	-3.830975	-4.430283
C	4.756233	-3.706047	-4.733536
C	5.681916	-4.520980	-4.091510
N	3.473051	-6.521247	-1.855273
C	3.274434	-7.798967	-2.169217
C	3.472412	-8.252500	-3.596276
C	1.469072	-4.843951	-3.175500
C	0.975347	-3.545641	-2.519179
C	6.332810	-6.305698	-2.428320
C	7.366899	-6.925113	-3.376888
C	2.895290	-8.786942	-1.237501
C	2.599026	-8.681164	0.129255
C	2.229083	-9.964603	0.835768
N	2.611816	-7.539980	0.835329
C	2.198818	-7.556174	2.209173
C	3.174408	-7.596270	3.227858
C	2.746556	-7.553380	4.558824
C	1.397505	-7.472722	4.881784
C	0.447525	-7.440457	3.866087
C	0.821247	-7.486569	2.520177
C	4.662086	-7.692890	2.923477
C	5.295593	-8.939842	3.558101
C	-0.247748	-7.438684	1.435978
C	-1.396484	-8.424035	1.688895
Zn	3.202804	-5.893613	0.004681
O	2.526161	-3.821615	2.051281
C	2.139917	-2.992706	3.169156
C	2.748727	-3.547504	4.448007
O	3.776432	-4.158496	0.214854
C	3.468714	-3.278578	1.179127
O	4.593883	-2.915249	1.950917
C	5.675292	-2.384133	1.185062
C	5.161984	-1.519401	0.031559
C	3.778081	-0.999900	0.401378
O	2.891321	-2.104160	0.611740
C	3.152358	-0.121433	-0.665836
C	0.615965	-2.944655	3.231693
C	0.000146	-2.217898	2.049018
O	-1.443168	-2.304357	2.075762
C	-2.063415	-1.406306	2.857576

O	-1.530897	-0.552654	3.523230
O	-3.396879	-1.547960	2.825477
C	-3.974771	-2.559947	2.001399
C	5.410132	-6.423325	3.355380
C	-0.790377	-6.013983	1.257771
C	0.629312	-5.184205	-4.414732
C	7.023362	-5.467400	-1.341529
H	1.042607	-2.703289	-3.217295
H	3.168095	-9.292018	-3.725903
H	6.892906	-7.506029	-4.174989
H	8.034470	-7.594228	-2.823382
H	5.001167	-5.526756	2.881196
H	6.348332	-9.022154	3.266669
H	5.260237	-8.896757	4.652097
H	4.787134	-9.858225	3.246963
H	6.471166	-6.497860	3.091206
H	4.771571	-7.791553	1.838170
H	3.855489	-0.428362	1.341685
H	6.252886	-1.786019	1.897842
H	6.315610	-3.196027	0.820888
H	5.348768	-6.282127	4.440311
H	3.486250	-7.583354	5.354821
H	1.085432	-7.438212	5.922039
H	-0.606243	-7.379518	4.124899
H	-1.988644	-8.144624	2.567008
H	-1.032992	-9.444407	1.848293
H	-2.077377	-8.438111	0.831069
H	-1.509345	-5.973451	0.431790
H	-1.301628	-5.673842	2.164930
H	0.014448	-5.303852	1.048642
H	0.223236	-7.722918	0.489838
H	1.179041	-9.954904	1.143692
H	2.819598	-10.091186	1.747384
H	2.389710	-10.826625	0.187039
H	2.810682	-9.787364	-1.644185
H	1.566725	-3.290801	-1.634925
H	-0.075172	-3.641743	-2.221540
H	1.327974	-5.656466	-2.454863
H	-0.427027	-5.288199	-4.143497
H	0.952041	-6.121813	-4.878838
H	0.697475	-4.397823	-5.174340
H	2.899182	-7.625308	-4.284973
H	4.522293	-8.158118	-3.891080
H	2.685431	-3.187029	-4.927507
H	5.087387	-2.973382	-5.464578
H	6.738061	-4.412570	-4.323498
H	5.818956	-7.129761	-1.923103
H	6.290357	-5.046112	-0.647251
H	7.734922	-6.076631	-0.772427
H	7.576236	-4.633174	-1.788554
H	7.994543	-6.163214	-3.851128
H	5.846563	-0.685793	-0.160404
H	5.074008	-2.109983	-0.885455
H	3.736203	0.795218	-0.798765
H	3.109034	-0.652553	-1.621382
H	2.134051	0.158138	-0.380815
H	2.525114	-1.983285	2.989682
H	2.469285	-2.925587	5.305423
H	2.398680	-4.567967	4.629560
H	3.837014	-3.559321	4.364373
H	0.231830	-3.969831	3.280447
H	0.317805	-2.432298	4.152729
H	0.285792	-1.163347	2.044658
H	0.294839	-2.671705	1.103355
H	-3.646194	-3.556816	2.307080
H	-3.720863	-2.407866	0.948901
H	-5.052520	-2.465269	2.140853

TS($\mathbf{VI}^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VII}^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.131292 kcal.mol^{-1}

O	1.907808	-4.214329	-0.174322	C	2.668839	-6.778332	-4.044553	C	1.363215	-5.996162	-4.246605
C	3.186243	-3.318590	0.884555	C	2.933825	-7.676146	-5.263787	C	7.660861	-6.069028	-1.195867
O	3.741813	-2.494897	-0.024549	C	6.491356	-5.082259	-1.045937	C	3.257055	-1.059552	4.331383
C	2.937501	-1.491984	-0.705053	C	7.002495	-3.714666	-0.581986	O	1.266017	-3.519068	6.938393
C	1.531965	-2.005751	-1.008643	C	2.974883	-0.163704	0.031839	H	1.436774	-5.311553	-5.099045
C	1.544102	-3.497494	-1.331782	C	4.301196	-7.989152	-1.405861	H	5.843038	-9.354037	-2.012936
O	2.407563	-2.642289	1.762250	C	5.138401	-8.657967	-2.476469	H	7.315157	-7.076963	-1.442275
C	1.712188	-3.436178	2.737623	C	3.782401	-8.865135	-0.433578	H	8.234000	-6.129521	-0.263817
C	1.212367	-2.549995	3.864619	C	2.970990	-8.621805	0.688906	H	4.533942	-5.282470	3.318958
C	2.284532	-2.096922	4.855548	C	2.570015	-9.832979	1.499517	H	5.306962	-8.664540	4.757657
O	1.625893	-1.479124	5.997655	N	2.564703	-7.412998	1.075658	H	3.936325	-8.140219	5.738810
C	1.173544	-2.315468	6.946005	C	1.792570	-7.236155	2.267083	H	3.704322	-9.379526	4.505342
O	0.582577	-1.659879	7.954190	C	0.392094	-7.070502	2.162165	H	5.738225	-6.239255	4.200701
C	0.506838	-0.234003	7.917156	C	-0.334861	-6.766657	3.317951	H	4.344864	-7.674302	2.736059
O	3.851123	-4.335258	1.238692	C	0.292107	-6.623421	4.550207	H	2.240672	-3.687576	-2.163202
Zn	3.074623	-5.811130	0.034083	C	1.666078	-6.814398	4.644095	H	0.542351	-3.811224	-1.662532
N	4.086411	-6.673255	-1.440147	C	2.439222	-7.131935	3.522399	H	3.477852	-1.389636	-1.653118
C	4.552549	-5.868799	-2.527713	C	-0.345717	-7.231394	0.840133	H	4.292414	-5.663849	5.039639
C	3.851768	-5.860707	-3.758246	C	-1.073188	-5.943665	0.429876	H	2.149099	-6.703617	5.611100
C	4.277126	-4.981845	-4.760346	C	3.937249	-7.348285	3.698212	H	-0.282087	-6.367248	5.435917
C	5.365909	-4.140389	-4.572527	C	4.664458	-6.051838	4.084176	H	-1.412412	-6.637505	3.248162
C	6.058016	-4.174031	-3.367052	C	4.233415	-8.447891	4.730409	H	-2.113256	-8.259978	1.619183
C	5.672873	-5.025736	-2.328190	C	-1.319247	-8.418895	0.881059	H	-0.809458	-9.352070	1.140862

H	-1.797457	-8.556548	-0.095201
H	-1.572859	-6.078651	-0.536436
H	-1.841950	-5.667905	1.160726
H	-0.366244	-5.113678	0.340226
H	0.401873	-7.445985	0.069541
H	3.179303	-9.905619	2.406303
H	2.708929	-10.750477	0.925080
H	1.528127	-9.766825	1.821771
H	4.048210	-9.905910	-0.583909
H	1.109649	-5.404824	-3.363935
H	0.532788	-6.683389	-4.443783
H	2.524709	-7.427521	-3.175583
H	2.119276	-8.397518	-5.392491
H	3.870088	-8.232838	-5.165253
H	2.998390	-7.087258	-6.185322
H	4.498485	-9.244823	-3.143603
H	5.693290	-7.940585	-3.081367
H	3.743937	-4.961462	-5.707688
H	5.680229	-3.466672	-5.365272
H	6.917786	-3.525467	-3.228271
H	5.838189	-5.461662	-0.254290
H	6.182370	-2.999590	-0.487459
H	7.477584	-3.815289	0.399499
H	7.757156	-3.302607	-1.261992
H	8.343186	-5.745957	-1.990789
H	0.865851	-1.831958	-0.157134
H	1.136291	-1.439129	-1.859773
H	2.495450	0.610988	-0.576578
H	2.450332	-0.232954	0.986941
H	4.008597	0.140789	0.219499
H	2.377430	-4.217811	3.112390
H	0.871260	-3.921930	2.234500
H	0.684762	-1.678604	3.457633
H	0.484163	-3.148168	4.422407
H	2.815677	-2.978623	5.228684
H	3.971204	-0.776343	5.109801
H	2.724904	-0.160517	4.004434
H	3.804186	-1.460680	3.476459
H	-0.011608	0.050609	8.833475
H	-0.058169	0.110562	7.047040
H	1.503134	0.215494	7.897946

TS(**VI**$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$→**VII**$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.119763 kcal.mol^{-1}

C	3.951700	-6.325991	-4.340292
C	4.628480	-6.123132	-3.111789
C	5.794472	-5.324567	-3.049162
C	6.248470	-4.719062	-4.224980
C	5.579265	-4.885458	-5.431665
C	4.445328	-5.687036	-5.482318
N	4.094628	-6.685493	-1.910455
C	4.210188	-8.000388	-1.698437
C	5.068901	-8.844162	-2.618599
C	6.591101	-5.170779	-1.760181
C	7.099899	-3.744914	-1.524029
C	2.709201	-7.204837	-4.466105
C	2.828991	-8.208817	-5.622764
C	3.551999	-8.714249	-0.685491
C	2.653288	-8.280019	0.305025
C	2.033750	-9.370199	1.151303
N	2.344906	-7.005112	0.538439
Zn	3.116179	-5.540851	-0.600023
O	4.038497	-4.143402	0.612739
C	3.464447	-3.059997	0.307864
O	2.713820	-2.367966	1.197499
C	1.965126	-3.118312	2.159782
C	1.552430	-2.212656	3.306402
C	2.699269	-1.766088	4.214192
O	2.139581	-1.270192	5.464101
C	1.846394	-2.195339	6.391072

