Electronic Supplementary Material (ESI) for Polymer Chemistry
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DFT Investigations on the Ring-Opening Polymerization of Cyclic Carbonates Catalyzed by Zinc-{β-diiminate} Complexes

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Cartesian coordinates of all optimized structures as they appear in the text

1 Introduction

TMC

G = -381,493855 u.a.

C	1.334655	-0.218365	-2.056752
O	1.196327	0.119536	-0.671386
C	-0.007619	0.232030	-0.068768
O	-1.126952	0.114758	-0.816503
C	-1.092272	-0.214501	-2.210643
C	0.168143	0.309700	-2.861136
O	-0.081304	0.461023	1.105747
H	-1.158866	-1.305822	-2.312738
H	-1.998986	0.223583	-2.634833
H	0.232968	-0.028638	-3.900302
H	0.170279	1.405233	-2.859256
H	1.406397	-1.310665	-2.144775
H	2.290041	0.212129	-2.366155

7CC

G = -420,760534 u.a.

O	-1.858848	0.634909	3.572028
C	-1.038023	-0.098985	3.097690
O	-0.949291	-1.416209	3.422370
C	-1.066554	-2.443491	2.416463
H	-2.080346	-2.852055	2.497807
H	-0.360707	-3.226197	2.715251
C	-0.802017	-1.986955	0.991093
H	-1.539865	-1.224432	0.715075
H	-0.985307	-2.839520	0.327330
H	1.341806	-2.256638	0.734736
C	0.611259	-1.439427	0.776576
H	0.656798	-0.919350	-0.186021
H	1.814490	0.175602	1.612054
C	1.005528	-0.495821	1.908854
H	1.326625	-1.053379	2.794026
O	-0.081260	0.368242	2.266010

3 Results and Discussion

3.1 Ring-opening polymerization of cyclic carbonates by metal dialkylamide as catalyst

(BDI)Zn($N(SiMe_3)_2$)

G = -2338,489821 u.a.

C	0.068344	-0.687799	0.103228
C	-0.078583	-0.118604	1.389561
C	1.062465	0.193193	2.173147
C	2.326381	-0.118914	1.661370
C	2.480519	-0.707283	0.412559
C	1.356766	-0.974378	-0.359248
N	-1.388917	0.102502	1.927562
C	-1.898383	1.336954	1.964590

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C	-1.252828	2.466437	1.187999
C	0.979062	0.909191	3.518016
C	1.665465	0.139787	4.655875
C	-1.119051	-0.912935	-0.820576
C	-1.129259	-2.308555	-1.452889
Zn	-2.465534	-1.429050	2.628892
N	-2.333024	-3.286247	2.253714
N	-3.824461	-0.368797	3.682502
C	-4.695639	-1.029626	4.612638
C	-6.074938	-1.199902	4.335275
C	-6.860552	-1.893126	5.264150
C	-6.322849	-2.412207	6.432578
C	-4.970260	-2.235143	6.697174
C	-4.139081	-1.548655	5.809097
C	-6.765434	-0.655652	3.089192
C	-7.432098	-1.769822	2.268051
C	-2.681476	-1.310502	6.175645
C	-2.059369	-2.442094	6.999752
C	-3.844945	0.961433	3.573018
C	-4.765273	1.809642	4.427452
C	-3.035168	1.705929	2.697022
C	-7.825935	0.402758	3.439515
C	-2.513659	0.030817	6.907337
C	1.582471	2.321328	3.424368
C	-1.168129	0.170209	-1.910921
H	-5.510978	2.302998	3.796508
H	-5.283182	1.234353	5.193755
H	-4.185118	2.600392	4.911964
H	-1.946007	2.799374	0.407637
H	-1.066813	3.325621	1.838072
H	-0.316985	2.171798	0.714798
H	-3.271569	2.764872	2.658581
H	-7.919470	-2.028112	5.060426
H	-6.953093	-2.950028	7.135435
H	-4.553245	-2.635489	7.615744
H	3.207753	0.111751	2.254262
H	3.472340	-0.942502	0.036287
H	1.480665	-1.405644	-1.348709
H	1.443023	2.861085	4.367701
H	2.659127	2.273039	3.226853
H	1.128959	2.912289	2.624751
H	1.547765	0.683467	5.599930
H	1.246729	-0.860354	4.783316
H	2.740708	0.030880	4.475885
H	-1.460321	0.210110	7.149459
H	-2.867371	0.868965	6.301722
H	-3.081304	0.030468	7.844732
H	-0.980677	-2.283016	7.098533
H	-2.467534	-2.480995	8.015619
H	-2.217365	-3.418387	6.532562
H	-8.244130	0.839216	2.525646
H	-8.655170	-0.047037	3.996476
H	-7.425232	1.214121	4.050850
H	-7.837782	-1.362059	1.335566
H	-6.729995	-2.565206	2.016830
H	-8.265286	-2.220960	2.817970
H	-2.053606	0.040223	-2.543130
H	-1.203250	1.176212	-1.483034
H	-0.284349	0.115899	-2.556848
H	-2.022238	-2.435429	-2.074836
H	-0.262041	-2.470797	-2.102188
H	-1.132417	-3.085695	-0.685305
H	-0.078312	1.011575	3.780437
H	-2.113149	-1.237256	5.239749
H	-2.028805	-0.815416	-0.219051
H	-6.005389	-0.183195	2.457598
Si	-3.727362	-4.001715	1.492646
Si	-0.973866	-4.235321	2.789415
C	-1.507284	-5.727704	3.833876
C	0.108236	-4.894859	1.379734

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C	0.172072	-3.176417	3.851023
C	-3.306976	-5.469545	0.366832
C	-4.989443	-4.649640	2.746953
C	-4.538210	-2.706980	0.365537
H	-4.230953	-5.848959	-0.086458
H	-2.632560	-5.184812	-0.446795
H	-2.848182	-6.302991	0.908664
H	-5.894737	-5.024301	2.254045
H	-4.559478	-5.479771	3.318410
H	-5.287481	-3.881712	3.467420
H	-5.476853	-3.077776	-0.061795
H	-4.768038	-1.766022	0.879612
H	-3.867854	-2.473521	-0.467820
H	-0.628085	-6.266753	4.206573
H	-2.101816	-5.415373	4.699100
H	-2.109072	-6.443357	3.263461
H	1.009538	-3.774486	4.228805
H	0.597728	-2.360616	3.257364
H	-0.341904	-2.749523	4.718470
H	0.932230	-5.492692	1.788341
H	-0.442729	-5.529648	0.679428
H	0.550566	-4.069755	0.811597

I_{TMC}

G = -2719,973884 u.a.

Zn	-3.917855	-6.580846	-2.035493
N	-2.935468	-6.029993	-0.369466
C	-1.919492	-6.783981	0.064149
C	-1.238137	-6.511393	1.388670
C	-1.405777	-7.899824	-0.615971
C	-1.948871	-8.667985	-1.653602
C	-1.170085	-9.927698	-1.971832
N	-3.075884	-8.372391	-2.310033
C	-3.483012	-7.536146	-6.509098
C	-2.890464	-8.052672	-5.195380
C	-1.431552	-8.485538	-5.414262
C	-3.701073	-9.351599	-3.145469
C	-3.696912	-9.169913	-4.550780
H	-3.565583	-12.272853	0.284991
C	-3.723880	-12.145075	-0.790608
C	-4.395368	-10.081826	-5.346536
C	-5.081805	-11.154224	-4.787391
C	-5.055630	-11.339066	-3.412137
C	-4.368970	-10.460420	-2.566083
C	-4.347978	-10.767361	-1.071740
C	-5.744442	-10.703550	-0.436071
C	-7.113563	-7.671613	-2.187642
C	-7.230076	-6.799939	-5.063438
Si	-6.795646	-6.194881	-3.320051
N	-5.151886	-5.649718	-3.146774
C	-2.186993	-10.504797	3.253662
O	-1.872000	-9.993922	2.211654
O	-1.951275	-9.874215	4.420241
C	-8.050603	-4.843419	-2.868970
C	-2.268515	-10.457713	5.692823
C	-3.455898	-11.387225	5.581642
C	-3.144632	-12.379305	4.484177
C	-5.344865	-3.761586	-5.526279
Si	-4.583467	-4.154139	-3.832620
C	-2.712799	-4.272786	-4.132305
C	-4.954130	-2.655889	-2.733501
C	-6.867204	-6.078535	1.362649
C	-1.367203	-2.366058	-1.384307
C	-5.354652	-6.281180	1.225549
C	-3.364772	-4.893712	0.391884
C	-1.302921	-3.512255	-0.363710
C	-4.833787	-7.155511	2.377620
C	-0.131289	-3.255231	0.599413
C	-2.621267	-3.686757	0.381820

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C	-4.571136	-4.980045	1.131029
C	-5.011946	-3.857498	1.836482
C	-4.292337	-2.668782	1.830001
C	-3.109053	-2.595172	1.109873
O	-2.806065	-11.701881	3.264871
H	-1.489646	-1.398510	-0.885065
H	-1.288094	-7.418959	1.998499
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H	-5.411303	-8.084722	2.442128
H	-6.199596	-9.717254	-0.548534
H	-4.377835	-12.954583	-1.134765
H	-2.759686	-12.268044	-1.291098
H	-5.679311	-10.930911	0.633909
H	-3.729418	-10.018664	-0.569665
H	-3.997188	-13.014309	4.233509
H	-2.304200	-13.026630	4.766096
H	-1.382680	-10.994543	6.056006
H	-2.454365	-9.612531	6.359408
H	-6.422322	-11.435574	-0.889796
H	-5.577665	-12.188187	-2.977883
H	-5.624932	-11.847677	-5.423843
H	-4.400405	-9.953063	-6.424407
H	-1.380265	-9.343275	-6.094926
H	-0.946339	-8.771197	-4.477910
H	-0.850705	-7.668456	-5.857107
H	-2.928927	-6.652609	-6.843392
H	-3.410527	-8.276921	-7.313591
H	-4.532670	-7.254329	-6.394451
H	-2.883215	-7.214080	-4.491545
H	-0.120636	-9.667829	-2.142453
H	-1.552264	-10.450803	-2.848210
H	-1.196162	-10.607838	-1.115336
H	-0.527873	-8.337037	-0.152460
H	-2.197021	-2.487540	-2.081504
H	-0.437594	-2.320901	-1.962531
H	-1.097382	-4.438127	-0.910828
H	0.813210	-3.210737	0.045702
H	-0.040177	-4.030190	1.363481
H	-0.254570	-2.296395	1.115360
H	-0.178147	-6.293747	1.224366
H	-1.684491	-5.682526	1.936646
H	-2.543389	-1.667011	1.109022
H	-4.652562	-1.806605	2.384644
H	-5.934683	-3.914645	2.405323
H	-5.180070	-6.839029	0.296861
H	-7.259744	-5.408257	0.592518
H	-7.382839	-7.040193	1.271478
H	-7.137367	-5.666080	2.341182
H	-4.932190	-6.626701	3.332831
H	-3.625316	-11.905944	6.530524
H	-4.361698	-10.821636	5.337474
H	-9.072483	-5.239754	-2.903836
H	-7.873339	-4.457757	-1.859333
H	-8.008693	-3.992301	-3.557221
H	-8.150907	-8.012173	-2.286318
H	-6.468541	-8.513042	-2.461830
H	-6.948053	-7.430703	-1.132774
H	-8.285506	-7.095968	-5.107749
H	-7.068795	-6.037752	-5.831481
H	-6.630338	-7.678668	-5.323212
H	-4.915477	-2.826431	-5.906248
H	-5.133083	-4.545494	-6.260463
H	-6.430401	-3.624150	-5.484280
H	-2.297993	-3.303554	-4.432092
H	-2.152157	-4.603359	-3.249737
H	-2.504843	-4.981188	-4.941057
H	-4.525422	-1.735394	-3.148356
H	-6.036510	-2.507216	-2.652509
H	-4.568382	-2.782166	-1.717058

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$TS(I_{TMC} \rightarrow II_{TMC})$

G = -2719,90313 u.a.

Zn	-3.646006	-7.291950	-0.976729
N	-2.241738	-5.961731	-0.150325
C	-0.989794	-6.387858	0.029025
C	-0.000062	-5.598641	0.869386
C	-0.439936	-7.567255	-0.496166
C	-0.980445	-8.535664	-1.346295
C	0.039156	-9.518645	-1.895493
N	-2.263928	-8.615149	-1.722518
C	-2.954142	-7.269060	-5.010952
C	-1.793924	-8.167094	-4.563416
C	-0.775533	-8.328530	-5.698816
C	-2.547936	-9.682361	-2.637247
C	-2.305249	-9.495092	-4.017513
H	-2.260456	-11.728236	1.183004
C	-1.999649	-11.511790	0.140839
C	-2.538988	-10.565295	-4.886925
C	-2.967963	-11.797799	-4.409939
C	-3.186396	-11.972174	-3.048134
C	-2.996001	-10.928022	-2.137412
C	-3.266092	-11.142659	-0.650827
C	-4.340992	-12.203372	-0.382951
C	-5.889422	-9.689821	-3.134094
C	-6.740010	-7.105986	-4.375201
Si	-6.633981	-8.021495	-2.709134
N	-5.775706	-7.094557	-1.427782
C	-5.809425	-8.063940	0.419110
O	-4.582394	-8.005101	0.680551
O	-6.372082	-9.244564	-0.017273
C	-8.448164	-8.438966	-2.303625
C	-7.036201	-9.952197	1.046169
C	-8.224275	-9.139848	1.580429
C	-8.020980	-7.690921	1.146068
C	-8.199573	-5.109341	-1.693250
Si	-6.338246	-5.390858	-1.397533
C	-5.474779	-4.390392	-2.748808
C	-6.049095	-4.527064	0.247819
C	-4.300168	-5.867937	3.350178
C	-2.424796	-2.538759	-2.844289
C	-2.904002	-5.631211	2.757870
C	-2.543423	-4.660289	0.379569
C	-1.944405	-3.663882	-1.918536
C	-1.911997	-5.376221	3.906492
C	-0.407851	-3.723312	-1.992569
C	-2.447068	-3.536537	-0.482201
C	-2.885237	-4.491312	1.743829
C	-3.182954	-3.201752	2.200603
C	-3.134543	-2.101376	1.357839
C	-2.759220	-2.273956	0.030061
O	-6.632530	-7.352693	1.223477
H	-1.910347	-1.595519	-2.627609
H	0.013887	-6.015441	1.881634
H	-0.908520	-5.128030	3.551295
H	-1.838168	-6.263536	4.544950
H	-5.245195	-12.032874	-0.974352
H	-1.522145	-12.406343	-0.276365
H	-1.266885	-10.702856	0.152282
H	-4.617254	-12.185855	0.676465
H	-3.634698	-10.192413	-0.249326
H	-8.532117	-6.980822	1.798182
H	-8.363548	-7.542452	0.119963
H	-7.339251	-10.903090	0.606448
H	-6.307575	-10.156723	1.838898
H	-3.981894	-13.216265	-0.599590
H	-3.524044	-12.939258	-2.688712
H	-3.132000	-12.622509	-5.098424
H	-2.364840	-10.437435	-5.951375
H	-1.237472	-8.712105	-6.615086

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H	0.036707	-9.009908	-5.425147
H	-0.333872	-7.357257	-5.945809
H	-2.582370	-6.310096	-5.389404
H	-3.533894	-7.747060	-5.808413
H	-3.634633	-7.062929	-4.180168
H	-1.287678	-7.646318	-3.744512
H	0.316012	-9.236907	-2.917433
H	-0.336712	-10.541012	-1.941293
H	0.946536	-9.500638	-1.289155
H	0.606580	-7.713122	-0.257583
H	-3.500232	-2.363784	-2.769734
H	-2.195632	-2.793621	-3.884189
H	-2.318255	-4.617515	-2.312326
H	-0.083958	-3.727478	-3.039549
H	-0.001571	-4.618715	-1.520834
H	0.035776	-2.846115	-1.508186
H	1.008571	-5.704072	0.463719
H	-0.240895	-4.539482	0.946038
H	-2.697592	-1.405778	-0.618184
H	-3.373501	-1.110222	1.734065
H	-3.455154	-3.063180	3.243739
H	-2.609775	-6.549224	2.240723
H	-5.021501	-6.153509	2.585203
H	-4.257472	-6.676633	4.088922
H	-4.669064	-4.971874	3.862994
H	-2.245839	-4.546883	4.540421
H	-9.176882	-9.506005	1.183824
H	-8.267299	-9.215621	2.671457
H	-8.895571	-8.832717	-3.225067
H	-8.520753	-9.227153	-1.549511
H	-9.063688	-7.593632	-1.989405
H	-6.630158	-10.233172	-3.733963
H	-4.974789	-9.626820	-3.725633
H	-5.685485	-10.279451	-2.240792
H	-7.153702	-7.816258	-5.102055
H	-7.401312	-6.235394	-4.362898
H	-5.767087	-6.786645	-4.755852
H	-8.347877	-4.022740	-1.646608
H	-8.574515	-5.446274	-2.662391
H	-8.830218	-5.544874	-0.911782
H	-5.666242	-3.323509	-2.586419
H	-4.392798	-4.538714	-2.733072
H	-5.829710	-4.642603	-3.750552
H	-6.089285	-3.443983	0.085103
H	-6.820811	-4.788767	0.975882
H	-5.082706	-4.748626	0.696961

II_{TMC}

G = -2719,964772 u.a.

C	-3.315941	-3.611419	2.338289
C	-2.796836	-4.828241	1.884065
C	-2.288196	-4.891554	0.569125
C	-2.291300	-3.750681	-0.267380
C	-2.827192	-2.561695	0.234052
C	-3.337007	-2.485984	1.525275
C	-2.789992	-6.028244	2.819665
C	-4.214016	-6.417454	3.239876
N	-1.779490	-6.132987	0.058498
Zn	-2.970115	-7.420818	-0.842670
O	-5.787050	-7.537710	0.308739
C	-6.785343	-8.314570	0.959718
C	-6.436807	-9.804601	0.839600
C	-5.499293	-9.945938	-0.361543
O	-5.887150	-9.087191	-1.416367
C	-5.803991	-7.683059	-1.120215
N	-6.996289	-7.113300	-1.720638
Si	-7.967588	-8.175939	-2.776424
C	-9.380058	-7.174970	-3.554067
C	-1.754823	-3.795653	-1.692072

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C	-0.868824	-2.591025	-2.036263
C	-1.907933	-5.787449	4.053832
C	-0.458737	-6.344139	0.097805
C	0.434230	-5.312175	0.747549
C	0.189044	-7.455272	-0.462728
C	-0.334649	-8.570738	-1.137911
N	-1.638130	-8.830340	-1.277276
C	-2.046361	-10.050284	-1.912132
C	-2.250830	-10.081288	-3.308089
C	-2.707060	-11.270683	-3.885639
C	-2.933079	-12.405585	-3.118133
C	-2.706398	-12.366564	-1.746313
C	-2.269405	-11.199067	-1.113177
C	-1.981154	-8.874653	-4.195988
C	-1.026085	-9.212695	-5.350272
C	-2.024465	-11.193321	0.393674
C	-0.580361	-11.587290	0.748587
C	-2.987373	-12.097965	1.173994
C	0.692486	-9.472343	-1.788824
O	-4.660879	-7.129997	-1.578452
C	-3.284608	-8.264232	-4.728885
Si	-7.208866	-5.344272	-1.630646
C	-6.729634	-4.517756	-3.262078
C	-6.193624	-4.578726	-0.244345
C	-9.002997	-4.893193	-1.211444
C	-2.902502	-3.931381	-2.702976
C	-8.870847	-9.581238	-1.881940
C	-7.001298	-8.870088	-4.241574
H	-0.769847	-8.305028	-5.907299
H	-2.773035	-13.159238	1.006309
H	0.062779	-5.036529	1.737578
H	-0.065472	-2.451962	-1.305100
H	-0.409850	-2.731469	-3.020742
H	-0.453057	-11.622072	1.836328
H	-3.565237	-3.060294	-2.658328
H	-0.875810	-5.547759	3.779366
H	-1.886675	-6.679986	4.689090
H	-4.032408	-11.922683	0.907087
H	-0.343263	-12.580327	0.350414
H	0.151940	-10.880807	0.354323
H	-2.876568	-11.917671	2.248365
H	-2.174485	-10.163758	0.741871
H	-6.811231	-7.974537	1.998142
H	-7.758176	-8.097377	0.503380
H	-5.501550	-10.954993	-0.780502
H	-4.465652	-9.725643	-0.059956
H	-2.880251	-13.260562	-1.155029
H	-3.282769	-13.321526	-3.586660
H	-2.882100	-11.306566	-4.957549
H	-1.482019	-9.911259	-6.060167
H	-0.096316	-9.666539	-4.992223
H	-3.068783	-7.384001	-5.345535
H	-3.826250	-8.983193	-5.353183
H	-3.946214	-7.959948	-3.913380
H	-1.489827	-8.113179	-3.580898
H	1.629382	-9.464602	-1.227565
H	0.908872	-9.089618	-2.793507
H	0.345761	-10.499386	-1.901206
H	1.270399	-7.434044	-0.395979
H	-3.511233	-4.817849	-2.502316
H	-2.511837	-4.005604	-3.724314
H	-1.132130	-4.691131	-1.787557
H	-1.442417	-1.659078	-2.079203
H	1.454859	-5.685504	0.842416
H	0.456803	-4.390736	0.156833
H	-2.846454	-1.678634	-0.398445
H	-3.748568	-1.551149	1.895943
H	-3.711287	-3.548332	3.348933
H	-2.363361	-6.873448	2.269199
H	-4.840917	-6.598029	2.363278

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H	-4.196381	-7.325940	3.852971
H	-4.682087	-5.626837	3.837027
H	-2.289271	-4.958839	4.660773
H	-7.345108	-10.399120	0.699039
H	-5.935856	-10.177037	1.740918
H	-9.655630	-9.978430	-2.537137
H	-8.205367	-10.405674	-1.617162
H	-9.362707	-9.226385	-0.969444
H	-6.579954	-8.059488	-4.845687
H	-6.181997	-9.513469	-3.916161
H	-7.669994	-9.452263	-4.887341
H	-9.826714	-7.816964	-4.323572
H	-10.171860	-6.929816	-2.841016
H	-9.068285	-6.252552	-4.051088
H	-9.014792	-3.872909	-0.809317
H	-9.682436	-4.915963	-2.065930
H	-9.408794	-5.552946	-0.436771
H	-5.695423	-4.766184	-3.516825
H	-7.361724	-4.837522	-4.096008
H	-6.809850	-3.427084	-3.184543
H	-6.309385	-3.489199	-0.291308
H	-6.545161	-4.912537	0.735427
H	-5.131050	-4.812296	-0.315412

TS(II_{TMC}→III_{TMC})

G = -2719,949423 u.a.

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C	-2.286781	-3.866589	-0.438813
C	-2.849793	-2.592850	-0.312944
C	-3.821935	-2.319567	0.640235
C	-4.118268	-5.656311	2.457229
C	-5.635400	-5.726741	2.661547
N	-2.233153	-6.227426	0.254922
Zn	-3.270108	-7.671505	-0.695723
O	-5.087792	-7.907094	0.208157
C	-5.578854	-8.822599	1.156022
C	-5.378041	-10.275554	0.695836
C	-5.356023	-10.328128	-0.834167
O	-6.252074	-9.370344	-1.383613
C	-5.816083	-8.049458	-1.423601
N	-6.963828	-7.256820	-1.538502
Si	-8.558920	-8.113556	-1.506766
C	-9.965239	-6.843777	-1.413261
C	-1.191304	-4.072946	-1.479438
C	0.017403	-3.162531	-1.206012
C	-3.412363	-5.388394	3.797004
C	-0.990070	-6.496931	0.662680
C	-0.257077	-5.550699	1.593969
C	-0.233323	-7.610635	0.265799
C	-0.503278	-8.601259	-0.694852
N	-1.718289	-8.893373	-1.164874
C	-1.830171	-9.942293	-2.138531
C	-1.839484	-9.631921	-3.516760
C	-1.926581	-10.680478	-4.438857
C	-1.993819	-12.003973	-4.027738
C	-1.997640	-12.297921	-2.669054
C	-1.930038	-11.289532	-1.702807
C	-1.731075	-8.208101	-4.041983
C	-0.432802	-7.997837	-4.836373
C	-1.969344	-11.668873	-0.224330
C	-0.586926	-12.018792	0.352295
C	-2.922973	-12.839358	0.059027
C	0.730696	-9.281298	-1.254748
O	-4.732962	-7.757277	-2.068687
C	-2.951944	-7.822790	-4.889285
Si	-6.878970	-5.580382	-2.193265
C	-7.718693	-5.529799	-3.889447

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C	-5.146821	-4.931308	-2.479913
C	-7.681828	-4.369451	-0.988233
C	-1.693930	-3.850884	-2.912791
C	-8.928364	-9.188269	0.002547
C	-8.807335	-9.106024	-3.092594
H	-0.343236	-6.952810	-5.152556
H	-2.502859	-13.791752	-0.282560
H	-0.860396	-4.692559	1.887024
H	0.393218	-3.274885	-0.185255
H	0.834328	-3.394892	-1.898176
H	-0.688287	-12.371737	1.384817
H	-2.047903	-2.823922	-3.056850
H	-2.323697	-5.385863	3.691664
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H	-3.893943	-12.713540	-0.426774
H	-0.115055	-12.818930	-0.229381
H	0.089816	-11.163558	0.364704
H	-3.089579	-12.935651	1.137167
H	-2.334144	-10.789043	0.319195
H	-5.085745	-8.646839	2.121166
H	-6.646641	-8.624442	1.307211
H	-5.689153	-11.295959	-1.216989
H	-4.353602	-10.150570	-1.234129
H	-2.061316	-13.334554	-2.351684
H	-2.049542	-12.804383	-4.760569
H	-1.932005	-10.450882	-5.501298
H	-0.414778	-8.618298	-5.739309
H	0.453752	-8.250682	-4.246761
H	-2.867041	-6.782120	-5.222531
H	-3.027485	-8.447376	-5.786550
H	-3.872892	-7.928798	-4.311135
H	-1.701069	-7.535109	-3.178798
H	1.512466	-9.348089	-0.494349
H	1.125340	-8.661165	-2.067978
H	0.539425	-10.272158	-1.663992
H	0.783155	-7.614164	0.645420
H	-2.518593	-4.522947	-3.158366
H	-0.882943	-4.023494	-3.629274
H	-0.847379	-5.108927	-1.412091
H	-0.240368	-2.106921	-1.345963
H	0.037660	-6.099606	2.494641
H	0.662493	-5.185946	1.127406
H	-2.514572	-1.799012	-0.975780
H	-4.247620	-1.322942	0.719844
H	-4.969475	-3.103896	2.269688
H	-3.787964	-6.632418	2.090174
H	-6.144608	-5.949490	1.721343
H	-5.881718	-6.517904	3.378354
H	-6.039073	-4.792826	3.067767
H	-3.708510	-4.416050	4.206976
H	-6.180130	-10.905070	1.098524
H	-4.435720	-10.679724	1.079841
H	-9.971812	-9.518479	-0.076049
H	-8.299084	-10.076239	0.073318
H	-8.845093	-8.619666	0.934441
H	-8.780628	-8.454866	-3.972176
H	-8.031590	-9.865670	-3.212245
H	-9.782859	-9.606084	-3.079449
H	-10.896975	-7.409731	-1.539300
H	-10.012216	-6.371776	-0.426641
H	-9.965762	-6.055251	-2.168112
H	-7.650891	-3.363826	-1.424584
H	-8.719581	-4.589463	-0.734143
H	-7.101347	-4.337891	-0.060360
H	-7.156092	-6.151799	-4.594472
H	-8.757426	-5.867777	-3.904635
H	-7.700431	-4.502270	-4.271941
H	-5.232788	-3.894074	-2.826876
H	-4.551013	-4.920798	-1.565332
H	-4.621640	-5.516438	-3.235794

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III_{TMC}

G = -2720,013522 u.a.