O	1.332858	-1.649814	7.501654	O	2.008894	-3.387642	6.286715	H	-0.228852	-4.408379	-0.529169
C	1.169672	-0.232541	7.577135	H	1.476596	-5.717602	-5.491246	H	0.298324	-6.823065	-0.670120
C	1.494575	-6.674734	1.640891	H	5.525924	-9.660521	-2.054270	H	2.083516	-10.331472	0.636596
C	2.027467	-6.605381	2.951918	H	7.420924	-7.203194	-1.799535	H	0.991837	-9.145340	1.389517
C	1.192881	-6.165961	3.985623	H	8.320321	-6.066105	-0.786942	H	2.564857	-9.470735	2.103101
C	-0.136050	-5.829396	3.752692	H	4.411256	-5.074909	2.846211	H	3.739641	-9.782240	-0.691280
C	-0.656967	-5.940969	2.468881	H	4.543997	-8.413586	4.528962	H	1.234679	-5.760124	-3.737869
C	0.137553	-6.360454	1.396844	H	3.200381	-7.630904	5.362653	H	0.559090	-7.040372	-4.752169
C	3.464714	-6.992488	3.286168	H	2.875401	-8.909749	4.191850	H	2.603221	-7.780560	-3.542424
C	4.320145	-5.778010	3.678209	H	5.329574	-6.102092	3.956837	H	1.994373	-8.917798	-5.596902
C	-0.488896	-6.496023	0.016739	H	3.915624	-7.426439	2.388479	H	3.762273	-8.778299	-5.573812
C	-1.027074	-5.155381	-0.500436	H	0.799697	-3.131576	-2.234758	H	2.799778	-7.710618	-6.597803
O	2.190905	-3.784456	-0.876519	H	3.291639	-0.303781	-0.224425	H	4.459665	-9.294572	-3.409371
C	1.844453	-2.922438	-1.951958	H	3.894012	-0.709402	-1.842714	H	5.852816	-8.259958	-3.101725
C	1.900445	-1.482535	-1.420081	H	3.888510	-5.256816	4.540348	H	3.931216	-5.821573	-6.430450
C	3.313488	-1.081349	-0.995041	H	1.592883	-6.069251	4.990729	H	5.945995	-4.399897	-6.332072
O	4.091141	-2.202055	-0.524047	H	-0.762763	-5.492114	4.573786	H	7.145638	-4.107629	-4.193999
C	2.716387	-3.096547	-3.190852	H	-1.702538	-5.700289	2.292077	H	5.925788	-5.414438	-0.926321
C	-1.586874	-7.570050	0.000999	H	-2.420715	-7.299477	0.658261	H	6.280103	-3.023517	-1.533777
C	3.518772	-8.049198	4.401908	H	-1.207020	-8.541724	0.332304	H	7.581809	-3.685228	-0.542576
C	7.762244	-6.166725	-1.724411	H	-1.989229	-7.692401	-1.010894	H	7.846164	-3.443881	-2.268265
C	1.422959	-6.379207	-4.619442	H	-1.432197	-5.270180	-1.512415	H	8.457372	-5.982205	-2.551707
C	3.549692	-0.635190	3.669701	H	-1.835215	-4.775362	0.134961	H	1.215919	-1.399246	-0.572298

H	1.554339	-0.787600	-2.193935
H	2.389172	-2.414300	-3.984638
H	3.768240	-2.899041	-2.972464
H	2.649606	-4.112046	-3.581706
H	2.569501	-3.952006	2.518942
H	1.081220	-3.529247	1.662519
H	1.008828	-1.337733	2.928912
H	0.855252	-2.800286	3.912251
H	3.317686	-2.634468	4.461713
H	4.328092	-0.360174	4.387030
H	2.934958	0.248144	3.468180
H	4.020714	-0.945494	2.735338
H	0.738288	-0.044485	8.560951
H	0.494223	0.130580	6.798103
H	2.129990	0.281829	7.486805

TS($\mathbf{VI}^{\gamma\alpha,\alpha\gamma}_{\text{TMC-}\gamma(R)} \rightarrow \mathbf{VII}^{\gamma\alpha,\alpha\gamma}_{\text{TMC-}\gamma(R)}$)

G = -2422.125604 kcal.mol^{-1}

C	4.048762	-4.886545	-4.979726
C	4.540593	-5.315852	-3.723240
C	5.822852	-4.914189	-3.274152
C	6.569272	-4.048902	-4.080713
C	6.080096	-3.586154	-5.297085
C	4.834457	-4.013833	-5.740557
N	3.719870	-6.112465	-2.864462
C	3.636637	-7.434150	-3.032405
C	2.842584	-8.295113	-2.256159
C	1.982725	-8.031369	-1.174780
C	1.225206	-9.222072	-0.630295
C	6.439707	-5.465304	-1.993892
C	7.478335	-6.549088	-2.329300
C	2.721402	-5.370591	-5.552342
C	1.700248	-4.236274	-5.713809
Zn	2.730253	-5.240733	-1.371580
O	3.802433	-4.075977	-0.113591
C	3.104475	-3.015824	-0.003962
O	3.523689	-1.817972	-0.494166
C	4.004087	-1.844612	-1.856287
C	4.915986	-0.647095	-2.028041
N	1.789156	-6.826671	-0.636888
C	0.905528	-6.689968	0.481370
C	1.440314	-6.701933	1.790504
C	0.560376	-6.558513	2.868005
C	-0.805198	-6.393592	2.671928
C	-1.314476	-6.366325	1.378580
C	-0.481109	-6.514739	0.265797
C	2.925561	-6.899097	2.061929
C	3.208559	-8.290854	2.649459
C	-1.080749	-6.458057	-1.132310
C	-1.463279	-5.017268	-1.502877
O	1.808093	-3.453200	-1.251833
C	1.543012	-2.402447	-2.147993
C	2.809512	-1.856165	-2.822309
C	-2.282929	-7.397076	-1.302497
C	3.500526	-5.806091	2.971955
C	4.413615	-8.112814	-4.141005
C	7.064715	-4.389032	-1.099173
C	2.921384	-6.086681	-6.898097
O	2.434244	-2.866874	1.154287
C	1.872963	-1.584489	1.526457
C	2.887697	-0.818233	2.362038
C	0.584896	-1.861455	2.289143
C	-0.463157	-2.565917	1.443697
O	-1.708011	-2.685139	2.165529
C	-2.491219	-1.594141	2.146179
O	-2.252243	-0.557760	1.575756
O	-3.618813	-1.771285	2.848276
C	-3.846081	-3.017811	3.506615
H	-2.042480	-8.426372	-1.017040
H	-2.382127	-6.230798	1.227541

H	-1.470598	-6.284868	3.524068
H	0.956436	-6.578704	3.879873
H	3.323757	-4.814493	2.551212
H	3.064477	-5.844526	3.977124
H	4.582014	-5.942979	3.081480
H	3.447214	-6.830358	1.102701
H	2.703962	-8.423358	3.613502
H	4.283452	-8.423423	2.815889
H	2.873156	-9.093802	1.986064
H	7.478618	-4.853664	-0.197822
H	6.316949	-3.660987	-0.778351
H	7.886069	-3.861445	-1.596886
H	1.674359	-10.157666	-0.967556
H	8.311116	-6.128699	-2.904854
H	7.044654	-7.361888	-2.919118
H	1.187979	-9.215120	0.460796
H	7.890263	-6.982373	-1.411129
H	0.187580	-9.199091	-0.981260
H	4.818266	-9.064618	-3.787977
H	5.229874	-7.495466	-4.516815
H	3.746528	-8.335247	-4.981031
H	2.896232	-9.337653	-2.549000
H	-0.307902	-6.781091	-1.837075
H	-3.136925	-7.078022	-0.695262
H	2.295864	-6.092980	-4.849024
H	4.464548	-3.671199	-6.703810
H	1.979766	-6.532285	-7.237294
H	3.670069	-6.881143	-6.830792
H	0.765256	-4.621218	-6.135756
H	1.466180	-3.766730	-4.755310
H	-1.850638	-4.970943	-2.527338
H	-2.243074	-4.635548	-0.833909
H	-0.597925	-4.353242	-1.425488
H	-2.613495	-7.403621	-2.346857
H	2.072529	-3.457134	-6.388165
H	0.818318	-2.731871	-2.905428
H	1.055229	-1.587141	-1.592785
H	4.580700	-2.765111	-1.977487
H	3.251925	-5.389152	-7.675480
H	6.675389	-2.910464	-5.905337
H	7.557072	-3.738381	-3.751211
H	5.639642	-5.938382	-1.416866
H	2.601356	-0.843493	-3.191702
H	3.081767	-2.464642	-3.690891
H	5.305523	-0.625632	-3.050173
H	4.370331	0.284860	-1.847284
H	5.761251	-0.696729	-1.336087
H	1.647634	-1.024724	0.614162
H	2.475527	0.148645	2.668074
H	3.146502	-1.384956	3.261938
H	3.797873	-0.640287	1.786035
H	0.806049	-2.458915	3.181248
H	0.181447	-0.898022	2.618778
H	-0.651328	-2.016854	0.517293
H	-0.171431	-3.589403	1.211521
H	-3.069841	-3.220835	4.249104
H	-3.879885	-3.843246	2.790852
H	-4.813584	-2.911835	3.998934

TS($\mathbf{VI}^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}\rightarrow\mathbf{VII}^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.119507 kcal.mol^{-1}

C	-0.515106	-7.294216	1.416571
C	0.733352	-7.487796	0.782345
C	1.748589	-8.254207	1.403208
C	1.482359	-8.820425	2.653809
C	0.259803	-8.637786	3.288337
C	-0.725308	-7.877293	2.670177
N	0.993439	-6.890582	-0.494107
C	0.626011	-7.535881	-1.602078
C	0.926640	-7.115962	-2.910023