C	-3.631400	-0.051232	-0.157771
C	-4.600028	-0.068277	1.000966
N	-4.450022	0.822375	1.981830
N	-6.856173	-0.627961	3.006748
C	-5.617231	-1.042559	0.963355
C	-6.650839	-1.311208	1.876262
C	-7.579779	-2.453863	1.541291
H	-7.555947	-3.214470	2.327993
C	-6.517697	-4.094072	5.299786
C	-6.372666	-2.575346	5.132896
C	-7.711917	-1.878678	4.941273
C	-7.936205	-0.968550	3.884174
C	-9.184140	-0.323059	3.734097
C	-9.475543	2.109714	3.140481
C	-5.605307	-1.970078	6.317996
C	-8.750044	-2.113871	5.847508
C	-9.979111	-1.477823	5.719639
H	-8.589935	-2.804144	6.671714
C	-10.188917	-0.593370	4.668222
C	-10.735701	0.350473	1.837313
H	-2.770054	-0.511948	3.052119
C	-4.922656	3.411786	0.715020
C	-0.641948	-0.552000	2.920704
C	-4.794035	4.027614	-0.683774
C	-3.583012	3.028210	1.325099
C	-1.142273	2.430593	2.568163
C	-2.536868	3.955160	1.342454
H	-2.680523	4.926741	0.877380
H	-0.198050	2.212232	3.059838
C	-1.322420	3.663048	1.951922
C	-2.156040	1.468133	2.577334
C	-2.004111	0.386108	4.835742
C	-5.683948	4.353932	1.661979
Zn	-5.693981	0.860500	3.495719
O	-5.608338	2.100108	4.825084
C	-6.434776	2.155452	5.960678
H	-7.464878	1.820911	5.754550
H	-6.053162	1.499663	6.762536
C	-6.490768	3.590369	6.481246
H	-7.188431	3.673222	7.322700
H	-6.875654	4.232405	5.678286
C	-5.136904	4.140144	6.897371
H	-5.187672	5.218033	7.066787
H	-4.388213	3.911349	6.136419
O	-4.644446	3.513630	8.103137
O	-5.849694	4.994184	9.314801
C	-5.053576	4.066662	9.268219
N	-4.480870	3.467517	10.371927
Si	-5.313375	4.013752	11.886118
Si	-3.056434	2.392673	10.113556
C	-4.800902	2.951709	13.361122
C	-3.604441	0.744232	9.389340
C	-2.166458	2.048678	11.741033
C	-4.853932	5.799531	12.260540
C	-7.173782	3.764105	11.723957
C	-1.780844	3.250927	9.021581
C	-9.448170	0.668248	2.609665
C	-3.377724	1.772733	1.938215
C	-1.943950	0.156002	3.317098
H	-0.574780	-1.526691	3.416059
H	-5.515976	2.496922	0.613979
H	-9.639176	2.820046	2.322438
H	-10.838428	1.022952	0.978918
H	-6.158075	-2.107358	7.253904
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H	-2.601054	-0.155838	0.195145

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H	-3.846031	-0.853836	-0.864614
H	0.242094	0.023266	3.215884
H	-0.583567	-0.718285	1.840049
H	-5.595904	-1.690064	0.095326
H	-4.241559	3.373840	-1.366685
H	-5.786698	4.202377	-1.112567
H	-4.278137	4.993657	-0.659761
H	-0.522006	4.397946	1.955052
H	-6.680910	4.579551	1.266395
H	-5.146543	5.301981	1.778096
H	-5.795388	3.914013	2.658234
H	-8.616507	0.596411	1.901162
H	-1.182331	1.032594	5.163817
H	-2.940951	0.870398	5.129605
H	-1.919744	-0.563670	5.375959
H	-7.306480	-2.920849	0.594204
H	-8.615598	-2.106678	1.476529
H	-11.151944	-0.098992	4.571414
H	-10.771606	-1.671255	6.437365
H	-5.444490	-0.895552	6.186178
H	-5.775578	-2.401582	4.231792
H	-4.626277	-2.448418	6.432288
H	-5.530593	-4.567214	5.338411
H	-7.074684	-4.541786	4.470368
H	-7.039326	-4.354545	6.227028
H	-10.740508	-0.678431	1.463305
H	-11.627163	0.480018	2.460245
H	-10.283038	2.244533	3.868729
H	-8.535758	2.374525	3.635221
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H	-5.142513	6.449122	11.430908
H	-5.459649	3.234364	14.191628
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H	-3.773397	3.110329	13.694595
H	-7.658485	3.987281	12.681690
H	-7.603932	4.407026	10.955041
H	-7.405412	2.722580	11.474334
H	-1.239594	1.519674	11.487164
H	-1.879494	2.963622	12.268447
H	-2.725618	1.412703	12.430469
H	-2.746417	0.075683	9.254824
H	-4.316790	0.243530	10.053941
H	-4.084855	0.885167	8.418117
H	-0.849996	2.671803	9.020265
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H	-1.546167	4.248213	9.409741

I_{7CC}

G = -2759,239195 u.a.

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C	4.908480	1.761537	1.053489
C	5.653548	2.956921	0.958972
C	7.045058	2.871166	0.834127
C	7.693829	1.645265	0.790493
C	4.783787	-0.811360	1.108541
C	4.359141	-1.329592	-0.276345
N	3.484404	1.791188	1.212750
C	2.709405	1.713145	0.122038
C	3.316736	1.947635	-1.244482
C	5.003240	4.332158	0.971981
C	5.408481	5.127265	2.220442
Zn	2.626646	1.990194	3.000178
N	3.316593	2.758386	4.594668
Si	2.507644	4.196452	5.149084
C	1.113825	3.825353	6.377274
N	0.777567	1.340289	2.505953
C	0.478293	1.145513	1.223207

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C	1.336722	1.442449	0.144056
O	-0.729780	-3.583267	7.203337
C	-0.971011	-3.573065	8.381374
O	-1.686319	-2.578919	8.956088
C	-2.798012	-2.809785	9.850258
C	-2.992738	-4.246931	10.302292
C	-1.850910	-4.760857	11.182924
C	-0.507831	-4.322657	10.614852
O	-0.464182	-4.520203	9.194761
C	-0.168501	0.999357	3.533760
C	0.054408	-0.175683	4.294594
C	-0.831205	-0.491459	5.328601
C	-1.914378	0.328611	5.620442
C	-2.132430	1.471114	4.864180
C	-1.282214	1.830679	3.811458
C	1.182274	-1.141811	3.962014
C	0.706490	-2.201131	2.954266
C	-1.634097	3.077716	3.007562
C	-2.987858	2.926725	2.291285
C	-0.853630	0.558615	0.803806
C	-1.676708	4.341122	3.879492
C	1.788059	-1.821882	5.194754
C	5.546239	-1.922204	1.843005
C	5.328038	5.132789	-0.298432
Si	4.582894	1.977054	5.498450
C	4.099023	1.698320	7.312481
C	4.976796	0.296738	4.734459
C	6.222915	2.928593	5.497066
C	3.663111	5.419734	6.025928
C	1.819858	5.118718	3.639901
H	0.873739	1.349976	-0.832452
H	2.667254	1.568121	-2.035377
H	3.440732	3.025453	-1.399522
H	4.304583	1.495362	-1.345118
H	-1.434241	0.184403	1.646186
H	-1.446472	1.314491	0.279018
H	-0.684370	-0.260522	0.099040
H	7.627265	3.786433	0.763009
H	8.774799	1.600167	0.688823
H	7.463745	-0.482976	0.849643
H	-0.685098	-1.398062	5.907378
H	-2.588679	0.068062	6.431552
H	-2.988198	2.103373	5.086976
H	1.524371	-2.882447	2.693960
H	-0.105362	-2.797533	3.384527
H	0.338743	-1.746677	2.030143
H	2.676972	-2.392722	4.905318
H	2.086911	-1.089065	5.950391
H	1.091778	-2.524542	5.662189
H	3.851351	-2.295777	-0.179629
H	3.673040	-0.648068	-0.782807
H	5.234663	-1.473736	-0.919904
H	6.386467	-2.300085	1.249666
H	5.933912	-1.586389	2.807893
H	4.878011	-2.770899	2.022749
H	4.773637	6.077680	-0.305729
H	6.394235	5.378524	-0.353711
H	5.072157	4.581688	-1.208554
H	4.928154	6.112488	2.222298
H	5.116639	4.597937	3.130919
H	6.491797	5.289378	2.252061
H	-3.174403	3.789334	1.641702
H	-3.041070	2.022644	1.680761
H	-3.807686	2.879672	3.016540
H	-1.862235	5.224534	3.258281
H	-2.484364	4.283587	4.617533
H	-0.742650	4.494495	4.420053
H	1.979862	-0.568337	3.472033
H	3.868107	-0.604081	1.674801
H	-0.859556	3.221648	2.246471

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H	3.918332	4.185171	1.008140
H	-0.306653	-3.269652	10.837297
H	0.317284	-4.919527	11.009580
H	-1.899218	-5.852507	11.251115
H	-1.941340	-4.369693	12.203645
H	-3.105722	-4.889184	9.421143
H	-3.945293	-4.300632	10.841230
H	-3.686022	-2.460191	9.313455
H	-2.638995	-2.146665	10.708158
H	4.889292	1.153063	7.842240
H	3.940030	2.641288	7.847239
H	3.175723	1.114547	7.391557
H	6.975204	2.382121	6.079154
H	6.609192	3.039039	4.478291
H	6.131636	3.928283	5.931558
H	5.750397	-0.215411	5.318749
H	4.106893	-0.365541	4.691878
H	5.368706	0.426756	3.720319
H	1.214108	5.982909	3.935328
H	2.645364	5.490856	3.024342
H	1.190024	4.487347	3.001817
H	3.095448	6.313883	6.311342
H	4.095893	5.005687	6.942658
H	4.486213	5.740943	5.379982
H	0.539713	4.726712	6.624249
H	0.418657	3.070899	5.996377
H	1.531774	3.436500	7.312425

$TS(I_{7CC} \rightarrow II_{7CC})$

G = -2759,167244 u.a.

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C	4.723907	3.215853	2.210156
C	6.020057	3.739826	2.231199
C	7.133577	2.928803	2.046383
C	5.594077	-0.504422	1.504832
C	6.085518	-0.829583	0.082429
N	3.213891	1.289430	2.003149
C	2.655977	1.201795	0.783105
C	3.469922	1.430245	-0.482770
C	3.535263	4.170112	2.274490
C	3.789845	5.431928	3.107207
Zn	2.103192	0.842740	3.721181
N	2.960151	1.151330	5.681346
Si	2.839854	2.763207	6.422614
C	2.383574	2.787217	8.266557
N	0.252117	0.666757	2.668483
C	0.221757	0.665234	1.338548
C	1.326131	0.891404	0.503588
O	1.326761	-0.649918	4.989406
C	1.422097	-0.167368	6.142048
O	0.573122	0.806848	6.611907
C	-0.768950	0.377593	6.954208
C	-0.853127	-0.996698	7.598408
C	0.081559	-1.196119	8.791536
C	1.512898	-0.750989	8.474761
O	1.857074	-1.019445	7.108767
C	-0.990899	0.359674	3.319714
C	-1.394576	-0.988470	3.498073
C	-2.644151	-1.237680	4.077386
C	-3.496477	-0.206343	4.451918
C	-3.093507	1.110824	4.265633
C	-1.844020	1.419720	3.715538
C	-0.580888	-2.183889	3.011397
C	-1.311431	-2.928721	1.879714
C	-1.457538	2.879403	3.515696
C	-1.934451	3.425015	2.160130
C	-1.053114	0.402157	0.550394

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C	-1.970338	3.794954	4.635204
C	-0.251230	-3.182424	4.129807
C	6.411095	-1.352400	2.490636
C	3.079306	4.601285	0.869235
Si	4.457686	0.237226	6.020846
C	4.860986	0.098217	7.872463
C	4.319064	-1.522633	5.344342
C	6.037513	1.022639	5.335393
C	4.467332	3.740318	6.368223
C	1.508832	3.789085	5.570895
H	1.093567	0.848054	-0.555340
H	3.682446	0.460918	-0.944419
H	2.882678	2.001549	-1.205592
H	4.414071	1.944492	-0.316075
H	-1.950562	0.350300	1.163033
H	-1.185109	1.185623	-0.201598
H	-0.949033	-0.540161	0.003802
H	6.160633	4.806387	2.376188
H	8.132141	3.356883	2.062599
H	7.825764	0.941816	1.656720
H	-2.964490	-2.267463	4.214176
H	-4.470151	-0.426896	4.881547
H	-3.761533	1.916508	4.555228
H	-0.666486	-3.710543	1.463493
H	-2.218338	-3.417441	2.253848
H	-1.610974	-2.266526	1.064578
H	0.315278	-4.026300	3.719413
H	0.354644	-2.712060	4.904680
H	-1.161496	-3.594110	4.581568
H	5.930040	-1.891647	-0.137363
H	5.579744	-0.246247	-0.688306
H	7.159037	-0.630031	-0.009362
H	7.484779	-1.169664	2.370344
H	6.150513	-1.140795	3.525918
H	6.239054	-2.418473	2.305493
H	2.267156	5.333049	0.945861
H	3.905192	5.071418	0.323329
H	2.711402	3.763230	0.276921
H	2.849861	5.975359	3.248710
H	4.200725	5.207892	4.092966
H	4.477481	6.117640	2.599337
H	-1.680290	4.486968	2.066804
H	-1.473376	2.899196	1.322411
H	-3.022145	3.330035	2.063822
H	-1.494473	4.777894	4.561358
H	-3.051977	3.956384	4.564772
H	-1.756124	3.391097	5.628974
H	0.366436	-1.803620	2.618611
H	4.542473	-0.801474	1.585438
H	-0.363643	2.924040	3.518035
H	2.701543	3.621678	2.726882
H	1.654473	0.309434	8.684601
H	2.236450	-1.320266	9.062814
H	0.068717	-2.253900	9.076517
H	-0.269496	-0.628923	9.662745
H	-0.640787	-1.756443	6.840240
H	-1.894866	-1.153823	7.901790
H	-1.384840	0.404419	6.054228
H	-1.118177	1.154327	7.642447
H	5.774677	-0.502632	7.963782
H	5.079682	1.073496	8.319743
H	4.091102	-0.388928	8.471548
H	6.825791	0.260307	5.308145
H	5.933650	1.426935	4.328345
H	6.395200	1.826292	5.984536
H	5.279765	-2.035752	5.470887
H	3.555286	-2.085600	5.882344
H	4.061224	-1.559052	4.281616
H	1.445644	4.781477	6.032236
H	1.688904	3.938407	4.502512

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H	0.540699	3.299730	5.691862
H	4.251589	4.794736	6.580518
H	5.165779	3.395672	7.138120
H	4.981255	3.683273	5.405857
H	2.495559	3.816637	8.629500
H	1.347041	2.486730	8.437210
H	3.037473	2.159174	8.878884

II_{7CC}

G = -2759,234211 u.a.

C	-3.388559	-0.266063	4.394753
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C	-1.165494	0.336043	2.815553
C	-1.461276	-1.013243	3.115749
C	-2.575434	-1.286856	3.915617
C	-1.704219	2.842610	2.959672
C	-2.923008	3.568215	2.372993
N	0.011941	0.647876	2.058051
C	-0.086239	0.686668	0.721316
C	-1.432338	0.434765	0.081911
C	-0.601485	-2.161249	2.604229
C	-1.430050	-3.245962	1.901968
C	-1.175862	3.581128	4.197900
C	0.241252	-2.774156	3.732456
Zn	1.718954	1.066811	2.952963
O	2.345536	1.701779	4.579732
C	2.263701	1.149798	5.815757
O	0.991418	1.408918	6.433100
C	-0.045259	0.467392	6.212625
C	-0.024231	-0.679514	7.238887
C	1.375568	-0.907263	7.805689
C	2.453941	-1.127482	6.753239
O	2.409331	-0.255280	5.625116
N	2.864865	1.198743	1.336801
C	2.339078	1.160478	0.112721
C	3.238183	1.347456	-1.086773
C	4.282430	1.356018	1.481506
C	4.818506	2.643098	1.703659
C	6.194820	2.758236	1.921515
C	7.024631	1.643749	1.905140
C	6.485140	0.386893	1.656578
C	5.115127	0.214287	1.437762
C	3.950416	3.893254	1.692488
C	3.842420	4.520917	3.089190
C	4.561985	-1.179530	1.166443
C	4.479257	-2.015635	2.451804
C	4.443924	4.925715	0.668244
C	0.975535	0.944920	-0.155787
C	5.361005	-1.929371	0.091205
N	3.218615	1.734241	6.750102
Si	2.573256	3.016890	7.819953
C	1.644319	2.394199	9.348807
C	4.005215	4.041727	8.532457
C	1.513018	4.300071	6.927178
Si	4.963764	1.408303	6.616788
C	5.615525	0.749650	8.272238
C	5.999039	2.919620	6.137060
C	5.364247	0.112974	5.313113
H	8.091444	1.754837	2.079120
H	-1.932188	3.599642	4.991240
H	-0.279056	3.104350	4.603398
H	7.140504	-0.479578	1.636549
H	3.940623	0.513090	-1.178322
H	0.709321	0.954053	-1.205459
H	2.655604	1.410578	-2.006955
H	3.842146	2.253208	-0.985204
H	-3.322659	3.052246	1.493806
H	-0.914884	2.866208	2.201266

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H	-3.734894	3.655912	3.102996
H	-2.646992	4.584272	2.071464
H	4.517741	4.501382	-0.338495
H	3.755140	5.776526	0.625546
H	5.431426	5.317926	0.934543
H	2.942244	3.591674	1.389843
H	6.622749	3.740441	2.104772
H	-0.927682	4.619279	3.950754
H	3.460845	3.798715	3.816907
H	4.820360	4.875579	3.434549
H	3.168017	5.384809	3.068562
H	6.371424	-2.177606	0.433041
H	5.458867	-1.343464	-0.828557
H	4.863700	-2.872518	-0.159780
H	3.540283	-1.065057	0.790311
H	3.856903	-1.532997	3.210515
H	5.473186	-2.160508	2.888868
H	4.056982	-3.004356	2.238477
H	0.886986	-2.027183	4.204203
H	0.877904	-3.577300	3.344875
H	-0.400117	-3.203210	4.510756
H	0.094235	-1.750256	1.865823
H	-2.812530	-2.318362	4.162913
H	-4.250358	-0.499383	5.014149
H	-2.097198	-3.763708	2.599349
H	-0.769531	-4.001289	1.462707
H	-2.048603	-2.831650	1.099297
H	-1.372149	0.526948	-1.003182
H	-1.799996	-0.566024	0.327290
H	-2.181198	1.140003	0.454044
H	-3.741143	1.848104	4.440235
H	0.019601	0.069003	5.196914
H	2.358645	-2.125347	6.310023
H	3.440839	-1.072267	7.230605
H	-0.980558	1.029673	6.275757
H	-0.409293	-1.590198	6.763428
H	1.375826	-1.780147	8.471244
H	-0.701499	-0.454812	8.071724
H	1.652311	-0.046343	8.416229
H	6.972654	2.572613	5.771189
H	6.183013	3.607614	6.964896
H	5.523641	3.476229	5.324853
H	4.990806	0.417358	4.333278
H	4.965976	-0.877994	5.537363
H	6.455751	0.033270	5.244388
H	4.807843	3.476264	9.012087
H	6.705395	0.638329	8.220083
H	4.450822	4.697110	7.779130
H	3.566539	4.688709	9.302404
H	5.196149	-0.235398	8.503636
H	5.393236	1.404971	9.119253
H	1.927930	4.529862	5.941150
H	0.487902	3.953423	6.787174
H	0.704863	1.900550	9.089951
H	2.249668	1.700328	9.942514
H	1.408520	3.250647	9.992362
H	1.491678	5.228968	7.509724

TS(II_{7CC}→III_{7CC})

G = -2759,217103 u.a.

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C	-1.180047	0.254589	2.998794
C	-1.475687	-1.072510	3.400607
C	-2.649497	-1.300093	4.125612
C	-1.769468	2.761949	2.907348
C	-2.978261	3.406463	2.211496
N	0.028780	0.503500	2.272197

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C	-0.062867	0.572038	0.939383
C	-1.417661	0.472252	0.266647
C	-0.555864	-2.233829	3.039597
C	-0.839886	-2.786432	1.632478
C	-1.322766	3.624258	4.098244
C	-0.599350	-3.390212	4.045951
Zn	1.792895	0.899093	3.209486
O	2.043477	2.325773	4.586805
C	2.175700	1.765873	5.740771
O	1.068652	1.659758	6.569973
C	-0.063074	0.891820	6.195006
C	-0.034659	-0.457415	6.913909
C	1.379991	-1.029155	7.033952
C	2.158819	-1.127222	5.724732
O	2.311792	0.105268	5.045936
N	2.920039	1.026699	1.545900
C	2.377855	0.971184	0.327698
C	3.261840	1.105988	-0.893116
C	4.333281	1.243510	1.636501
C	4.822735	2.557661	1.821832
C	6.202669	2.735651	1.966845
C	7.081541	1.660453	1.913589
C	6.588114	0.379437	1.694709
C	5.218280	0.143416	1.546803
C	3.911208	3.778395	1.795625
C	3.998698	4.615367	3.077578
C	4.722415	-1.276328	1.299245
C	4.744844	-2.117510	2.583353
C	4.203076	4.656449	0.567369
C	1.013767	0.775373	0.064556
C	5.505766	-1.985264	0.185208
N	3.240669	2.119857	6.607839
Si	2.685956	3.089554	8.030521
C	2.119222	2.037067	9.493510
C	4.113333	4.160683	8.671284
C	1.369790	4.354848	7.544624
Si	4.964176	1.684784	6.460755
C	5.499456	0.868493	8.085642
C	6.081915	3.161464	6.091375
C	5.321852	0.422037	5.129165
H	8.149869	1.821760	2.030027
H	-2.087565	3.633131	4.883594
H	-0.384550	3.265818	4.529029
H	7.281004	-0.455821	1.639080
H	3.849983	0.193867	-1.039732
H	0.747608	0.787178	-0.985338
H	2.661589	1.268313	-1.789689
H	3.976049	1.925052	-0.789278
H	-3.360191	2.790079	1.391388
H	-0.941936	2.748227	2.191096
H	-3.805733	3.572749	2.909914
H	-2.700456	4.383504	1.802005
H	4.105309	4.101876	-0.370986
H	3.507197	5.501912	0.529763
H	5.219205	5.064873	0.605457
H	2.880816	3.420076	1.711616
H	6.594447	3.739385	2.111811
H	-1.166653	4.660074	3.776168
H	3.704950	4.025504	3.948504
H	5.009651	5.009720	3.232653
H	3.321756	5.474563	3.009652
H	6.539152	-2.192941	0.482948
H	5.541723	-1.389905	-0.732875
H	5.038302	-2.947006	-0.052240
H	3.678414	-1.212402	0.976724
H	4.125004	-1.667772	3.362797
H	5.763190	-2.204139	2.978073
H	4.371789	-3.129188	2.386194
H	-0.470237	-3.050523	5.077613
H	0.200316	-4.104267	3.823367

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H	-1.543639	-3.943106	3.989353
H	0.467235	-1.837189	3.027424
H	-2.897591	-2.309708	4.438346
H	-4.411824	-0.455886	5.028254
H	-1.881347	-3.117761	1.549764
H	-0.196337	-3.649415	1.428053
H	-0.653052	-2.045952	0.852698
H	-1.305835	0.187400	-0.781201
H	-2.082030	-0.238255	0.760034
H	-1.913907	1.448312	0.294613
H	-3.874580	1.849620	4.328144
H	-0.086749	0.763934	5.114355
H	1.650974	-1.827354	5.046368
H	3.147340	-1.562928	5.944032
H	-0.948976	1.470379	6.472948
H	-0.698728	-1.143017	6.374560
H	1.332732	-2.035272	7.470800
H	-0.451754	-0.350479	7.923047
H	1.950500	-0.413405	7.735947
H	7.115310	2.802405	6.012430
H	6.062015	3.947645	6.848044
H	5.816337	3.606094	5.128287
H	4.984359	0.743196	4.143960
H	4.877197	-0.549530	5.348701
H	6.409586	0.293473	5.078574
H	5.026840	3.633083	8.952765
H	6.562986	0.607756	8.026085
H	4.376266	4.946190	7.956094
H	3.738764	4.660820	9.573470
H	4.941615	-0.062452	8.235772
H	5.363356	1.483400	8.978697
H	1.529295	4.698141	6.517493
H	0.358123	3.948875	7.606056
H	1.209091	1.480747	9.257906
H	2.889138	1.319799	9.796349
H	1.911299	2.680478	10.356783
H	1.435401	5.227791	8.204191

III_{7CC}

G = -2759,284972 u.a.