C	1.681307	-6.028042	-3.381311	C	4.350647	-4.175956	-3.389520	H	5.160029	-5.017323	4.523609
C	1.976800	-6.068227	-4.867368	C	0.814709	-2.604987	-3.473814	H	5.462790	-3.552486	3.564516
C	3.091370	-8.522693	0.736998	C	0.410253	-1.147339	-3.218114	H	1.819468	-2.053559	1.883267
C	3.156529	-9.954611	0.181560	C	5.077020	-5.470787	-3.046278	H	0.010506	-2.366896	-0.554777
C	-1.622543	-6.457558	0.792454	C	5.719570	-6.093938	-4.296918	H	2.736465	-5.728231	4.979171
C	-1.769140	-5.121563	1.533305	O	1.813367	-3.795301	0.839078	H	0.154905	-0.891642	0.418190
Zn	2.014311	-5.186447	-0.633413	C	1.661115	-2.387812	0.845552	H	2.461188	-4.126580	5.688016
O	3.748819	-5.109054	0.390189	C	0.252305	-1.982620	0.440799	H	-0.482718	-2.375350	1.147103
C	3.505332	-4.309232	1.351983	C	2.735824	-1.715759	-0.020209	H	0.846251	-5.391426	3.421668
O	3.342037	-4.873116	2.563813	C	4.120966	-2.331122	0.234370	H	0.647468	-3.710629	3.989550
C	3.373063	-4.066226	3.766084	O	4.123744	-3.099113	1.445839	H	-0.549930	-6.887548	7.099231
C	2.411431	-4.704738	4.759124	C	4.797208	-4.009323	4.299302	H	-1.972433	-6.468908	6.113732
C	0.974015	-4.716407	4.266786	C	6.138696	-5.273671	-1.954391	H	-2.089326	-6.450548	7.898125
O	0.085873	-5.221706	5.286780	C	0.039963	-3.126770	-4.695775	H	0.573058	-7.782066	-3.688755
C	-0.291759	-4.328496	6.216541	C	-0.179847	-8.811866	-1.493403	H	2.800620	-6.767202	-5.048717
O	-1.098390	-4.871772	7.138268	C	4.277693	-8.257071	1.671585	H	1.110891	-6.442845	-5.418975
C	-1.439798	-6.255036	7.043996	C	-2.968084	-7.194955	0.741514	H	-1.327950	-6.230267	-0.237199
N	2.171592	-5.044213	-2.621396	O	0.028151	-3.165484	6.255626	H	2.636687	-0.855602	-4.476911
C	2.955626	-4.007440	-3.223866	H	2.484693	-1.831867	-1.080069	H	-2.883398	-8.171084	0.253515
C	2.320800	-2.800517	-3.615902	H	2.740511	-0.640486	0.194703	H	-3.375285	-7.364237	1.744209
C	3.106835	-1.783696	-4.166707	H	4.889122	-1.570203	0.384825	H	-3.705036	-6.602154	0.188801
C	4.481110	-1.931883	-4.320390	H	4.430918	-2.974485	-0.592223	H	-1.030758	-2.925246	-4.578796
C	5.089084	-3.117680	-3.932141	H	4.834618	-3.415888	5.218460	H	-1.680544	-7.734307	3.168522

H	2.249397	-9.419751	3.136742
H	5.217064	-8.370358	1.119568
H	4.306873	-8.965610	2.507697
H	3.186358	-7.832849	-0.106341
H	6.660972	-6.218142	-1.764900
H	4.120380	-10.131180	-0.309002
H	2.368645	-10.147432	-0.552707
H	3.050967	-10.692590	0.985210
H	6.891689	-4.537692	-2.258715
H	3.028705	-3.057625	3.518260
H	0.533500	-0.530438	-4.115171
H	0.990648	-0.688438	-2.413091
H	-0.648071	-1.098138	-2.942074
H	0.496396	-3.203671	-2.611241
H	0.377741	-2.626239	-5.610338
H	0.159240	-4.202431	-4.833856
H	-0.821448	-4.577508	1.535806
H	-2.530435	-4.492733	1.057425
H	4.337497	-6.178791	-2.659286
H	5.001097	-6.220019	-5.112113
H	2.267619	-5.099157	-5.271996
H	-0.146892	-9.375228	-2.427347
H	0.172710	-9.447358	-0.678690
H	-1.227772	-8.574342	-1.279814
H	0.074693	-9.088152	4.259822
H	4.238571	-7.242250	2.071286
H	6.140079	-7.076959	-4.058463
H	-2.069341	-5.282527	2.574890
H	5.072967	-1.125916	-4.745800
H	6.162093	-3.234885	-4.060655
H	5.683493	-4.951184	-1.015641
H	6.537512	-5.470388	-4.674704

VII$^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$

G = -2422.146733 kcal.mol^{-1}

C	4.465621	-3.940821	-2.305327
C	3.157420	-4.134348	-2.814888
C	2.569882	-3.175929	-3.672877
C	3.306004	-2.031841	-3.998683
C	4.592159	-1.833354	-3.512874
C	5.162889	-2.786928	-2.677550
N	2.408979	-5.282437	-2.405045
Zn	1.129301	-5.119204	-0.869130
O	2.492648	-4.913536	0.918616
C	2.871299	-4.139256	1.786772
O	3.269961	-4.612665	2.963227
C	3.791976	-3.728869	4.002620
C	5.268725	-3.472374	3.755823
C	1.178253	-3.351218	-4.263262
C	1.208789	-3.325924	-5.799039
C	5.131450	-4.959959	-1.389718
C	5.856925	-4.304631	-0.207526
N	0.335970	-6.943315	-0.944559
C	0.756215	-7.828008	-1.851363
C	0.085835	-9.181716	-1.930015
C	-0.822369	-7.243880	-0.156900
C	-2.109126	-6.959003	-0.673348
C	-3.221920	-7.204008	0.136430
C	-3.088006	-7.731548	1.415301
C	-1.820510	-8.017544	1.906088
C	-0.673195	-7.777169	1.143074
C	-2.321283	-6.384626	-2.067731
C	-3.316625	-7.213134	-2.893394
C	0.690914	-8.098513	1.734427
C	0.936232	-7.306502	3.024840
C	1.760215	-7.586584	-2.804739
C	2.461359	-6.406809	-3.117513
C	3.257481	-6.458144	-4.404858
C	0.870834	-9.602191	1.989727
C	-2.762946	-4.915136	-1.999132

O	0.114540	-3.580256	-0.547651	H	-1.652244	-1.673028	-0.008674	H	1.448070	-7.785943	1.009306
C	0.029023	-2.869503	0.645073	H	3.995263	-5.429174	5.303068	H	6.162083	-5.067768	0.516124
C	1.042153	-1.709028	0.656817	H	-1.486337	-1.752937	1.761333	H	1.871381	-9.806935	2.387021
C	2.479755	-2.149954	0.493656	H	4.014677	-3.855111	6.116948	H	0.749417	-10.189423	1.074455
O	2.955720	-2.822126	1.696545	H	-2.104056	-3.151523	0.855755	H	0.141235	-9.972585	2.718735
C	-1.388474	-2.325427	0.831160	H	1.530861	-5.170827	4.911708	H	6.764938	-3.780100	-0.524940
C	0.197500	-2.303405	-3.717091	H	1.583048	-3.575625	5.715887	H	3.233179	-2.789403	3.960063
C	6.115494	-5.860478	-2.153500	H	2.234237	-7.158870	8.544204	H	0.536137	-1.286858	-3.950379
C	3.532043	-4.436108	5.324665	H	0.509806	-6.711856	8.493328	H	0.089260	-2.403642	-2.632971
C	2.051606	-4.562353	5.651839	H	1.332872	-6.910520	10.068429	H	-0.790466	-2.435213	-4.172913
O	1.853472	-5.251962	6.898374	H	1.961638	-8.418283	-3.470330	H	0.808387	-4.335034	-3.957098
C	2.008616	-4.496536	8.003706	H	4.070557	-5.732465	-4.429827	H	1.496135	-2.339512	-6.180013
O	2.295757	-3.324856	8.018477	H	3.661500	-7.459836	-4.569352	H	1.917530	-4.054688	-6.205280
O	1.804676	-5.196786	9.122840	H	-1.359988	-6.412053	-2.590363	H	-2.010327	-4.303455	-1.492742
C	1.449011	-6.579180	9.036189	H	2.861459	-1.285927	-4.652790	H	-2.913897	-4.514745	-3.008549
H	0.810424	-1.049609	-0.189657	H	-3.039045	-8.271743	-2.931840	H	4.339546	-5.595769	-0.982509
H	0.948046	-1.111182	1.572999	H	-4.331129	-7.153885	-2.484206	H	5.623205	-6.430242	-2.944814
H	3.158502	-1.301221	0.389277	H	-3.359338	-6.837272	-3.921500	H	2.591772	-6.232439	-5.246235
H	2.605202	-2.813554	-0.363740	H	0.216362	-3.555134	-6.202320	H	0.680359	-9.876900	-2.525331
H	5.669466	-2.825649	4.542032	H	-4.214218	-6.979011	-0.245887	H	-0.077049	-9.607947	-0.937932
H	5.828220	-4.412511	3.761897	H	-1.715206	-8.436381	2.904059	H	-0.900414	-9.091068	-2.397717
H	5.424430	-2.975469	2.795939	H	1.957154	-7.468064	3.386052	H	-3.967749	-7.920070	2.024946
H	0.244001	-3.509819	1.524278	H	0.244733	-7.610104	3.819217	H	0.805360	-6.235701	2.850004

H	6.586532	-6.577450	-1.471521
H	-3.712129	-4.818789	-1.458743
H	5.149522	-0.941223	-3.786069
H	6.171661	-2.630993	-2.304563
H	5.219702	-3.579503	0.305675
H	6.910604	-5.263235	-2.614647

VII$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.144898 kcal.mol^{-1}

C	4.421046	-3.949563	-2.529041
C	3.072265	-4.093306	-2.926685
C	2.442751	-3.100342	-3.714018
C	3.186574	-1.977333	-4.088334
C	4.509197	-1.817640	-3.692934
C	5.113862	-2.798504	-2.916846
N	2.354658	-5.280973	-2.574452
C	1.520874	-5.266857	-1.535505
C	0.660743	-6.323482	-1.182286
C	0.397608	-7.544947	-1.828051
C	-0.780143	-8.323268	-1.278886
C	1.000110	-3.224982	-4.185089
C	0.936743	-3.554134	-5.684100
C	5.122836	-4.995488	-1.675660
C	5.282811	-4.524181	-0.221954
Zn	2.413131	-6.843105	-3.812468
O	2.532322	-6.659355	-5.669346
C	3.701930	-6.802364	-6.417984
C	3.707013	-5.804739	-7.576949
N	1.063350	-8.001862	-2.888801
C	0.714261	-9.258999	-3.472558
C	1.403147	-10.428485	-3.062993
C	1.081447	-11.642248	-3.678661
C	0.125362	-11.713078	-4.685911
C	-0.530702	-10.556903	-5.088436
C	-0.261096	-9.319300	-4.494626
C	2.460714	-10.391337	-1.966906
C	1.879271	-10.761981	-0.593267
C	-1.023915	-8.090155	-4.967687
C	-0.627900	-7.701031	-6.399691
O	4.319196	-7.964168	-3.500020
C	5.162266	-8.663705	-4.043322
O	5.032533	-9.362406	-5.155297
C	3.783735	-9.312440	-5.906118
C	3.817311	-8.236493	-6.968205
O	6.356608	-8.808845	-3.476456
C	7.341424	-9.665710	-4.087267
C	8.668795	-9.373003	-3.413859
C	9.246859	-7.993575	-3.720565
O	9.689301	-7.961427	-5.104812
C	8.875359	-7.366569	-5.996854
O	9.424040	-7.310328	-7.214513
C	10.745314	-7.814653	-7.421914
H	7.044849	-10.708088	-3.929869
C	-2.543512	-8.282916	-4.852277
C	3.664173	-11.294446	-2.269232
C	1.409082	-4.022038	-0.682112
C	0.170066	-1.972620	-3.867502
C	6.485443	-5.397110	-2.253872
O	7.772790	-6.929636	-5.773065
H	2.957262	-8.417508	-7.627035
H	4.725596	-8.352181	-7.573308
H	3.714035	-10.311620	-6.340941
H	2.953398	-9.169163	-5.212230
H	4.606638	-6.600503	-5.816457
H	2.827669	-5.962459	-8.211939
H	8.542909	-9.468164	-2.329239
H	4.608619	-5.905676	-8.192202
H	9.392268	-10.137808	-3.721955
H	3.667110	-4.783306	-7.189577
C	10.462715	-7.665351	-2.873018

H	8.470656	-7.232937	-3.605340
H	10.799864	-8.884429	-7.203968
H	11.472683	-7.283590	-6.802762
H	10.956285	-7.639228	-8.477125
H	0.042703	-6.131145	-0.312354
H	-0.700506	-9.394609	-1.466175
H	-0.891344	-8.151788	-0.205763
H	0.544035	-4.063856	-3.649798
H	-1.274468	-10.611998	-5.879357
H	0.225477	-1.700018	-2.808260
H	0.504671	-1.105691	-4.447733
H	-0.882368	-2.143324	-4.119326
H	-3.063286	-7.350592	-5.098667
H	2.717712	-1.212181	-4.701770
H	6.148125	-2.672102	-2.607547
H	6.895820	-6.237946	-1.684282
H	7.209271	-4.575770	-2.196929
H	4.494018	-5.890656	-1.670310
H	4.471980	-11.090093	-1.558398
H	5.780766	-5.293352	0.379666
H	4.317480	-4.310178	0.245910
H	5.888677	-3.612087	-0.168306
H	3.413776	-12.357141	-2.173419
H	7.375923	-9.475379	-5.160787
H	-0.839849	-8.516988	-7.101089
H	0.436055	-7.450293	-6.454521
H	-1.201984	-6.826243	-6.726409
H	-0.746713	-7.255970	-4.315374
H	-2.906966	-9.050638	-5.544488
H	-2.841861	-8.582578	-3.842417
H	1.452735	-4.494335	-5.901698
H	-0.105967	-3.646672	-6.010632
H	2.825284	-9.361204	-1.907605
H	1.097596	-10.067155	-0.278305
H	-1.699974	-7.975574	-1.763759
H	1.011346	-4.264988	0.305333
H	2.369380	-3.515740	-0.569744
H	0.724869	-3.306587	-1.151724
H	5.066651	-0.933444	-3.990687
H	6.402851	-5.702616	-3.299936
H	2.664430	-10.746153	0.171256
H	1.401179	-2.756885	-6.276669
H	-0.105775	-12.665983	-5.154781
H	1.593096	-12.548608	-3.366733
H	4.049065	-11.137807	-3.281182
H	1.447907	-11.769658	-0.611878
H	10.870751	-6.689426	-3.148320
H	10.184906	-7.633544	-1.815567
H	11.247468	-8.417983	-3.000913

VII$^{\gamma\alpha,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$

G = -2422.147983 kcal.mol^{-1}

C	4.385088	-5.106613	-5.093036
C	4.705106	-5.277489	-3.725671
C	5.812751	-4.603262	-3.153883
C	6.583790	-3.770851	-3.971360
C	6.272240	-3.586046	-5.314048
C	5.180354	-4.249070	-5.860840
N	3.870653	-6.074640	-2.884167
C	4.036618	-7.395156	-2.807815
C	3.261253	-8.251313	-2.006110
C	2.188304	-7.974305	-1.138092
C	1.543267	-9.188914	-0.504475
C	6.197382	-4.800205	-1.693575
C	7.328179	-5.831130	-1.546661
C	3.217434	-5.824406	-5.755794
C	2.084395	-4.851543	-6.114933
Zn	2.319063	-5.199226	-1.977252
O	1.191477	-4.063819	-2.950044
C	0.773538	-2.787565	-2.619366

C	1.690776	-1.694222	-3.184247
C	3.112054	-1.733734	-2.647774
O	3.061353	-1.461861	-1.203130
C	2.978042	-2.468308	-0.352892
O	2.765519	-2.088028	0.902455
C	2.585583	-0.683837	1.257687
C	3.943223	-0.033043	1.458368
N	1.708504	-6.756802	-0.892003
C	0.650069	-6.548940	0.047149
C	0.970693	-6.257452	1.395714
C	-0.071900	-5.953530	2.276586
C	-1.395909	-5.929884	1.851626
C	-1.696713	-6.239455	0.531201
C	-0.694592	-6.564243	-0.389125
C	2.400129	-6.329607	1.917433
C	2.628876	-7.624355	2.714926
C	-1.089367	-6.958748	-1.805640
C	-1.721527	-5.792543	-2.577956
O	3.110343	-3.659863	-0.605272
C	1.733305	-0.681237	2.517924
C	0.353942	-1.289788	2.305554
O	-0.422174	-1.241804	3.516064
C	-1.004611	-0.056004	3.779463
O	-0.915530	0.937220	3.100230
O	-1.718279	-0.087246	4.908703
C	-1.803160	-1.303074	5.656294
C	-2.021158	-8.181064	-1.801156
C	2.793902	-5.117459	2.769271
C	5.084682	-8.073973	-3.663543
C	6.591624	-3.493790	-0.994582
C	3.664138	-6.619495	-6.992292
C	4.024056	-0.676569	-3.236735
H	-1.590455	-9.020265	-1.245618
H	-2.733764	-6.239507	0.204798
H	-2.191136	-5.685160	2.551014
H	0.158473	-5.737392	3.316599
H	2.667741	-4.184621	2.216901
H	2.205870	-5.059225	3.692424
H	3.846521	-5.195747	3.064021
H	3.063768	-6.348575	1.047528
H	1.981328	-7.657931	3.598871
H	3.667693	-7.684896	3.058886
H	2.420991	-8.516680	2.118682
H	6.714196	-3.665682	0.080029
H	5.829950	-2.720839	-1.128023
H	7.542389	-3.096383	-1.367524
H	0.944712	-8.934194	0.370278
H	8.228636	-5.501193	-2.077660
H	7.043569	-6.807843	-1.946488
H	0.878589	-9.665668	-1.234253
H	7.590489	-5.966719	-0.491301
H	2.299577	-9.925807	-0.222885
H	4.648442	-8.347203	-4.631222
H	5.437326	-8.992283	-3.189197
H	5.936667	-7.423393	-3.866555
H	3.520641	-9.301898	-2.081617
H	-0.175742	-7.240788	-2.338595
H	-2.989272	-7.946238	-1.344832
H	2.811964	-6.538179	-5.031743
H	4.940112	-4.105581	-6.911306
H	2.831421	-7.217508	-7.378283
H	4.494340	-7.296716	-6.767021
H	1.268819	-5.389031	-6.612959
H	1.682437	-4.376980	-5.214501
H	-2.049227	-6.129408	-3.568335
H	-2.599857	-5.397006	-2.054768
H	-0.992497	-4.990054	-2.718175
H	-2.215145	-8.514715	-2.826534
H	2.437972	-4.075223	-6.804318

H	-0.235937	-2.603397	-3.029379
H	0.665938	-2.629356	-1.527153
H	3.544116	-2.728542	-2.780226
H	3.990698	-5.957762	-7.802162
H	6.882110	-2.932548	-5.932378
H	7.444893	-3.259756	-3.549172
H	5.316948	-5.196023	-1.178019
H	1.263939	-0.699927	-2.990325
H	1.748411	-1.820150	-4.271804
H	4.121144	-0.845053	-4.312389
H	3.617896	0.327483	-3.077571
H	5.023668	-0.727544	-2.796994
H	2.049381	-0.197524	0.437322
H	3.814872	1.015527	1.743154
H	4.499698	-0.541397	2.251450
H	4.529333	-0.065966	0.537336
H	2.257709	-1.219694	3.315736
H	1.610843	0.359199	2.835394
H	-0.188308	-0.757937	1.517934
H	0.415979	-2.350369	2.057666
H	-0.817086	-1.624575	6.001283
H	-2.254119	-2.101354	5.061463
H	-2.438974	-1.070419	6.510996

VII$^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.146669 kcal.mol^{-1}

C	-0.938049	-7.425873	-1.400283
C	0.070247	-6.965656	-0.520433
C	-0.256938	-6.524022	0.782142
C	-1.592642	-6.590679	1.192803
C	-2.590619	-7.051235	0.343415
C	-2.259299	-7.453735	-0.944428
N	1.426867	-6.898241	-0.975662
Zn	2.054168	-5.272934	-1.929522
O	2.642109	-3.696294	-0.461533
C	2.499618	-2.523668	-0.149301
O	2.518253	-2.181785	1.137578
C	2.351770	-0.800899	1.515915
C	2.416254	-0.733045	3.029767
C	3.731442	-1.225069	3.635201
O	3.636412	-1.097249	5.077035
C	3.054030	-2.123612	5.726612
O	3.016921	-1.923069	7.048394
C	3.572449	-0.727225	7.599114
C	0.793521	-5.996314	1.749057
C	0.377172	-4.659243	2.376259
C	-0.642453	-7.860192	-2.829536
C	-1.205744	-9.253414	-3.145294
N	3.831478	-5.922425	-2.550107
C	4.204693	-7.177717	-2.299091
C	5.455077	-7.740926	-2.941666
C	4.635149	-5.071707	-3.370954
C	4.401480	-5.007975	-4.764327
C	5.166241	-4.122237	-5.530737
C	6.146536	-3.323909	-4.955091
C	6.367619	-3.394826	-3.584339
C	5.619866	-4.249896	-2.768186
C	3.356027	-5.871304	-5.455163
C	3.978390	-6.746472	-6.553487
C	5.900042	-4.294391	-1.271668
C	6.034472	-2.895512	-0.655171
C	3.477797	-8.085695	-1.508582
C	2.191284	-7.988995	-0.943459
C	1.656404	-9.262118	-0.324247
C	7.158689	-5.115851	-0.949270
C	2.205073	-5.022833	-6.015749
O	0.918490	-4.207373	-2.963863
C	0.232731	-3.100155	-2.488063
C	0.919814	-1.791418	-2.901793
C	2.352737	-1.674176	-2.412899