C	-4.171830	-0.927812	2.933966
C	-3.830940	0.375543	2.591965
C	-2.625991	0.665253	1.944712
C	-1.747908	-0.401367	1.648971
C	-2.088482	-1.733445	1.975465
C	-3.305907	-1.969064	2.620899
C	-2.280574	2.107124	1.601034
C	-3.405735	2.812937	0.832219
N	-0.459641	-0.116793	1.091699
C	-0.266755	-0.141088	-0.230873
C	-1.439893	-0.447403	-1.131181
C	-1.160293	-2.900537	1.669058
C	-1.874834	-4.041679	0.931675
C	-1.902293	2.898817	2.861895
C	-0.487873	-3.422318	2.947604
Zn	1.005122	0.338905	2.306416
O	4.200081	3.865058	6.230594
C	3.886675	3.231225	7.228220
O	2.679638	2.640823	7.363631
C	1.751209	2.870001	6.280219
C	0.458607	2.145900	6.612055
C	0.519527	0.620681	6.453535
C	0.203907	0.121555	5.043482
O	1.139935	0.599804	4.110435
N	2.454760	0.549243	1.008019
C	2.227394	0.395723	-0.297293
C	3.379792	0.541899	-1.262859
C	3.779853	0.840585	1.474006
C	4.206751	2.184269	1.563963

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C	5.488430	2.439586	2.058239
C	6.327927	1.406184	2.459389
C	5.885857	0.091796	2.382675
C	4.612717	-0.217957	1.894803
C	3.283406	3.337699	1.199069
C	2.554701	3.846001	2.453657
C	4.145001	-1.665406	1.879776
C	3.856968	-2.147825	3.310582
C	3.998900	4.489990	0.483794
C	0.968448	0.097575	-0.855526
C	5.131557	-2.602646	1.171336
N	4.707075	3.030202	8.323010
Si	3.959252	2.474617	9.864180
C	3.551151	0.638389	9.784605
C	5.129331	2.750557	11.318417
C	2.435927	3.516020	10.255912
Si	6.417423	3.462647	7.917942
C	7.603875	2.844897	9.251284
C	6.602672	5.330374	7.781692
C	6.941779	2.565611	6.347292
H	7.319708	1.627993	2.842947
H	-2.741326	2.934726	3.565862
H	-1.050893	2.445026	3.379273
H	6.538446	-0.711975	2.713436
H	4.171508	-0.176346	-1.027911
H	0.954063	0.028856	-1.936456
H	3.055101	0.383072	-2.292018
H	3.830619	1.535914	-1.184687
H	-3.696151	2.254436	-0.063519
H	-1.401677	2.089129	0.948335
H	-4.302746	2.941218	1.447607
H	-3.081459	3.810935	0.518339
H	4.567901	4.140375	-0.384158
H	3.266683	5.225853	0.134925
H	4.691037	5.017796	1.148162
H	2.522285	2.952761	0.511434
H	5.833383	3.465908	2.139527
H	-1.633152	3.929627	2.606001
H	1.970165	3.050270	2.926496
H	3.267305	4.207402	3.202404
H	1.874185	4.667236	2.200279
H	6.085034	-2.670170	1.706160
H	5.346638	-2.267167	0.151543
H	4.718772	-3.615781	1.113734
H	3.203681	-1.704622	1.321540
H	3.134598	-1.495997	3.812677
H	4.772922	-2.148535	3.912208
H	3.459852	-3.169358	3.303322
H	0.085599	-2.636308	3.448546
H	0.195660	-4.247131	2.717430
H	-1.233367	-3.791747	3.660489
H	-0.367778	-2.530865	1.010618
H	-3.578003	-2.987018	2.887398
H	-5.111406	-1.132011	3.440096
H	-2.630977	-4.522698	1.561191
H	-1.154688	-4.813926	0.640722
H	-2.376378	-3.687941	0.025191
H	-1.151792	-0.406796	-2.182441
H	-1.845389	-1.441270	-0.917832
H	-2.254345	0.263925	-0.961815
H	-4.512881	1.186656	2.833862
H	2.185360	2.492729	5.353138
H	-0.825978	0.434593	4.790771
H	0.187532	-0.982472	5.073600
H	1.596536	3.949982	6.184007
H	-0.324845	2.548939	5.956901
H	-0.202465	0.152366	7.135955
H	0.166085	2.413670	7.634897
H	1.511444	0.257468	6.749475
H	7.637775	5.601457	7.544178

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H	6.337821	5.822050	8.724188
H	5.951811	5.719470	6.995388
H	6.324536	2.840312	5.491075
H	6.875227	1.480703	6.485543
H	7.987724	2.804799	6.120598
H	5.991978	2.081562	11.327310
H	8.617137	2.973971	8.850905
H	5.489303	3.782093	11.382935
H	4.552676	2.552650	12.230259
H	7.479941	1.778833	9.466918
H	7.554495	3.397553	10.191723
H	2.674309	4.584100	10.204092
H	1.608378	3.318883	9.573146
H	2.845737	0.424783	8.978003
H	4.455109	0.044430	9.611808
H	3.106409	0.301036	10.727952
H	2.098806	3.303749	11.277181

3.2 Ring-opening polymerization of cyclic carbonates by metal alkoxide as catalyst

(BDI)Zn(OBn)

G = -1811,507656 u.a.

C	-3.702149	-0.679292	-1.779577
C	-2.699564	0.015824	-2.456234
C	-2.999723	0.604875	-3.689991
C	-4.276229	0.502716	-4.236011
C	-5.274941	-0.194142	-3.553647
C	-4.982152	-0.783738	-2.325766
C	-1.305968	0.152118	-1.871911
O	-1.163949	-0.583651	-0.692948
Zn	0.396410	-0.856491	0.205916
N	2.281444	-0.447318	-0.068346
C	3.196698	-0.821455	0.831159
C	2.904078	-1.510176	2.020445
C	1.671024	-1.965149	2.529545
C	1.707099	-2.685254	3.856383
N	0.498694	-1.799950	1.916285
C	-0.705618	-2.313264	2.501086
C	-1.136363	-3.616901	2.170983
C	-2.341515	-4.075307	2.711033
C	-3.109262	-3.274201	3.547707
C	-2.681496	-1.986527	3.847649
C	-1.483865	-1.480227	3.334131
C	-0.361909	-4.499211	1.203398
C	-0.106481	-5.908933	1.752190
C	-1.085731	-0.042317	3.630524
C	-1.119868	0.290721	5.127669
C	-1.969295	0.929219	2.830935
C	-1.083283	-4.561085	-0.152636
C	2.659955	0.255989	-1.257680
C	2.903713	-0.470467	-2.444654
C	3.156033	0.243061	-3.620298
C	3.177126	1.632609	-3.631686
C	2.951624	2.333305	-2.452589
C	2.693280	1.668673	-1.250167
C	2.875195	-1.991941	-2.476330
C	4.130879	-2.587602	-3.127657
C	2.425860	2.471228	0.015461
C	3.473730	3.566895	0.253456
C	1.605607	-2.507332	-3.170876
C	1.011352	3.070362	-0.001461
C	4.646645	-0.491173	0.569202
H	5.289031	-0.872851	1.363779
H	4.974275	-0.917533	-0.384011
H	4.790759	0.591131	0.491823
H	2.724570	-2.750197	4.244058
H	1.081935	-2.169874	4.592168
H	1.301325	-3.696917	3.759497

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H	3.763008	-1.730974	2.642418
H	3.336312	-0.300899	-4.543723
H	3.371194	2.168409	-4.556828
H	2.971882	3.419702	-2.465808
H	-3.294132	-1.355896	4.486465
H	-4.043875	-3.648640	3.956428
H	-2.688676	-5.074932	2.463215
H	-0.749174	1.307258	5.298431
H	-2.136535	0.244115	5.532565
H	-0.499254	-0.397489	5.710864
H	-1.640969	1.964179	2.979953
H	-1.942040	0.705786	1.759645
H	-3.013911	0.859757	3.154791
H	3.305611	4.046266	1.223753
H	4.491336	3.163034	0.247170
H	3.424235	4.352061	-0.508436
H	0.814826	3.628005	0.920959
H	0.888694	3.759204	-0.844525
H	0.245323	2.294107	-0.096298
H	4.118572	-3.679739	-3.045528
H	4.193133	-2.342448	-4.193326
H	5.046173	-2.222968	-2.650227
H	1.579452	-3.602584	-3.167044
H	0.698731	-2.147079	-2.674758
H	1.565918	-2.174653	-4.214027
H	0.519876	-6.478325	1.056937
H	0.403436	-5.881961	2.720804
H	-1.037551	-6.470581	1.883999
H	-0.499422	-5.140825	-0.876559
H	-2.062501	-5.042370	-0.050049
H	-1.250736	-3.560601	-0.563700
H	-1.118187	1.229208	-1.705989
H	-0.583089	-0.152433	-2.649766
H	-0.053709	0.093591	3.290363
H	2.478124	1.780953	0.863686
H	0.614982	-4.033450	1.036898
H	2.848140	-2.343457	-1.439749
H	-2.224461	1.148107	-4.228659
H	-4.493100	0.964787	-5.196053
H	-6.271965	-0.276317	-3.978615
H	-5.754020	-1.329272	-1.787969
H	-3.458057	-1.133731	-0.825044

(BDI)Zn(OMe)

G = -1580,610511 u.a.

Zn	0.346589	0.000217	0.369384
N	0.354310	-0.000789	2.331910
N	2.268983	0.000848	0.037338
C	1.501865	-0.000906	3.009357
C	3.139919	0.000448	1.051727
C	2.777315	-0.000312	2.408865
C	4.617497	0.000859	0.738609
C	1.463018	-0.001731	4.519465
H	5.214766	0.000898	1.651339
H	4.887921	-0.876048	0.141913
H	4.887537	0.877971	0.142044
H	2.469159	-0.000479	4.940765
H	0.922934	0.873543	4.893374
H	0.925619	-0.879078	4.892421
H	3.608666	-0.000433	3.103299
C	2.726115	0.001667	-1.319919
C	2.907293	-1.227142	-1.992980
C	3.253766	-1.198716	-3.347050
C	3.424328	0.003210	-4.024039
C	3.252689	1.204353	-3.345960
C	2.906174	1.231237	-1.991857
C	2.702030	-2.562038	-1.291565
H	3.388918	-2.135618	-3.880753
H	3.690932	0.003807	-5.077423

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H	3.387044	2.141865	-3.878791
C	2.699920	2.565328	-1.289210
C	-0.896350	-0.001582	3.032360
C	-1.521937	1.226707	3.338033
C	-2.761447	1.198600	3.983706
C	-3.376918	-0.003049	4.313140
C	-2.760336	-1.203968	3.983086
C	-1.520799	-1.230613	3.337408
C	-0.915377	2.558495	2.923681
H	-3.256928	2.135373	4.224749
H	-4.340501	-0.003623	4.815477
H	-3.254997	-2.141309	4.223589
C	-0.913136	-2.561608	2.922102
C	-0.872245	-3.587442	4.061610
C	-1.660310	-3.124309	1.701571
C	-0.875265	3.583434	4.064039
C	-1.663039	3.121581	1.703649
C	3.861561	-3.539415	-1.526253
C	1.364760	-3.196807	-1.702762
C	3.859194	3.543392	-1.522299
C	1.362595	3.199955	-1.700463
H	-0.357375	4.492049	3.738104
H	-1.880319	3.880526	4.382059
H	-0.351292	3.193049	4.942703
H	-1.191447	4.046864	1.353174
H	-1.679267	2.402722	0.877988
H	-2.703484	3.351759	1.960008
H	3.720217	4.445284	-0.916601
H	4.823322	3.100151	-1.252707
H	3.921927	3.862093	-2.568341
H	1.203145	4.146718	-1.172394
H	1.342617	3.407004	-2.776291
H	0.518021	2.540980	-1.474937
H	3.723647	-4.441642	-0.920807
H	3.923357	-3.857666	-2.572489
H	4.825768	-3.095844	-1.257484
H	1.205893	-4.144072	-1.175414
H	0.520075	-2.538305	-1.476293
H	1.344417	-3.402954	-2.778755
H	-0.354258	-4.495656	3.734714
H	-0.347982	-3.197656	4.940370
H	-1.877068	-3.885064	4.379853
H	-1.187637	-4.048643	1.350050
H	-2.700443	-3.356009	1.957813
H	-1.677462	-2.404596	0.876675
O	-1.190278	0.000154	-0.598043
C	-1.284718	0.000422	-1.995043
H	-2.346537	0.002288	-2.284274
H	-0.822810	0.884332	-2.466257
H	-0.825992	-0.885125	-2.466259
H	0.119539	2.371302	2.618659
H	2.651081	2.368929	-0.213164
H	0.121626	-2.373369	2.617199
H	2.653619	-2.366796	-0.215289

3.2.1 Ring-opening polymerization of 7CC

Initiation Step of the 7CC ROP reaction

A_{7CC}

G = -2001,353842 u.a.