C	3.099742	-0.478439	-2.971256
O	2.347582	-1.487011	-0.952308
H	3.131295	-0.199457	1.038670
C	1.115995	-7.016089	2.852461
C	-1.161872	-6.820710	-3.835392
O	2.608135	-3.121888	5.217809
H	-0.871820	-10.004286	-2.421655
H	-3.042694	-7.799106	-1.614301
H	-3.622790	-7.091127	0.681585
H	-1.853177	-6.271707	2.198393
H	0.121249	-3.924398	1.607132
H	-0.493381	-4.773081	3.031972
H	1.190871	-4.254327	2.984646
H	1.710279	-5.820646	1.177773
H	0.221764	-7.254064	3.440049
H	1.868303	-6.612185	3.538626
H	1.503889	-7.952974	2.441642
H	6.072939	-2.970206	0.436938
H	5.193160	-2.251153	-0.925351
H	6.953099	-2.392501	-0.977525
H	0.996292	-9.061223	0.520892
H	8.042187	-4.682927	-1.432920
H	7.068781	-6.151763	-1.284420
H	1.070410	-9.819635	-1.063632
H	7.340475	-5.130616	0.131356
H	2.476061	-9.905038	0.003261
H	5.184718	-8.243938	-3.877559
H	5.920663	-8.486680	-2.293135
H	6.186067	-6.970251	-3.187652
H	3.950861	-9.053967	-1.387604
H	0.444557	-7.911963	-2.947852
H	-2.301270	-9.258400	-3.141992
H	2.929707	-6.541568	-4.701945
H	4.991810	-4.065136	-6.602349
H	3.225969	-7.424783	-6.970526
H	4.807336	-7.351050	-6.171569
H	1.474074	-5.664327	-6.521257
H	1.689496	-4.487336	-5.212723
H	-0.953154	-7.145981	-4.861525
H	-2.247045	-6.696077	-3.740473
H	-0.681610	-5.849984	-3.676373
H	-0.883399	-9.575616	-4.141608
H	2.571797	-4.296962	-6.751526
H	-0.792417	-3.078158	-2.898250
H	0.104377	-3.101386	-1.388438
H	2.892242	-2.601218	-2.622915
H	4.365991	-6.140620	-7.380226
H	6.737081	-2.650737	-5.571052
H	7.138209	-2.772927	-3.136414
H	5.045682	-4.784506	-0.795902
H	0.346177	-0.918210	-2.560498
H	0.950795	-1.755637	-3.997531
H	3.172537	-0.574617	-4.057853
H	2.576696	0.455595	-2.741914
H	4.114952	-0.421574	-2.569186
H	1.383584	-0.441738	1.154559
H	1.600583	-1.330914	3.448059
H	2.252585	0.310544	3.326751
H	3.859404	-2.285832	3.404075
C	4.956459	-0.427817	3.227406
H	3.063705	0.159993	7.213250
H	4.641360	-0.651647	7.383296
H	3.415527	-0.806935	8.675188
H	5.837241	-0.787643	3.765584
H	5.151179	-0.540376	2.157499
H	4.828528	0.637019	3.448116

TS(**VII**$^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$⟶**VIII**$^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.140812 kcal.mol^{-1}

C	-0.745013	-6.748297	-1.042691

C	0.502971	-6.724217	-0.376570	C	6.868856	-4.295750	-4.151421	C	1.777741	-7.435124	2.962006
C	0.586563	-6.389448	0.994713	C	6.076199	-5.076987	-3.304373	C	-1.263193	-6.069973	-3.434992
C	-0.586105	-6.010685	1.656623	C	3.271407	-6.046512	-5.787782	O	1.363870	-2.540203	5.222737
C	-1.810824	-5.977761	1.001171	C	3.598429	-6.956623	-6.980881	H	-1.647874	-9.196825	-1.929565
C	-1.885141	-6.359674	-0.333282	C	6.521288	-5.277969	-1.861825	H	-2.848665	-6.360788	-0.836828
N	1.697868	-6.958987	-1.133874	C	6.492119	-3.960227	-1.073899	H	-2.707380	-5.671148	1.533380
Zn	2.408832	-5.492471	-2.228894	C	3.387766	-8.495514	-1.950769	H	-0.533803	-5.734138	2.706577
O	1.690782	-3.981933	-2.980462	C	2.239665	-8.176928	-1.204522	H	2.522902	-4.386712	1.460397
C	0.819291	-3.050044	-2.416083	C	1.584490	-9.311618	-0.453816	H	1.604444	-4.633930	2.957968
C	1.224899	-1.638338	-2.848327	C	7.919140	-5.911004	-1.774967	H	3.278487	-5.178878	2.846967
C	2.592719	-1.212106	-2.336012	C	2.260852	-4.960382	-6.185285	H	2.666977	-6.831413	1.106512
C	3.118674	0.062279	-2.968685	O	2.485292	-0.934016	-0.902362	H	1.082363	-7.061693	3.721350
C	1.889455	-6.456866	1.780618	C	2.829831	-1.898707	-0.052048	H	2.753059	-7.558795	3.445272
C	2.343089	-5.080250	2.284016	O	3.290269	-2.984538	-0.329640	H	1.424344	-8.424617	2.653572
C	-0.887741	-7.216429	-2.485533	O	2.619333	-1.547888	1.225071	H	6.807985	-4.129860	-0.038166
C	-1.893796	-8.371496	-2.605686	C	2.065036	-0.259067	1.538126	H	5.490024	-3.526756	-1.051274
N	4.008522	-6.381523	-2.969524	C	1.691095	-0.262877	3.009272	H	7.177401	-3.226229	-1.513768
C	4.203596	-7.685301	-2.763013	C	2.831171	-0.629522	3.959515	H	1.639356	-9.143254	0.625492
C	5.366149	-8.372616	-3.440435	O	2.347033	-0.490508	5.322103	H	8.688943	-5.233487	-2.160676
C	4.890867	-5.644786	-3.826693	C	1.638569	-1.524191	5.811650	H	7.990081	-6.842308	-2.345772
C	4.527132	-5.439463	-5.177962	O	1.248294	-1.309726	7.074484	H	0.522449	-9.382990	-0.706157
C	5.356807	-4.650772	-5.980419	C	1.612781	-0.093531	7.729196	H	8.171476	-6.133891	-0.732496
C	6.518103	-4.077221	-5.477742	H	2.804187	0.515085	1.303908	H	2.065828	-10.263957	-0.680341

H	5.315026	-9.454128	-3.306921
H	6.316182	-8.019583	-3.028659
H	5.385789	-8.146476	-4.510088
H	3.688490	-9.534895	-1.899340
H	0.085622	-7.600523	-2.807929
H	-2.913267	-8.046403	-2.371155
H	2.798766	-6.671373	-5.022978
H	5.084091	-4.483808	-7.019454
H	2.686387	-7.434165	-7.355626
H	4.305908	-7.746914	-6.709261
H	1.357054	-5.417287	-6.605160
H	1.974272	-4.361342	-5.315653
H	-1.393133	-6.446944	-4.455950
H	-2.205095	-5.598927	-3.131584
H	-0.483887	-5.303066	-3.454940
H	-1.902377	-8.762877	-3.628907
H	2.679405	-4.294162	-6.948835
H	-0.218228	-3.219076	-2.754636
H	0.783563	-3.100977	-1.315652
H	3.297815	-2.037309	-2.460338
H	4.037121	-6.390865	-7.810240
H	7.148801	-3.465616	-6.117569
H	7.779564	-3.849154	-3.760033
H	5.812397	-5.961817	-1.383972
H	0.474412	-0.902515	-2.527768
H	1.254578	-1.620004	-3.944513
H	3.262313	-0.093122	-4.041703
H	2.415461	0.890651	-2.832857
H	4.080438	0.348122	-2.533047
H	1.181853	-0.073450	0.921143
H	0.873727	-0.971994	3.171765
H	1.322443	0.738841	3.264526
H	3.100969	-1.677799	3.808903
C	4.054527	0.261966	3.861100
H	1.201782	0.775442	7.208605
H	2.698919	0.009588	7.797366
H	1.183012	-0.165070	8.728884
H	4.780946	-0.006605	4.632588
H	4.537531	0.136310	2.888432
H	3.790077	1.317051	3.987704

TS(**VII**$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$→**VIII**$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.14028 kcal.mol^{-1}

C	4.466928	-4.321689	-2.818366
C	3.102244	-4.344746	-3.191599
C	2.538769	-3.300542	-3.961002
C	3.356126	-2.222597	-4.316059
C	4.689362	-2.170332	-3.930596
C	5.234828	-3.215381	-3.193477
N	2.304841	-5.483031	-2.849913
C	1.406078	-5.405761	-1.865000
C	0.478968	-6.415153	-1.550025
C	0.236668	-7.658142	-2.164000
C	-0.932793	-8.452666	-1.630245
C	1.098783	-3.339979	-4.457722
C	1.045331	-3.741045	-5.940207
C	5.090687	-5.463200	-2.026370
C	4.807580	-5.337751	-0.521100
Zn	2.402446	-7.081396	-3.982781
O	3.163952	-7.512650	-5.583747
C	4.433599	-7.143005	-6.063247
C	4.357433	-5.910380	-6.961389
N	0.961333	-8.156605	-3.166769
C	0.642986	-9.436854	-3.726427
C	1.113219	-10.619732	-3.109132
C	0.850860	-11.844180	-3.731541
C	0.142551	-11.916088	-4.924709
C	-0.320717	-10.747149	-5.515027
C	-0.084023	-9.496295	-4.937442
C	1.905016	-10.611876	-1.808182