C	-1.801423	0.342403	3.919145
C	-0.677479	-0.297112	3.348734
C	-0.503635	-1.698032	3.470492
C	-1.479456	-2.433376	4.149068
C	-2.591296	-1.816735	4.711690
C	-2.739666	-0.440264	4.600280
N	0.259752	0.460205	2.578352
C	1.446729	0.781009	3.096556

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C	1.716154	0.512900	4.561334
C	0.695370	-2.426580	2.872864
C	1.358774	-3.381742	3.875639
C	-1.996176	1.850431	3.849057
C	-1.759827	2.504043	5.219783
C	2.519245	1.318467	2.364878
C	2.645606	1.588640	0.987805
C	4.052883	1.892546	0.518168
N	1.645689	1.532838	0.109798
Zn	-0.129953	0.816838	0.665674
O	-1.561985	2.562697	0.425067
C	-2.158773	2.339874	-0.621806
O	-3.463183	2.086608	-0.567707
C	-4.372363	1.950390	-1.682227
C	-4.070273	2.829647	-2.883581
C	-2.945031	2.275790	-3.764149
C	-1.857052	1.640851	-2.915802
O	-1.530192	2.479494	-1.786369
C	1.867004	1.892846	-1.257405
C	2.199049	0.898997	-2.204392
C	2.365009	1.278778	-3.541312
C	2.220937	2.602086	-3.939404
C	1.887284	3.569432	-2.996756
C	1.690642	3.242170	-1.652199
C	2.379915	-0.562281	-1.819925
C	3.760830	-1.095654	-2.227394
C	1.305862	4.328637	-0.654985
C	2.531243	5.107953	-0.150377
O	-1.297799	-0.150673	-0.458153
C	-2.362644	-0.900297	0.059329
C	0.274052	5.315807	-1.216625
C	1.257846	-1.435476	-2.401694
C	0.318047	-3.178410	1.587705
C	-3.376735	2.237959	3.304414
H	1.994089	-0.534860	4.718771
H	2.539086	1.134199	4.920253
H	0.831197	0.702317	5.172233
H	4.558293	0.949200	0.278582
H	4.075482	2.509488	-0.380220
H	4.630040	2.380951	1.306558
H	3.422082	1.484835	2.941709
H	-3.602743	0.042029	5.051877
H	-3.335776	-2.407261	5.239115
H	-1.365409	-3.510499	4.239425
H	2.621852	0.522815	-4.279369
H	2.367697	2.880281	-4.979985
H	1.769127	4.601783	-3.314209
H	3.898788	-2.117659	-1.857495
H	3.877498	-1.124566	-3.316436
H	4.569686	-0.476763	-1.825779
H	1.408776	-2.484638	-2.121852
H	0.281187	-1.118387	-2.021756
H	1.247795	-1.384001	-3.497104
H	2.286225	-3.786131	3.455665
H	1.603172	-2.879664	4.817416
H	0.714473	-4.234550	4.115527
H	-0.466149	-3.918978	1.782000
H	-0.046303	-2.494198	0.816555
H	1.188395	-3.709456	1.185237
H	-1.873998	3.591642	5.150208
H	-2.479372	2.138883	5.961700
H	-0.755703	2.297575	5.602734
H	-3.448955	3.326686	3.208769
H	-3.548982	1.807120	2.315816
H	-4.183249	1.912394	3.971496
H	2.221502	5.891788	0.550086
H	3.247473	4.466921	0.368314
H	3.055087	5.591372	-0.983528
H	-0.090361	5.966033	-0.414151
H	0.706586	5.967123	-1.985047

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H	-0.580792	4.793558	-1.650897
H	-3.118741	-0.279521	0.569179
H	-2.879982	-1.431766	-0.758855
H	-2.051622	-1.669819	0.782225
H	2.310732	-0.627935	-0.729266
H	1.442001	-1.676911	2.594688
H	0.845279	3.826831	0.201370
H	-1.249755	2.248328	3.155573
H	-2.117043	0.655037	-2.521901
H	-0.915126	1.543254	-3.458048
H	-2.531423	3.077256	-4.385006
H	-3.332247	1.510647	-4.448516
H	-3.820394	3.834492	-2.525494
H	-4.992512	2.933036	-3.466419
H	-5.335073	2.219305	-1.241754
H	-4.411763	0.889643	-1.953713

TS(A_{7CC}→B_{7CC})

G = -2001,345352 u.a.

C	-1.885074	0.330201	3.711597
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C	-1.583703	-2.435981	4.045420
C	-2.724501	-1.803194	4.523704
C	-2.863129	-0.430727	4.359686
N	0.255805	0.419029	2.503140
C	1.409963	0.751276	3.087868
C	1.608020	0.478320	4.563271
C	0.656031	-2.480641	2.901839
C	1.319658	-3.305377	4.015239
C	-2.071990	1.835545	3.589422
C	-1.842656	2.531995	4.939908
C	2.513202	1.316989	2.425271
C	2.716406	1.615964	1.063514
C	4.130148	1.990485	0.677880
N	1.772600	1.546346	0.126243
Zn	-0.038426	0.898351	0.603008
O	-1.498444	2.386794	0.185111
C	-2.111426	1.862681	-0.764130
O	-3.396145	1.417842	-0.652142
C	-4.430817	2.372852	-0.952070
C	-4.226125	3.119861	-2.265451
C	-3.754265	2.219497	-3.409292
C	-2.417071	1.522061	-3.086990
O	-1.718751	2.168206	-2.013208
C	2.072214	1.907486	-1.226920
C	2.429422	0.903256	-2.154142
C	2.679689	1.273557	-3.479051
C	2.587787	2.597965	-3.888674
C	2.228085	3.574690	-2.967846
C	1.957034	3.257888	-1.633279
C	2.530342	-0.562757	-1.760814
C	3.910277	-1.156191	-2.077190
C	1.555341	4.372820	-0.676477
C	2.692670	5.383914	-0.461944
O	-1.269085	0.037229	-0.631645
C	-2.037801	-1.105084	-0.351692
C	0.287321	5.095344	-1.152303
C	1.412549	-1.385226	-2.419446
C	0.310575	-3.387128	1.711329
C	-3.444713	2.210362	3.017751
H	2.011946	-0.527875	4.716681
H	2.321369	1.188035	4.987645
H	0.669312	0.538084	5.116771
H	4.645453	1.106157	0.284504
H	4.158663	2.747699	-0.106453
H	4.691452	2.345633	1.544078
H	3.373760	1.496281	3.059824
H	-3.750138	0.065686	4.743957

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H	-3.499434	-2.376536	5.025457
H	-1.475681	-3.509891	4.175372
H	2.955647	0.508086	-4.200258
H	2.794063	2.867901	-4.921132
H	2.152095	4.609978	-3.290810
H	3.974953	-2.187726	-1.713482
H	4.103439	-1.176939	-3.155377
H	4.715703	-0.580772	-1.609315
H	1.466017	-2.432204	-2.098866
H	0.429473	-0.987298	-2.149852
H	1.503583	-1.367956	-3.511850
H	2.261117	-3.737563	3.658903
H	1.536574	-2.700058	4.900711
H	0.681675	-4.136014	4.336470
H	-0.440364	-4.134502	1.991132
H	-0.089257	-2.811064	0.873535
H	1.201567	-3.921692	1.363005
H	-1.956286	3.616884	4.835887
H	-2.566655	2.189106	5.688215
H	-0.840341	2.337200	5.333491
H	-3.496204	3.292199	2.854033
H	-3.618718	1.714521	2.060083
H	-4.259243	1.944144	3.701258
H	2.386572	6.154515	0.254386
H	3.599767	4.910685	-0.074284
H	2.957071	5.888949	-1.398009
H	-0.021458	5.842398	-0.412304
H	0.456840	5.620441	-2.099603
H	-0.531540	4.387309	-1.290073
H	-3.037312	-0.998151	-0.795529
H	-1.574028	-2.003836	-0.788308
H	-2.178818	-1.283125	0.723699
H	2.388412	-0.624272	-0.676954
H	1.388230	-1.747703	2.549854
H	1.324964	3.914932	0.289895
H	-1.319151	2.208398	2.889475
H	-2.552381	0.472736	-2.818951
H	-1.724751	1.575533	-3.929172
H	-3.650904	2.832712	-4.310803
H	-4.512543	1.459291	-3.631587
H	-3.501856	3.928430	-2.124612
H	-5.177041	3.596760	-2.531296
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H	-5.338208	1.763560	-0.988860

B_{7CC}

G = -2001,359938 u.a.

C	-1.533877	0.532548	4.076461
C	-0.654613	-0.243327	3.287542
C	-0.805276	-1.645478	3.196849
C	-1.842426	-2.249522	3.914614
C	-2.713900	-1.500847	4.696272
C	-2.556835	-0.121737	4.769719
N	0.365370	0.409169	2.519599
C	1.581182	0.587008	3.040485
C	1.849705	0.121235	4.451587
C	0.106260	-2.510664	2.337544
C	0.822550	-3.592358	3.159987
C	-1.416884	2.047238	4.171151
C	-1.351774	2.541214	5.623273
C	2.653540	1.195757	2.362213
C	2.734487	1.691808	1.049984
C	4.071567	2.245120	0.617731
N	1.721037	1.699068	0.177339
Zn	-0.055036	1.102801	0.728622
O	-1.779276	1.474820	0.136269
C	-2.354374	0.623378	-0.730653
O	-3.543994	1.129381	-1.266872
C	-3.454985	2.376931	-1.943452

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C	-2.501710	2.348470	-3.140756
C	-2.508633	1.001384	-3.868280
C	-2.019436	-0.156204	-2.963545
O	-1.426428	0.317309	-1.755056
C	1.926309	2.175683	-1.159684
C	2.389117	1.284206	-2.153223
C	2.490496	1.750198	-3.467164
C	2.153677	3.056867	-3.799813
C	1.718947	3.927533	-2.807518
C	1.602687	3.513457	-1.476899
C	2.755947	-0.159882	-1.841380
C	4.163129	-0.526174	-2.335063
C	1.131501	4.502059	-0.419594
C	1.951020	5.799948	-0.430140
O	-2.695782	-0.621812	-0.169964
C	-3.693187	-0.573712	0.839255
C	-0.367939	4.800863	-0.565375
C	1.714243	-1.132193	-2.413570
C	-0.664582	-3.145613	1.170030
C	-2.561709	2.736360	3.411829
H	1.665036	-0.952342	4.548435
H	2.879142	0.328254	4.746857
H	1.174659	0.616370	5.156328
H	4.516676	1.617910	-0.161034
H	3.959655	3.244489	0.187768
H	4.765530	2.295832	1.457838
H	3.568597	1.276211	2.936208
H	-3.243653	0.462298	5.376622
H	-3.514537	-1.989812	5.244724
H	-1.969423	-3.327483	3.854763
H	2.835976	1.073198	-4.244192
H	2.235414	3.397614	-4.828433
H	1.465436	4.951574	-3.068846
H	4.426507	-1.538519	-2.010014
H	4.226160	-0.508963	-3.428519
H	4.925163	0.160266	-1.951688
H	1.962851	-2.165164	-2.144784
H	0.713101	-0.905371	-2.037343
H	1.685553	-1.070421	-3.507711
H	1.519415	-4.151825	2.526443
H	1.392927	-3.167273	3.992240
H	0.112603	-4.312435	3.581550
H	-1.426310	-3.843293	1.537561
H	-1.168677	-2.390625	0.559912
H	0.018091	-3.713770	0.527786
H	-1.178733	3.622587	5.647788
H	-2.287185	2.349627	6.160372
H	-0.544720	2.057912	6.183686
H	-2.447468	3.825783	3.453188
H	-2.585568	2.431696	2.361095
H	-3.530991	2.487410	3.859153
H	1.650247	6.444644	0.402815
H	3.024028	5.603831	-0.335105
H	1.799007	6.369293	-1.353445
H	-0.700242	5.493614	0.216238
H	-0.580431	5.264935	-1.535304
H	-0.964877	3.886795	-0.489231
H	-4.652702	-0.241490	0.429848
H	-3.788715	-1.591446	1.222541
H	-3.395994	0.087058	1.660147
H	2.748423	-0.278386	-0.753228
H	0.875690	-1.859952	1.909554
H	1.279333	4.033766	0.559271
H	-0.478912	2.338829	3.687195
H	-2.836373	-0.840485	-2.716500
H	-1.234369	-0.732465	-3.460819
H	-1.865582	1.081968	-4.752261
H	-3.517796	0.775827	-4.234224
H	-1.481852	2.567029	-2.812780
H	-2.791818	3.147229	-3.834995

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H	-3.175807	3.171107	-1.240183
H	-4.480643	2.564240	-2.279027

TS(B_{7CC}→C_{7CC})

G = -2001,34812 u.a.

C	1.529006	3.601153	-1.580094
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C	2.399829	1.404404	-2.261622
C	2.486476	1.877194	-3.574634
C	2.100061	3.171226	-3.905516
C	1.644207	4.024860	-2.908476
N	1.647549	1.760430	0.052285
Zn	-0.141152	1.063607	0.554209
O	-1.801684	2.266627	0.394944
C	-2.673505	1.390998	0.094489
O	-3.267769	0.772133	1.134195
C	-4.200553	-0.269405	0.874346
C	2.902640	0.001092	-1.940525
C	1.980866	-1.092570	-2.495421
C	1.089351	4.601072	-0.517482
C	-0.327706	5.138013	-0.760180
C	2.646840	1.749406	0.941928
C	3.981772	2.341089	0.550091
C	2.569761	1.200573	2.229810
C	1.508159	0.549300	2.890743
C	1.817260	0.047894	4.283770
N	0.290727	0.376416	2.381785
C	-0.714115	-0.288441	3.158613
C	-1.505883	0.446504	4.071019
C	-2.521069	-0.225189	4.759038
C	-2.752602	-1.582785	4.572184
C	-1.955901	-2.295531	3.684179
C	-0.931464	-1.671896	2.965523
C	-1.295025	1.930885	4.339442
C	-2.483113	2.774774	3.854858
C	-0.073111	-2.508006	2.026407
C	-0.909043	-3.138092	0.904656
C	0.715167	-3.585023	2.786752
C	-1.024145	2.208283	5.826848
O	-3.519427	1.524270	-0.948594
C	-3.110172	2.332925	-2.062462
C	-1.747770	1.991042	-2.646313
C	-1.485242	0.516444	-2.957928
C	-1.793825	-0.440471	-1.795573
O	-1.520615	0.054940	-0.507915
C	4.339645	-0.216950	-2.438843
C	2.087281	5.765443	-0.408863
H	1.362766	-0.927191	4.470474
H	2.894803	-0.022710	4.441627
H	1.410668	0.735686	5.032406
H	4.637817	2.433043	1.416895
H	4.482183	1.710542	-0.191815
H	3.858983	3.325589	0.092554
H	3.482991	1.274050	2.808106
H	-3.142226	0.329962	5.457626
H	-3.544370	-2.084323	5.122673
H	-2.127296	-3.360605	3.547749
H	2.873301	1.221237	-4.350527
H	2.174193	3.518509	-4.932580
H	1.374929	5.047089	-3.162329
H	4.721204	-1.181229	-2.085980
H	4.391703	-0.226689	-3.532927
H	5.018977	0.565782	-2.086583
H	2.382191	-2.086038	-2.265584
H	0.980949	-1.026018	-2.060138
H	1.883652	-1.015278	-3.584341
H	1.364787	-4.140259	2.100817
H	1.345308	-3.151411	3.569509
H	0.044382	-4.307727	3.264768

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H	-1.656091	-3.833895	1.303372
H	-1.427904	-2.362545	0.336060
H	-0.266913	-3.702520	0.218553
H	-0.768369	3.263064	5.976057
H	-1.907374	1.997243	6.439991
H	-0.202466	1.601680	6.220837
H	-2.298734	3.836348	4.057047
H	-2.645536	2.648133	2.783434
H	-3.403837	2.492547	4.378621
H	1.806216	6.430544	0.414958
H	3.108788	5.417399	-0.225999
H	2.103777	6.364603	-1.326137
H	-0.585137	5.879418	0.004491
H	-0.407613	5.629688	-1.736614
H	-1.066338	4.335242	-0.704686
H	-3.709069	-1.094975	0.352759
H	-4.536212	-0.609917	1.854102
H	-5.049853	0.093290	0.288857
H	2.910265	-0.108824	-0.851788
H	0.653381	-1.837230	1.557220
H	1.081183	4.079109	0.444517
H	-0.414869	2.252039	3.773478
H	-2.863334	-0.692108	-1.832199
H	-1.249045	-1.384792	-1.945664
H	-0.432836	0.432384	-3.250140
H	-2.075779	0.190412	-3.825574
H	-0.974633	2.353311	-1.967219
H	-1.636759	2.581890	-3.564193
H	-3.130716	3.385283	-1.756658
H	-3.907314	2.171679	-2.794690

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G = -2001,357138 u.a.