C	1.278348	-11.523453	-0.741562	H	4.280616	-8.579909	-7.638261	H	-2.515495	-7.351969	-6.200672
C	-0.619198	-8.251112	-5.629582	H	5.951304	-8.089126	-7.318301	H	2.940950	-1.413210	-4.910645
C	0.040394	-8.045120	-7.000986	H	5.224895	-10.490657	-6.611813	H	6.282993	-3.177260	-2.915092
C	-2.150035	-8.281199	-5.749569	H	4.364192	-9.681288	-5.269827	H	6.930607	-6.565376	-1.823544
C	3.370314	-11.006129	-2.042754	H	5.125840	-6.914713	-5.238332	H	7.168671	-4.813649	-1.784667
C	1.307049	-4.140803	-1.040411	H	3.683022	-6.095573	-7.805602	H	4.623686	-6.395445	-2.366602
C	0.353956	-2.017047	-4.232746	H	10.085237	-9.341083	-2.612294	H	3.923530	-10.999360	-1.096690
C	6.596427	-5.619881	-2.259833	H	5.345940	-5.643246	-7.352017	H	5.281858	-6.161845	0.023135
C	4.996961	-8.342104	-6.840541	H	10.962766	-9.570801	-4.126160	H	3.737746	-5.369202	-0.301185
C	5.175468	-9.590135	-5.994873	H	3.974682	-5.053745	-6.398757	H	5.209773	-4.396899	-0.127255
O	6.449642	-9.586451	-5.298295	C	11.407822	-7.022886	-2.955295	H	3.440150	-12.016140	-2.463210
C	6.484868	-9.102884	-4.057917	H	9.326435	-7.062877	-3.554815	H	8.732556	-9.266471	-5.357822
O	7.725038	-9.118622	-3.544100	H	11.633326	-7.712299	-7.455699	H	-0.187708	-8.876838	-7.677738
C	8.828608	-9.602979	-4.323926	H	12.097497	-6.091157	-6.879783	H	1.127164	-7.965415	-6.901329
C	10.094973	-9.073993	-3.675206	H	11.498760	-6.305871	-8.550779	H	-0.334227	-7.127236	-7.468653
C	10.267188	-7.562775	-3.799099	H	-0.184536	-6.178157	-0.726427	H	-0.362138	-7.388053	-5.006401
O	10.584525	-7.246249	-5.182730	H	-1.557730	-8.821895	-2.448047	H	-2.487412	-9.109298	-6.382610
C	9.615637	-6.686400	-5.929453	H	-0.586098	-9.331130	-1.077893	H	-2.631637	-8.394338	-4.772654
O	10.047115	-6.383262	-7.159314	H	0.565910	-4.114003	-3.896888	H	1.508687	-4.717346	-6.109593
C	11.405016	-6.645115	-7.518729	H	-0.878120	-10.802491	-6.446847	H	0.007580	-3.790621	-6.289410
O	5.548267	-8.701601	-3.404973	H	0.413598	-1.686780	-3.190581	H	1.902481	-9.589335	-1.417753
H	8.815484	-10.698896	-4.320031	H	0.755970	-1.211732	-4.856920	H	0.218351	-11.304093	-0.577468
O	8.480561	-6.468431	-5.582772	H	-0.703903	-2.129427	-4.493557	H	-1.544833	-7.846731	-0.960472

H	0.866957	-4.354911	-0.064259
H	2.280887	-3.668226	-0.900146
H	0.663229	-3.410551	-1.542724
H	5.307406	-1.322913	-4.214962
H	6.846679	-5.638841	-3.324264
H	1.800940	-11.403715	0.213702
H	1.575196	-3.010206	-6.561383
H	-0.049153	-12.879006	-5.390724
H	1.212637	-12.759623	-3.270175
H	3.870659	-10.313752	-2.723385
H	1.352344	-12.579798	-1.022458
H	11.521722	-5.945821	-3.104268
H	11.205977	-7.201408	-1.895051
H	12.353849	-7.510320	-3.212587

TS(**VII**$^{m\alpha,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$→**VIII**$^{\gamma\alpha,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.143918 kcal.mol^{-1}

C	4.478514	-5.403680	-5.147946
C	4.857091	-5.624726	-3.803402
C	6.040240	-5.051323	-3.282456
C	6.814175	-4.245283	-4.123580
C	6.448007	-4.009707	-5.442835
C	5.290624	-4.591547	-5.944955
N	3.988001	-6.380606	-2.948973
C	4.200699	-7.681719	-2.748691
C	3.396674	-8.504929	-1.936281
C	2.244877	-8.203988	-1.190053
C	1.600093	-9.350907	-0.448805
C	6.502419	-5.272125	-1.848160
C	7.914149	-5.876735	-1.787465
C	3.227819	-6.021292	-5.757461
C	2.201967	-4.946053	-6.144777
Zn	2.380320	-5.513009	-2.202821
O	1.637971	-4.003346	-2.926369
C	0.800000	-3.063220	-2.322520
C	1.195476	-1.659118	-2.787521
C	2.599076	-1.248111	-2.366080
O	2.581961	-0.876823	-0.949061
C	2.916424	-1.802032	-0.051364
O	2.846811	-1.352303	1.208465
C	2.496467	0.026257	1.505335
C	3.728771	0.906805	1.378159
N	1.687446	-6.992247	-1.113451
C	0.483537	-6.783628	-0.364293
C	0.551852	-6.451877	1.008428
C	-0.634721	-6.120802	1.670672
C	-1.858428	-6.122504	1.012789
C	-1.914768	-6.487817	-0.326906
C	-0.760747	-6.833860	-1.036022
C	1.857049	-6.463651	1.793298
C	1.792496	-7.440468	2.978872
C	-0.883817	-7.274652	-2.488958
C	-1.279040	-6.112506	-3.411513
O	3.252322	-2.944374	-0.282105
C	1.925665	0.012854	2.916871
C	0.649436	-0.807481	3.025579
O	0.167670	-0.845275	4.381654
C	-0.531726	0.236326	4.774732
O	-0.776848	1.202012	4.094596
O	-0.947616	0.131541	6.041190
C	-0.637656	-1.045878	6.790000
C	-1.862754	-8.448479	-2.643761
C	2.247360	-5.064238	2.288251
C	5.370608	-8.352119	-3.430076
C	6.451472	-3.972673	-1.031691
C	3.563725	-6.919752	-6.957011
C	3.128225	-0.031828	-3.102825
H	-1.603542	-9.284312	-1.985698
H	-2.875404	-6.509252	-0.835186
H	-2.766724	-5.853138	1.545163

H	-0.595718	-5.856132	2.724481
H	2.401874	-4.366897	1.461939
H	1.475814	-4.654547	2.950864
H	3.180638	-5.111554	2.860775
H	2.649775	-6.805550	1.119895
H	1.072705	-7.104183	3.733339
H	2.770637	-7.510860	3.467091
H	1.494938	-8.448358	2.672242
H	6.786612	-4.155843	-0.004364
H	5.439488	-3.564416	-0.985777
H	7.111644	-3.212307	-1.464994
H	1.611638	-9.171447	0.629897
H	8.666357	-5.172925	-2.160340
H	8.000737	-6.790715	-2.383642
H	0.549835	-9.456917	-0.736707
H	8.179206	-6.121034	-0.753006
H	2.116398	-10.290482	-0.649861
H	5.315857	-9.436798	-3.326822
H	6.315438	-8.013584	-2.994395
H	5.405620	-8.096213	-4.492396
H	3.710572	-9.540621	-1.889191
H	0.100080	-7.629037	-2.813213
H	-2.891119	-8.151864	-2.410535
H	2.765532	-6.657593	-4.995621
H	5.006995	-4.412563	-6.979031
H	2.656675	-7.404139	-7.335022
H	4.279395	-7.704436	-6.690651
H	1.302546	-5.412337	-6.563613
H	1.910806	-4.355484	-5.270889
H	-1.390567	-6.465357	-4.443135
H	-2.235176	-5.673640	-3.104461
H	-0.519050	-5.326001	-3.403921
H	-1.854663	-8.815288	-3.675926
H	2.608116	-4.270096	-6.906401
H	-0.253811	-3.229592	-2.607767
H	0.825055	-3.107195	-1.222352
H	3.272362	-2.101545	-2.476492
H	3.996694	-6.343633	-7.782210
H	7.064310	-3.378914	-6.077973
H	7.722381	-3.792694	-3.733375
H	5.813011	-5.981070	-1.378351
H	0.476739	-0.909129	-2.429898
H	1.157799	-1.650549	-3.883589
H	3.212579	-0.257732	-4.169539
H	2.456622	0.825051	-2.985426
H	4.119197	0.249830	-2.735146
H	1.731151	0.347978	0.791991
H	3.477617	1.943824	1.620985
H	4.513214	0.570103	2.062834
H	4.116307	0.880629	0.357230
H	2.678173	-0.384579	3.607913
H	1.707965	1.045027	3.209069
H	-0.135608	-0.395516	2.384508
H	0.829071	-1.851098	2.763932
H	0.442757	-1.179753	6.887638
H	-1.069291	-1.935463	6.324074
H	-1.083345	-0.886967	7.772423

TS(**VII**$^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$→**VIII**$^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$)

G = -2422.142009 kcal.mol^{-1}

C	4.529201	-4.254696	-2.790953
C	3.170117	-4.316485	-3.180460
C	2.593845	-3.278806	-3.949283
C	3.390857	-2.185518	-4.301478
C	4.722780	-2.105971	-3.915908
C	5.279777	-3.137228	-3.169864
N	2.342263	-5.401365	-2.740517
Zn	1.065916	-5.108360	-1.265095
O	2.812718	-4.695031	1.559581
C	2.982652	-3.906099	2.463544

O	3.381056	-4.321689	3.673352	C	1.245566	-8.912091	1.460750	H	5.142928	-2.265981	3.584519
C	3.686736	-3.376750	4.735205	C	-2.842656	-5.058888	-2.449593	H	0.363170	-3.879816	1.375109
C	5.081111	-2.806491	4.531733	O	0.596657	-3.452538	-0.646087	H	-1.620522	-2.070982	-0.089170
C	1.146106	-3.314016	-4.418162	C	0.147459	-3.092942	0.633260	H	4.251371	-5.008022	6.016830
C	1.048657	-3.312160	-5.951161	C	0.902354	-1.821620	1.054100	H	-1.710409	-2.522437	1.628698
C	5.203490	-5.343981	-1.966882	C	2.405741	-2.000938	1.138743	H	3.851891	-3.501027	6.860345
C	5.527137	-4.852410	-0.548998	O	2.809313	-2.585063	2.406964	H	-1.897708	-3.760601	0.374499
N	0.218440	-6.879407	-1.196440	C	-1.360730	-2.845854	0.640844	H	1.818805	-5.336756	5.498910
C	0.590055	-7.836743	-2.050443	C	0.327485	-2.165080	-3.811683	H	1.443908	-3.821376	6.368841
C	-0.128165	-9.168358	-2.039563	C	6.477901	-5.878337	-2.639635	H	2.884378	-7.260397	9.073395
C	-0.915617	-7.076703	-0.346356	C	3.558770	-4.158432	6.035609	H	1.106487	-7.284883	8.957516
C	-2.219953	-6.921682	-0.870430	C	2.144491	-4.657760	6.287878	H	1.895665	-7.343536	10.561023
C	-3.306302	-7.082366	-0.004470	O	2.076630	-5.437978	7.495545	H	1.751797	-8.567668	-3.642990
C	-3.121275	-7.388686	1.337790	C	1.983630	-4.728233	8.636447	H	4.306713	-6.711039	-4.310952
C	-1.832362	-7.519276	1.842341	O	1.951139	-3.525019	8.716404	H	3.049533	-7.668042	-5.112033
C	-0.709966	-7.356487	1.024751	O	1.925483	-5.517235	9.714223	H	-1.541775	-6.692692	-2.880020
C	-2.473316	-6.545373	-2.324739	C	1.955911	-6.937082	9.550994	H	2.955637	-1.381562	-4.889682
C	-3.544422	-7.422452	-2.987773	H	0.704564	-1.057822	0.290517	H	-3.323398	-8.489290	-2.879671
C	0.691964	-7.485423	1.602968	H	0.528419	-1.430380	2.009083	H	-4.537415	-7.247051	-2.560015
C	0.786494	-7.034548	3.064184	H	2.925140	-1.039904	1.123302	H	-3.609420	-7.195561	-4.057327
C	1.588285	-7.689170	-3.029742	H	2.761896	-2.629245	0.320283	H	0.003234	-3.402209	-6.266390
C	2.360914	-6.568797	-3.386942	H	5.322912	-2.107885	5.338489	H	-4.315133	-6.961885	-0.389839
C	3.251388	-6.727759	-4.596998	H	5.826774	-3.607447	4.531369	H	-1.694950	-7.744089	2.895561