C	1.521876	3.598898	-1.610670
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C	2.425366	1.408895	-2.271699
C	2.518091	1.874660	-3.586662
C	2.117871	3.161765	-3.928706
C	1.644508	4.016219	-2.940599
N	1.639898	1.759080	0.028170
Zn	-0.070313	0.830884	0.422363
O	-1.902992	2.322297	0.449436
C	-2.861656	1.577338	0.252315
O	-3.359337	0.851502	1.238921
C	-4.304535	-0.183319	0.947861
C	2.945774	0.016312	-1.931979
C	2.020071	-1.097018	-2.440296
C	1.067922	4.602989	-0.557248
C	-0.347552	5.138525	-0.813267
C	2.620352	1.790294	0.938613
C	3.937032	2.435293	0.570497
C	2.541177	1.236032	2.222917
C	1.486556	0.558308	2.869281
C	1.791861	0.083443	4.272972
N	0.288202	0.337736	2.336003
C	-0.730235	-0.306663	3.111279
C	-1.495175	0.437756	4.041073
C	-2.540505	-0.208191	4.708648
C	-2.824264	-1.551330	4.491738
C	-2.044241	-2.277590	3.599700
C	-0.991881	-1.680479	2.899003
C	-1.221142	1.902147	4.363196
C	-2.355489	2.824062	3.893732
C	-0.131566	-2.542775	1.985690
C	-0.955653	-3.244598	0.899665
C	0.684282	-3.560835	2.798368
C	-0.968174	2.112335	5.865452
O	-3.559888	1.487830	-0.870145
C	-3.134879	2.264247	-2.016014

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C	-1.732605	1.977348	-2.524677
C	-1.396295	0.542820	-2.929218
C	-1.642504	-0.532768	-1.859377
O	-1.254901	-0.243387	-0.555996
C	4.375749	-0.199812	-2.450051
C	2.057065	5.775578	-0.450483
H	1.261029	-0.839415	4.513289
H	2.864784	-0.076911	4.396923
H	1.482125	0.836363	5.005057
H	4.599167	2.497062	1.435281
H	4.443972	1.861554	-0.211978
H	3.784709	3.440547	0.170535
H	3.441412	1.338064	2.817448
H	-3.142009	0.355134	5.417870
H	-3.637853	-2.033198	5.028028
H	-2.247980	-3.334752	3.448698
H	2.920400	1.219290	-4.354928
H	2.196486	3.503798	-4.957238
H	1.367629	5.034366	-3.202983
H	4.771511	-1.151735	-2.079838
H	4.410983	-0.237235	-3.544230
H	5.053056	0.597404	-2.126776
H	2.442801	-2.080927	-2.207008
H	1.033814	-1.036837	-1.973647
H	1.890274	-1.038633	-3.527142
H	1.340542	-4.139721	2.138813
H	1.310491	-3.073353	3.552324
H	0.029205	-4.268345	3.319340
H	-1.696684	-3.928118	1.329656
H	-1.465651	-2.500970	0.283110
H	-0.299846	-3.838744	0.252863
H	-0.645425	3.141809	6.056251
H	-1.878859	1.943364	6.450803
H	-0.201158	1.436911	6.256919
H	-2.134800	3.862489	4.167168
H	-2.480855	2.772306	2.811783
H	-3.306033	2.550893	4.366038
H	1.771547	6.440023	0.372404
H	3.082188	5.438126	-0.269168
H	2.067337	6.372922	-1.369070
H	-0.607598	5.889326	-0.058667
H	-0.422519	5.618506	-1.795824
H	-1.089410	4.339878	-0.753019
H	-3.848900	-0.912380	0.275736
H	-4.520346	-0.644622	1.910519
H	-5.214450	0.228769	0.504977
H	2.977112	-0.068221	-0.841258
H	0.577461	-1.881739	1.478055
H	1.052894	4.085968	0.407382
H	-0.317339	2.203139	3.824621
H	-2.726609	-0.748819	-1.856294
H	-1.161612	-1.461117	-2.221779
H	-0.339996	0.540996	-3.223110
H	-1.966348	0.254117	-3.824711
H	-1.011823	2.324246	-1.783798
H	-1.592687	2.633584	-3.393789
H	-3.231242	3.323674	-1.754861
H	-3.891648	2.020118	-2.766462

TS(C_{7CC}→D_{7CC})

G = -2001,355029 u.a.

C	-0.984944	-1.681132	2.903999
C	-0.722004	-0.307649	3.112491
C	-1.493701	0.445953	4.028263
C	-2.542237	-0.195585	4.695203
C	-2.824625	-1.540014	4.486288
C	-2.041828	-2.272772	3.601966
N	0.309058	0.327846	2.345190
C	1.499649	0.565125	2.886255

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C	1.812480	0.114427	4.296647
C	-1.218487	1.911575	4.341607
C	-0.899161	2.115222	5.831972
C	-0.120500	-2.547894	1.999490
C	0.701308	-3.551827	2.823448
C	2.555132	1.239717	2.235993
C	2.636947	1.781900	0.948691
C	3.939260	2.456816	0.586919
N	1.663783	1.724184	0.028417
Zn	-0.014114	0.763780	0.419106
O	-1.327670	-0.170403	-0.486924
C	-1.647827	-0.500728	-1.802238
C	-1.395798	0.570861	-2.872860
C	-1.791514	1.995563	-2.488385
C	-3.226274	2.239673	-2.050963
O	-3.668298	1.459611	-0.918921
C	-3.046553	1.652042	0.243655
O	-3.544901	0.911084	1.225554
C	-4.392474	-0.196898	0.912855
C	1.895971	2.244679	-1.286085
C	1.537863	3.577629	-1.597968
C	1.648250	4.001193	-2.926953
C	2.115467	3.153701	-3.923933
C	2.520462	1.865760	-3.592448
C	2.434805	1.391604	-2.279903
C	1.100715	4.581917	-0.537147
C	2.082711	5.763712	-0.462141
C	2.960562	-0.002786	-1.957038
C	4.417267	-0.178015	-2.413731
O	-2.172180	2.475711	0.461941
C	2.082818	-1.112830	-2.550244
C	-0.324442	5.108283	-0.758029
C	-2.380401	2.824037	3.924763
C	-0.940701	-3.263069	0.919271
H	1.100514	-0.625290	4.662829
H	2.820906	-0.306160	4.336052
H	1.792065	0.971751	4.977663
H	4.625181	2.467715	1.434996
H	4.426381	1.945094	-0.248448
H	3.766328	3.486356	0.263376
H	3.449211	1.356439	2.837928
H	-3.147306	0.373194	5.396869
H	-3.641213	-2.017874	5.021486
H	-2.246929	-3.330268	3.455744
H	2.919422	1.215293	-4.366823
H	2.185523	3.502201	-4.950873
H	1.367904	5.020305	-3.181333
H	4.807607	-1.142817	-2.072050
H	4.503957	-0.158552	-3.505494
H	5.068061	0.608794	-2.019114
H	2.504749	-2.097969	-2.321414
H	1.068922	-1.080184	-2.144022
H	2.013572	-1.024491	-3.640400
H	1.360702	-4.135694	2.171405
H	1.323694	-3.049567	3.570838
H	0.049891	-4.255604	3.353841
H	-1.668585	-3.956768	1.354882
H	-1.470711	-2.530392	0.306287
H	-0.281145	-3.848517	0.268419
H	-0.593436	3.150955	6.017375
H	-1.777484	1.918005	6.456661
H	-0.097725	1.456180	6.178922
H	-2.149822	3.865054	4.179522
H	-2.561309	2.763808	2.850832
H	-3.304195	2.552331	4.448267
H	1.822264	6.420279	0.375121
H	3.118395	5.437423	-0.324947
H	2.049768	6.366835	-1.376307
H	-0.561750	5.870958	-0.007818
H	-0.427735	5.573961	-1.744998

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H	-1.066801	4.313576	-0.662724
H	-3.847341	-0.911955	0.294261
H	-4.636627	-0.646515	1.874778
H	-5.301571	0.132124	0.403063
H	2.941565	-0.121617	-0.869118
H	0.587984	-1.889510	1.487003
H	1.115634	4.070389	0.430462
H	-0.341899	2.221413	3.764453
H	-2.722093	-0.751845	-1.830205
H	-1.122259	-1.418565	-2.125763
H	-0.329498	0.598421	-3.128087
H	-1.923270	0.258607	-3.786218
H	-1.123698	2.357861	-1.706009
H	-1.620552	2.655766	-3.348734
H	-3.367280	3.298573	-1.808289
H	-3.937022	1.962881	-2.834865

D_{7CC}

G = -2001,375211 u.a.

C	3.017472	1.146274	-2.222447
C	2.830925	2.038903	-1.143559
C	3.021036	3.429311	-1.309131
C	3.383680	3.903990	-2.573211
C	3.562452	3.038659	-3.646251
C	3.382537	1.672425	-3.465176
N	2.357100	1.539240	0.112473
Zn	0.430795	1.472884	0.421038
O	-1.058395	1.970856	-0.501181
C	-1.088582	2.382627	-1.842681
C	-2.340038	3.222590	-2.108999
C	-3.657864	2.531239	-1.748201
C	-3.960080	1.332113	-2.630561
O	-5.201691	0.701178	-2.246663
C	-6.312965	1.226495	-2.787443
O	-6.359676	2.132639	-3.582239
C	2.813252	4.409757	-0.163714
C	1.491930	5.176564	-0.328142
C	2.797168	-0.352167	-2.071370
C	1.476571	-0.780518	-2.729053
C	3.214419	1.148606	1.060254
C	4.695402	1.236104	0.779244
C	2.832668	0.657907	2.320597
C	1.550303	0.461911	2.870154
C	1.490402	-0.093931	4.273157
N	0.410104	0.732587	2.233026
C	-0.849986	0.482728	2.869251
C	-1.466508	-0.778887	2.717395
C	-2.717914	-0.982366	3.305916
C	-3.353619	0.027345	4.018638
C	-2.742996	1.269340	4.142936
C	-1.490987	1.524018	3.575051
C	-0.835357	-1.886187	1.886405
C	-1.558601	-2.015094	0.536358
C	-0.883482	2.914262	3.686009
C	-1.634272	3.899492	2.775639
C	-0.834739	3.428815	5.130587
C	-0.795514	-3.235361	2.615656
O	-7.421346	0.613219	-2.347016
C	-7.304264	-0.448274	-1.399370
C	3.988045	5.383727	-0.000418
C	3.967934	-1.180642	-2.617169
H	0.976456	-1.060283	4.285207
H	2.490152	-0.224887	4.689197
H	0.918331	0.569401	4.928792
H	5.280936	0.890200	1.632005
H	4.960282	0.634883	-0.096056
H	4.985615	2.265790	0.547969
H	3.654255	0.387983	2.972881
H	-3.250913	2.061229	4.687079

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H	-4.326443	-0.150768	4.468875
H	-3.206420	-1.947205	3.197339
H	3.523747	0.999725	-4.306975
H	3.842087	3.428309	-4.621209
H	3.526095	4.971354	-2.719980
H	3.814173	-2.242869	-2.398800
H	4.065759	-1.083851	-3.703691
H	4.920990	-0.878569	-2.171099
H	1.304079	-1.853672	-2.590807
H	0.623791	-0.241761	-2.303940
H	1.491065	-0.577570	-3.805640
H	-0.254157	-3.974886	2.015763
H	-0.295508	-3.157460	3.586564
H	-1.800124	-3.634269	2.792195
H	-2.600863	-2.320514	0.682062
H	-1.567992	-1.062569	-0.002931
H	-1.072668	-2.767368	-0.095325
H	-0.319861	4.394763	5.171488
H	-1.838004	3.578043	5.543637
H	-0.304164	2.735334	5.791251
H	-1.166502	4.890092	2.809551
H	-1.643912	3.555012	1.736677
H	-2.675717	4.010414	3.098397
H	3.845731	6.001251	0.892879
H	4.941429	4.855334	0.102037
H	4.076025	6.063789	-0.854344
H	1.336508	5.863906	0.510913
H	1.494926	5.767839	-1.250601
H	0.634003	4.498022	-0.371666
H	-6.827702	-0.105992	-0.476957
H	-8.327530	-0.765833	-1.194305
H	-6.730388	-1.284026	-1.808856
H	2.714854	-0.569096	-1.001349
H	0.200065	-1.597611	1.678149
H	2.741167	3.828724	0.761558
H	0.149308	2.854731	3.326935
H	-1.081465	1.511600	-2.523966
H	-0.208658	2.985885	-2.123276
H	-2.264307	4.145067	-1.520506
H	-2.346377	3.524532	-3.166330
H	-3.614212	2.206988	-0.703598
H	-4.482971	3.244890	-1.849131
H	-4.028292	1.620037	-3.683772
H	-3.212238	0.545117	-2.512978

Study of first Propagation step of the 7CC ROP reaction

E_{7CC}

G = -2422,114547 u.a.