H	1.838519	-6.946661	3.349486
H	0.313996	-7.749787	3.747722
H	1.348223	-6.823835	1.026624
H	6.010573	-5.647432	0.030146
H	2.246194	-8.976479	1.902086
H	1.326678	-9.217670	0.414561
H	0.601302	-9.633498	1.976795
H	6.212094	-3.997083	-0.578944
H	2.944367	-2.572896	4.703573
H	0.724483	-1.191017	-4.120119
H	0.336391	-2.216678	-2.718854
H	-0.712844	-2.219505	-4.152798
H	0.705368	-4.253618	-4.068342
H	1.442036	-2.382640	-6.377372
H	1.607977	-4.142007	-6.395472
H	-2.056950	-4.413455	-2.046225
H	-3.000449	-4.788821	-3.499994
H	4.501111	-6.177848	-1.868970
H	6.302057	-6.199318	-3.671360
H	3.103719	-5.900513	-5.297097
H	0.514000	-9.953302	-2.444249
H	-0.452594	-9.449744	-1.036290
H	-1.025747	-9.117075	-2.665793
H	-3.979203	-7.516022	1.992499
H	0.314399	-6.058480	3.212999
H	6.869619	-6.735062	-2.080744
H	-3.767617	-4.839082	-1.904433
H	5.325074	-1.246511	-4.198057
H	6.323280	-3.075425	-2.871630
H	4.622731	-4.555141	-0.014308
H	7.266688	-5.118581	-2.665355

VIII$^{\alpha\gamma,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$

G = -2422.161046 kcal.mol^{-1}

C	3.807006	3.509627	1.083188
C	2.400822	3.636407	1.050170
C	1.788478	4.901142	0.918922
C	2.608023	6.028312	0.806747
C	3.992871	5.919355	0.831052
C	4.581185	4.667988	0.972968
N	1.584793	2.472688	1.234779
Zn	1.049406	1.970456	3.066683
O	1.689470	3.022768	4.408250
C	1.598824	2.908683	5.804546
C	0.160788	2.765107	6.294677
C	0.277041	5.069904	0.950643
C	-0.165039	5.683681	2.288559
C	4.484291	2.163243	1.291971
C	5.644002	1.916792	0.318562
N	-0.040936	0.408790	2.663549
C	-0.150608	-0.041110	1.405788
C	-0.948907	-1.298798	1.156794
C	-0.714044	-0.264949	3.734419
C	-2.045758	0.087027	4.054424
C	-2.638740	-0.507218	5.172846
C	-1.950544	-1.428190	5.954029
C	-0.649894	-1.780224	5.614390
C	-0.010490	-1.217393	4.505683
C	-2.841240	1.092148	3.231850
C	-3.048089	2.407213	3.997390
C	1.413709	-1.635053	4.168226
C	2.415503	-1.080350	5.191236
C	0.425605	0.572688	0.284144
C	1.214009	1.738858	0.188977
C	1.651686	2.154273	-1.195507
C	1.557067	-3.158416	4.041051
C	-4.191952	0.525658	2.769899
C	2.251389	4.157403	6.415350
C	3.707010	4.332352	6.039560
O	4.458748	3.297554	6.713396

C	5.774630	3.323735	6.510442	H	0.098270	6.925261	-0.201859	H	-2.258699	1.325763	2.334947
O	6.319508	2.337205	7.239512	H	4.613035	6.807700	0.748077	H	-3.619353	2.241898	4.917654
C	7.758071	2.213009	7.164052	H	2.151301	7.009672	0.708030	H	-3.601935	3.126497	3.383817
C	8.126041	1.344479	5.971947	H	5.664155	4.589269	1.007924	H	-2.094531	2.862613	4.277803
C	-0.256053	5.889264	-0.231822	H	3.737213	1.383243	1.110456	H	-4.076811	-0.421104	2.232524
C	4.952088	2.021942	2.749218	H	5.396631	1.034284	2.918885	H	-4.865386	0.344848	3.614492
O	6.376807	4.103370	5.803429	H	6.479697	2.601778	0.496561	H	-4.691152	1.234803	2.100844
C	8.170573	1.644626	8.519243	H	6.029669	0.898816	0.440723	H	0.229024	0.076825	-0.658628
C	9.671091	1.506832	8.717412	H	5.332162	2.037344	-0.724242	H	2.743550	2.177902	-1.266226
O	10.353863	2.760941	8.536729	H	4.119152	2.153065	3.447400	H	1.304949	3.167560	-1.420405
C	10.417770	3.542184	9.622145	H	5.704492	2.779728	2.993877	H	1.705372	5.037397	6.051678
O	11.049420	4.667854	9.276148	H	2.204373	-1.460912	6.196687	H	3.844124	4.236291	4.960028
C	11.196737	5.611048	10.339631	H	1.390913	-3.663567	4.998637	H	2.379777	0.012235	5.238382
O	9.989149	3.279529	10.723808	H	2.567389	-3.417412	3.706590	H	2.168070	2.032013	6.161061
H	4.096512	5.305180	6.356494	H	0.845460	-3.574072	3.320356	H	2.157672	4.139135	7.508347
H	10.123026	0.842558	7.976909	H	1.663462	-1.201432	3.194313	H	8.177358	3.214207	7.028657
H	1.264788	1.473137	-1.954720	H	3.438318	-1.372553	4.929462	H	7.764592	2.283807	9.309886
H	-0.170011	4.072499	0.882587	H	-0.117206	-2.506571	6.222657	H	7.717875	0.653188	8.649803
H	0.229606	6.700136	2.399481	H	-2.428620	-1.873581	6.822167	H	9.883588	1.124962	9.719153
H	0.201337	5.093218	3.134152	H	-0.925919	-1.577143	0.102432	H	10.220663	5.915574	10.725839
H	-1.258075	5.740766	2.347246	H	-0.555416	-2.130481	1.749337	H	11.715414	6.464051	9.902476
H	-1.350919	5.919537	-0.210200	H	-1.991565	-1.167130	1.460642	H	11.784320	5.185623	11.157277
H	0.050936	5.462344	-1.192209	H	-3.658568	-0.240379	5.437930	H	0.114979	2.678068	7.386551

H	-0.429672	3.638991	5.995182
H	-0.306937	1.869819	5.870518
H	9.212397	1.258782	5.873575
H	7.701746	0.340165	6.074784
H	7.746241	1.796962	5.052992

VIII$^{\alpha\gamma,\gamma\alpha}{}_{\text{TMC-}\gamma(R)}$

G = -2422.158439 kcal.mol^{-1}

C	-2.050469	0.051916	4.006594
C	-0.696175	-0.269828	3.757789
C	-0.006638	-1.189028	4.580397
C	-0.684887	-1.749728	5.666935
C	-2.009555	-1.427431	5.936107
C	-2.682080	-0.538683	5.105523
N	0.009877	0.402973	2.707474
C	-0.015033	-0.079818	1.457477
C	0.604850	0.525484	0.354469
C	1.367450	1.709739	0.275532
C	1.884439	2.097484	-1.089406
C	1.442774	-1.574721	4.321227
C	1.626614	-3.095023	4.208644
C	-2.830284	1.021478	3.128434
C	-4.134796	0.406349	2.600817
Zn	1.014592	2.015927	3.130214
O	1.503729	3.137768	4.479970
C	1.408396	2.997946	5.873713
C	2.000720	4.262991	6.511675
C	3.440876	4.523693	6.126596
O	4.249988	3.487630	6.730691
C	5.555518	3.574585	6.496416
O	6.116354	4.426041	5.839673
N	1.653563	2.480261	1.321566
C	2.457644	3.655198	1.157314
C	1.830691	4.906180	0.973350
C	2.635225	6.046023	0.881878
C	4.018893	5.962820	0.976362
C	4.620960	4.725062	1.170019
C	3.862472	3.554904	1.263308
C	0.316849	5.047804	0.926625
C	-0.170203	5.828856	-0.300803
C	4.552562	2.226490	1.536209
C	4.945837	2.125216	3.018437
C	-0.025912	2.783863	6.349737
C	5.767391	1.983354	0.631608
C	-0.200213	5.683707	2.226695
C	-0.760104	-1.367231	1.196007
C	2.376168	-0.995347	5.393815
C	-3.118477	2.338335	3.863843
O	6.153862	2.543612	7.118017
C	7.580093	2.491920	6.979471
C	8.261408	3.343266	8.042695
C	9.781789	3.190032	8.042163
O	10.323999	3.939086	9.157522
C	10.345406	3.304911	10.333117
O	9.971720	2.173259	10.552592
C	10.469864	3.739257	6.805458
O	10.863876	4.142301	11.239272
C	10.954648	3.599186	12.557421
H	7.832337	1.434551	7.102499
H	3.792888	5.494403	6.490293
H	1.521317	1.415179	-1.859213
H	-0.108749	4.041012	0.860015
H	0.172838	6.708817	2.332776
H	0.133437	5.117508	3.101993
H	-1.295568	5.724212	2.230204
H	-1.265162	5.841553	-0.333090
H	0.189764	5.382978	-1.233845
H	0.166408	6.870982	-0.280104
H	4.626843	6.860812	0.908324
H	2.166710	7.017024	0.743546

H	5.701920	4.666754	1.261029
H	3.831543	1.427398	1.334204
H	5.397860	1.150061	3.234195
H	6.580161	2.686605	0.841914
H	6.163155	0.974747	0.792950
H	5.511045	2.080410	-0.428571
H	4.075340	2.255009	3.669276
H	5.669925	2.902788	3.284762
H	2.123462	-1.380410	6.387827
H	1.415492	-3.600455	5.157128
H	2.660183	-3.332699	3.934901
H	0.967775	-3.528865	3.449498
H	1.734737	-1.138172	3.360485
H	3.418101	-1.262021	5.185881
H	-0.163423	-2.450428	6.313757
H	-2.518011	-1.870569	6.787981
H	-0.666814	-1.670907	0.152552
H	-0.378401	-2.171524	1.832368
H	-1.822422	-1.259543	1.434541
H	-3.720185	-0.294151	5.315591
H	-2.206671	1.261846	2.261448
H	-3.736643	2.166571	4.752125
H	-3.656722	3.034214	3.210754
H	-2.195810	2.824622	4.192074
H	-3.958608	-0.539465	2.078502
H	-4.846080	0.207404	3.409649
H	-4.621416	1.093017	1.899785
H	0.476114	0.002122	-0.585162
H	2.978996	2.090897	-1.103035
H	1.577679	3.116234	-1.344244
H	1.408078	5.124470	6.177473
H	3.564452	4.488721	5.041757
H	2.310648	0.095952	5.437262
H	2.013541	2.142941	6.222695
H	1.917905	4.209853	7.604389
H	7.849782	2.815904	5.971023
H	8.001685	4.395770	7.886379
H	7.882290	3.036232	9.022749
H	10.043068	2.136890	8.195928
H	9.965635	3.325977	12.934385
H	11.389047	4.389847	13.169132
H	11.594530	2.713023	12.569865
H	-0.075926	2.683209	7.440292
H	-0.652981	3.633132	6.054266
H	-0.449636	1.873395	5.912435
H	11.555285	3.654193	6.904494
H	10.164344	3.181901	5.915451
H	10.215811	4.792670	6.654610

VIII$^{\gamma\alpha,\alpha\gamma}{}_{\text{TMC-}\gamma(R)}$

G = -2422.160679 kcal.mol^{-1}

C	4.128916	3.615517	1.954683
C	2.749343	3.728233	1.675016
C	2.143624	4.991128	1.499855
C	2.948497	6.131170	1.585255
C	4.310741	6.035781	1.842131
C	4.888937	4.786030	2.030171
N	1.938795	2.545465	1.647646
Zn	1.122329	1.918049	3.311928
O	1.260005	2.789618	4.905618
C	0.822573	2.304989	6.148292
C	0.938312	3.412262	7.194418
C	2.362834	3.896924	7.416097
O	3.069745	2.785598	8.038704
C	4.390094	2.752162	7.870957
O	4.851315	1.665561	8.512015
C	6.278481	1.442642	8.447211
C	6.468136	-0.057215	8.583551
C	0.645654	5.141323	1.281813
C	-0.029275	5.663338	2.560710

C	4.779216	2.270321	2.239814	O	5.065058	3.549050	7.253947	H	6.477693	1.052859	1.654707
C	6.099713	2.067040	1.486336	C	6.942526	2.272143	9.548298	H	5.977375	2.207301	0.407113
N	0.205569	0.326398	2.649444	C	8.438076	2.067366	9.689148	H	4.034383	2.208200	4.297882
C	0.267034	-0.009191	1.356911	O	9.051550	2.389044	8.428476	H	5.669936	2.838954	4.152145
C	-0.476854	-1.237682	0.890235	C	10.385376	2.303689	8.418091	H	2.153641	-1.969296	6.089254
C	-0.549840	-0.460714	3.577075	O	10.809062	2.621788	7.189879	H	1.449562	-4.016358	4.602443
C	-1.890014	-0.108323	3.853774	C	12.228022	2.581244	7.030171	H	2.722870	-3.636026	3.441881
C	-2.575596	-0.823441	4.840393	O	11.087925	1.993073	9.353920	H	1.038066	-3.746162	2.905832
C	-1.966055	-1.862011	5.534484	H	8.694718	1.036925	9.956412	H	1.853662	-1.374163	3.102115
C	-0.651080	-2.204605	5.243262	H	2.165048	1.772053	-1.612147	H	3.482128	-1.729467	4.941943
C	0.079668	-1.520525	4.267163	H	0.237571	4.145944	1.077688	H	-0.178799	-3.017326	5.789055
C	-2.584323	1.036788	3.130507	H	0.325548	6.671522	2.803098	H	-2.514811	-2.403505	6.300207
C	-2.724299	2.262931	4.045424	H	0.190880	5.020048	3.418628	H	-0.352011	-1.391592	-0.182359
C	1.526072	-1.910430	3.998643	H	-1.116736	5.712795	2.432362	H	-0.123045	-2.129641	1.416412
C	2.438260	-1.473367	5.154704	H	-0.779702	6.046555	-0.084631	H	-1.545339	-1.150536	1.110955
C	0.982421	0.709590	0.384764	H	0.777595	5.668884	-0.839885	H	-3.604385	-0.559339	5.070959
C	1.755870	1.881620	0.506057	H	0.624742	7.065427	0.232278	H	-1.949492	1.329319	2.287629
C	2.410484	2.398031	-0.753193	H	4.918862	6.933926	1.907037	H	-3.340171	2.030466	4.921538
C	1.687787	-3.411377	3.720952	H	2.496649	7.111262	1.456529	H	-3.200563	3.092310	3.510736
C	-3.946834	0.628805	2.554178	H	5.950200	4.717506	2.252282	H	-1.750323	2.608880	4.406308
C	2.456665	5.115652	8.319103	H	4.089737	1.489388	1.901644	H	-3.864737	-0.250476	1.907120
C	0.303383	6.029679	0.078764	H	5.385911	1.098204	3.975587	H	-4.670374	0.393380	3.342031
C	4.976974	2.090807	3.753690	H	6.875732	2.761012	1.826360	H	-4.367752	1.447494	1.960619

H	0.931485	0.298763	-0.616243
H	3.498679	2.427186	-0.638637
H	2.093642	3.424452	-0.961531
H	0.340459	4.268828	6.860155
H	2.838475	4.097373	6.452657
H	2.382568	-0.393973	5.325401
H	1.419736	1.441676	6.485517
H	-0.226692	1.965358	6.122809
H	0.519095	3.070675	8.150439
H	6.633807	1.790875	7.473504
H	6.739163	3.328879	9.347940
H	6.477064	2.019924	10.509326
H	8.851214	2.718105	10.466293
H	12.715625	3.287634	7.707061
H	12.412892	2.860271	5.992914
H	12.613440	1.577867	7.229499
H	3.499535	5.411908	8.457420
H	1.922551	5.957212	7.866928
H	2.010703	4.909991	9.298000
H	7.519739	-0.326141	8.451467
H	6.135971	-0.411161	9.565045
H	5.887566	-0.578554	7.818080

VIII$^{\gamma\alpha,\gamma\alpha}{}_{\text{TMC-}\gamma(R}$

G = -2422.159633 kcal.mol^{-1}

C	2.087089	4.844802	1.297920
C	2.660139	3.567544	1.477963
C	4.047179	3.417054	1.696922
C	4.846008	4.563823	1.707715
C	4.299281	5.826803	1.513572
C	2.930412	5.959850	1.316211
N	1.811564	2.412552	1.520043
Zn	1.057506	1.856004	3.240216
O	1.322878	2.783897	4.783874
C	0.959156	2.370390	6.074947
C	1.165014	3.526892	7.051880
C	2.610802	3.988673	7.152838
O	3.329770	2.906400	7.811617
C	4.637437	2.833511	7.575136
O	5.121780	1.792735	8.272785
C	6.535130	1.588951	8.138628
C	6.880525	0.382635	8.994356
C	8.375209	0.077844	9.081010
O	9.073735	1.209366	9.660176
C	9.113421	1.252664	10.996052
O	9.769712	2.363851	11.348135
C	9.896784	2.550235	12.759166
C	4.667403	2.058269	1.985076
C	5.950288	1.798987	1.185355
C	0.585855	5.039599	1.146981
C	-0.006111	5.624618	2.439436
N	0.055600	0.284234	2.666642
C	0.039395	-0.084275	1.381175
C	-0.771732	-1.294707	0.984344
C	-0.679781	-0.453112	3.650086
C	-0.053286	-1.516518	4.337120
C	-0.759754	-2.154160	5.361397
C	-2.048329	-1.762240	5.703268
C	-2.654959	-0.718866	5.013761
C	-1.992962	-0.048707	3.980612
C	1.366424	-1.960420	4.014976
C	2.338412	-1.548349	5.130672
C	-2.680185	1.106334	3.266469
C	-2.711574	2.360089	4.154312
C	1.461408	-3.468499	3.744766
C	-4.092482	0.747000	2.785443
C	0.730515	0.582146	0.355821
C	1.550815	1.727513	0.407143
C	2.162911	2.185890	-0.895093
C	2.787522	5.266127	7.956772
C	4.918927	1.902438	3.493466
C	0.215434	5.902432	-0.066344
O	5.295260	3.562438	6.863954
C	9.057562	-0.200260	7.752489
O	8.647546	0.436389	11.760406

H	1.849892	1.551071	-1.725057
H	0.135140	4.053272	0.994719
H	0.395795	6.626183	2.630463
H	0.235095	5.000232	3.305547
H	-1.096256	5.709691	2.363192
H	-0.873133	5.952721	-0.178458
H	0.631755	5.497257	-0.994502
H	0.579061	6.930324	0.038337
H	4.937662	6.705970	1.527400
H	2.503785	6.950617	1.183049
H	5.913860	4.466694	1.882747
H	3.941948	1.292261	1.690902
H	5.310364	0.903490	3.719162
H	6.762038	2.470257	1.485003
H	6.299740	0.774700	1.354496
H	5.791486	1.928702	0.109655
H	4.001220	2.054944	4.070430
H	5.644454	2.640726	3.850150
H	2.074841	-2.028483	6.079515
H	1.231085	-4.057040	4.639409
H	2.476527	-3.735098	3.431316
H	0.770836	-3.784063	2.956031
H	1.677076	-1.442765	3.101648
H	3.363703	-1.841361	4.878887
H	-0.288611	-2.969237	5.904765
H	-2.578632	-2.268323	6.505345
H	-0.713189	-1.474630	-0.089868
H	-0.419377	-2.188039	1.509185
H	-1.822258	-1.165463	1.262872
H	-3.662649	-0.415322	5.284988
H	-2.085705	1.348254	2.379278
H	-3.282401	2.175250	5.071154
H	-3.183964	3.196264	3.626858
H	-1.704009	2.672032	4.447676
H	-4.091770	-0.155087	2.165117
H	-4.776841	0.572928	3.622668
H	-4.509720	1.566561	2.190560
H	0.614378	0.148059	-0.629824
H	3.255683	2.170391	-0.833117
H	1.880013	3.219899	-1.114153
H	0.562816	4.377993	6.711690
H	3.030560	4.106702	6.150477
H	2.326281	-0.466645	5.295490
H	1.562709	1.512564	6.415553
H	-0.095288	2.051545	6.134000
H	0.804238	3.245960	8.050368
H	7.068869	2.484108	8.472654
H	6.775199	1.435466	7.081830
H	6.501373	0.541468	10.009154
H	6.368208	-0.504639	8.603525
H	8.507137	-0.770647	9.759298
H	8.913637	2.612632	13.232687
H	10.437866	3.488408	12.881452
H	10.455471	1.726581	13.211158
H	10.104174	-0.472450	7.912401
H	8.559591	-1.030845	7.243060
H	9.033395	0.673320	7.095169
H	3.843620	5.541862	8.012521
H	2.247528	6.087322	7.475074
H	2.396185	5.144494	8.972374