C	-1.239791	1.809779	4.461926
C	-0.582401	0.746571	3.795800
C	-1.033684	-0.583553	3.943023
C	-2.148860	-0.828367	4.750640
C	-2.798342	0.203006	5.417208
C	-2.338303	1.507346	5.272833
N	0.526802	1.035950	2.938243
C	1.756834	1.098686	3.448896
C	2.001078	0.674334	4.881339
C	-0.349830	-1.748819	3.244945
C	-1.228075	-2.297967	2.112305
C	-0.771812	3.255127	4.342990
C	0.012272	3.706459	5.585851
C	2.900561	1.493130	2.732099
C	3.075662	1.805440	1.372097
C	4.453595	2.323074	1.010912
N	2.128057	1.704388	0.437466
Zn	0.247079	1.267401	0.974912
O	-4.184331	-4.527623	-2.065197

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C	-3.867095	-3.991629	-3.097708
O	-3.517559	-4.693377	-4.183644
C	-3.156160	-4.004400	-5.381285
C	2.470436	1.892448	-0.941122
C	2.357011	3.164744	-1.544762
C	2.694634	3.296141	-2.896626
C	3.131803	2.211549	-3.643953
C	3.223407	0.960142	-3.044249
C	2.891514	0.769645	-1.700077
C	1.897039	4.397541	-0.780568
C	3.005814	5.458021	-0.693116
C	3.004768	-0.620682	-1.084378
C	2.617192	-1.744460	-2.054429
O	-1.057090	0.448631	-0.121477
C	-0.659729	-0.372570	-1.180590
C	-1.839801	-0.751289	-2.079786
C	-2.939767	-1.511045	-1.343116
C	-4.158371	-1.832585	-2.189030
O	-3.824509	-2.665462	-3.321055
O	-1.003166	3.113911	0.893715
C	-2.152859	2.885851	0.546493
O	-2.592103	3.355648	-0.620950
C	-3.670545	2.690889	-1.305920
C	-5.018542	3.236886	-0.871486
C	-5.106071	3.298200	0.657748
C	-4.399536	2.136497	1.333545
O	-2.959566	2.238853	1.378217
C	4.411917	-0.895041	-0.528930
C	0.631840	5.006904	-1.399590
C	0.050426	-2.861730	4.223525
C	-1.929097	4.229452	4.086938
H	1.157186	0.894361	5.535638
H	2.152717	-0.411540	4.908122
H	2.901659	1.143815	5.282304
H	3.803517	1.562809	3.328121
H	4.709352	2.155601	-0.035499
H	5.218273	1.868096	1.644674
H	4.483964	3.403883	1.190453
H	-2.842391	2.311328	5.802993
H	-3.655407	-0.008561	6.051510
H	-2.506832	-1.848507	4.864563
H	3.555662	0.111922	-3.635422
H	3.395990	2.337030	-4.690698
H	2.615757	4.272805	-3.367853
H	4.468307	-1.909841	-0.119116
H	5.164196	-0.810515	-1.321688
H	4.682276	-0.200373	0.268607
H	2.536001	-2.692207	-1.511819
H	1.658966	-1.550542	-2.543543
H	3.372619	-1.888650	-2.835236
H	0.625690	-3.635673	3.703744
H	0.662530	-2.477864	5.046120
H	-0.826173	-3.349546	4.663855
H	-2.173346	-2.691674	2.503622
H	-1.455541	-1.510636	1.387221
H	-0.718861	-3.117239	1.591472
H	0.329153	4.750199	5.479409
H	-0.608056	3.635552	6.486998
H	0.908733	3.103521	5.750101
H	-1.536790	5.228259	3.867175
H	-2.533847	3.904715	3.238013
H	-2.585106	4.324622	4.959899
H	2.678374	6.302988	-0.077134
H	3.924926	5.056409	-0.256717
H	3.258584	5.851213	-1.684426
H	0.295736	5.863536	-0.804887
H	0.818915	5.364657	-2.418726
H	-0.183326	4.281830	-1.430257
H	0.100316	0.111362	-1.818669
H	-0.204537	-1.314866	-0.816542

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H	2.307662	-0.655450	-0.238955
H	0.569603	-1.365557	2.790332
H	1.645644	4.084172	0.237104
H	-0.102845	3.310299	3.479717
H	-3.576360	1.616610	-1.126364
H	-3.477583	2.871707	-2.365253
H	-5.186142	4.230463	-1.299338
H	-5.796519	2.578442	-1.277354
H	-4.676065	4.234616	1.030313
H	-6.153134	3.293459	0.979947
H	-4.669127	2.076267	2.389886
H	-4.651456	1.176829	0.869060
H	-1.466825	-1.357680	-2.915656
H	-2.253345	0.166115	-2.523317
H	-3.268902	-0.915553	-0.482312
H	-2.545233	-2.446639	-0.928563
H	-4.925113	-2.344448	-1.601670
H	-4.582976	-0.929502	-2.639447
H	-2.918971	-4.786966	-6.102986
H	-3.983664	-3.394124	-5.752823
H	-2.282671	-3.366252	-5.224098

TS(E_{7CC}→F_{7CC})

G = -2422,106982 u.a.

C	-1.683678	0.750419	4.033313
C	-0.565908	0.083476	3.482196
C	-0.475465	-1.328445	3.525984
C	-1.525071	-2.047332	4.105254
C	-2.630146	-1.403517	4.649075
C	-2.697423	-0.016340	4.616794
N	0.458477	0.837031	2.824435
C	1.607000	1.090671	3.453867
C	1.768896	0.694456	4.904995
C	0.711673	-2.087655	2.946940
C	0.340350	-2.768367	1.622375
C	-1.797805	2.267615	4.042199
C	-1.573617	2.837924	5.451435
C	2.735832	1.673115	2.851829
C	2.988413	2.027545	1.512869
C	4.394295	2.522625	1.243023
N	2.093415	1.968702	0.525646
Zn	0.221375	1.436430	0.946907
O	-3.880590	-4.682548	0.207380
C	-4.307945	-4.302683	-0.854604
O	-4.480643	-5.139899	-1.887851
C	-5.006398	-4.638934	-3.116815
C	2.456433	2.323699	-0.812514
C	2.507012	3.678556	-1.213981
C	2.821232	3.966806	-2.546674
C	3.080196	2.960505	-3.466736
C	3.023303	1.631546	-3.061364
C	2.710086	1.286424	-1.744246
C	2.232524	4.836422	-0.263825
C	3.425424	5.801786	-0.175300
C	2.692075	-0.176830	-1.322547
C	2.246664	-1.131722	-2.435483
O	-1.220902	0.788407	-0.169715
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H	-0.996453	4.317619	-0.832323
H	-4.118510	-0.626478	-0.298884
H	-4.197741	-0.929249	1.450314
C	-5.792352	0.336879	0.701258
H	3.058616	-0.075595	-0.793971
H	0.452822	-1.896712	1.401179
H	1.101822	4.076317	0.406240
H	-0.388351	2.218373	3.721454
H	-2.571799	-0.769977	-2.070610
H	-0.987034	-1.474863	-2.350313
H	-0.123477	0.522509	-3.318652
H	-1.720658	0.241359	-3.995828
H	-0.863781	2.301074	-1.899840
H	-1.343290	2.620457	-3.540908
H	-3.070894	3.319784	-2.003644
H	-3.679175	2.026072	-3.059939
C	-6.191134	0.920587	2.056322
C	-7.622798	1.423883	2.109706
O	-8.578218	0.371396	1.856250
C	-8.913536	-0.371863	2.928328
O	-9.800495	-1.325326	2.619974
O	-8.492276	-0.225756	4.048528
C	-10.285144	-1.432740	1.280443
H	-10.994794	-2.260583	1.296968
H	-10.790190	-0.515388	0.966978
H	-9.473984	-1.652827	0.581324
H	-5.922731	1.084363	-0.090939
H	-6.453416	-0.502042	0.449855
H	-6.048803	0.179297	2.850817
H	-5.534006	1.763219	2.302053
H	-7.842908	1.864115	3.085331
H	-7.818815	2.159100	1.323758

TS($G_{7CC}\rightarrow H_{7CC}$)

G = -2422,118503 u.a.

C	2.519505	1.378344	-2.238568
C	1.976521	2.238496	-1.252456
C	1.666690	3.583563	-1.562696
C	1.828222	4.015488	-2.883843
C	2.299850	3.163337	-3.874651
C	2.657299	1.861193	-3.543301
N	1.688924	1.713100	0.048696
Zn	-0.034815	0.808740	0.381629
O	-2.080842	2.532128	0.366063

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C	-2.993296	1.757795	0.118200
O	-3.545397	1.031739	1.081047
C	-4.455645	-0.043377	0.774070
C	-5.901508	0.424181	0.747763
C	-6.363995	1.031816	2.071614
C	-7.807335	1.503067	2.059768
O	-8.729051	0.423844	1.792815
C	-9.093659	-0.301447	2.867193
O	-8.724101	-0.120574	4.000541
C	1.224546	4.589428	-0.506027
C	-0.176109	5.160106	-0.769202
C	2.998910	-0.032207	-1.913618
C	2.116764	-1.114676	-2.549586
C	2.636211	1.722245	0.997069
C	3.967547	2.368765	0.691702
C	2.497502	1.166781	2.273866
C	1.396382	0.534782	2.890342
C	1.649596	0.069247	4.308056
N	0.213476	0.348059	2.314265
C	-0.865879	-0.239687	3.052654
C	-1.187010	-1.599154	2.834900
C	-2.284786	-2.143032	3.509193
C	-3.054113	-1.375957	4.376578
C	-2.716623	-0.045170	4.592182
C	-1.624523	0.547876	3.950798
C	-0.344050	-2.501824	1.945784
C	-1.176580	-3.189761	0.857390
C	-1.290291	1.999606	4.271257
C	-2.393373	2.964859	3.814917
C	-1.009258	2.193443	5.770445
C	0.427848	-3.532779	2.784416
O	-1.324815	-0.106907	-0.581553
C	-1.616045	-0.422412	-1.905043
C	-1.303132	0.645539	-2.964117
C	-1.651068	2.082052	-2.578015
C	-3.084389	2.384395	-2.175305
O	-3.596598	1.618096	-1.061827
C	2.239362	5.738784	-0.384607
C	4.466354	-0.237691	-2.321299
O	-9.946514	-1.281376	2.544703
C	-10.369324	-1.431152	1.188466
H	0.894465	-0.636087	4.654871
H	2.635814	-0.398288	4.373576
H	1.652006	0.926585	4.989376
H	4.674081	2.216585	1.508718
H	4.402315	1.970777	-0.228755
H	3.844083	3.445217	0.539474
H	3.377837	1.242479	2.901968
H	-3.311471	0.549225	5.281055
H	-3.903235	-1.815937	4.892990
H	-2.532761	-3.190615	3.358439
H	3.060337	1.206031	-4.311538
H	2.410451	3.518283	-4.895801
H	1.584295	5.044455	-3.136329
H	4.821347	-1.215492	-1.977958
H	4.591765	-0.207867	-3.409100
H	5.121378	0.528117	-1.893980
H	2.508407	-2.111646	-2.318233
H	1.090866	-1.063298	-2.177080
H	2.086965	-1.013198	-3.640417
H	1.069934	-4.146836	2.142913
H	1.062064	-3.051528	3.535648
H	-0.257352	-4.206209	3.311755
H	-1.930707	-3.860203	1.284866
H	-1.675439	-2.439916	0.239243
H	-0.529689	-3.795980	0.212891
H	-0.661892	3.214526	5.963592
H	-1.914536	2.038558	6.367805
H	-0.250005	1.499199	6.142639
H	-2.118257	3.995808	4.066533

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H	-2.546242	2.902743	2.736471
H	-3.342898	2.745092	4.316513
H	1.974643	6.392701	0.453410
H	3.259352	5.376794	-0.222285
H	2.253443	6.354302	-1.291022
H	-0.418209	5.919952	-0.017624
H	-0.232049	5.640340	-1.752966
H	-0.942482	4.384797	-0.710539
H	-4.161103	-0.502092	-0.170766
H	-4.285849	-0.759882	1.581416
H	2.939144	-0.162151	-0.828617
H	0.394640	-1.872289	1.439821
H	1.189965	4.066748	0.455226
H	-0.382341	2.266514	3.721833
H	-2.696389	-0.643717	-1.967923
H	-1.109126	-1.354078	-2.219047
H	-0.231681	0.635097	-3.197285
H	-1.822769	0.359307	-3.890411
H	-0.987198	2.412903	-1.778635
H	-1.433569	2.740028	-3.429602
H	-3.185298	3.446692	-1.927258
H	-3.784911	2.145526	-2.980549
H	-11.060130	-2.274959	1.194104
H	-10.880746	-0.533488	0.831304
H	-9.523441	-1.647834	0.530693
H	-6.033008	1.143656	-0.069660
H	-6.523630	-0.445461	0.501250
H	-6.235234	0.314160	2.889937
H	-5.735696	1.895931	2.318732
H	-8.075140	1.958464	3.016328
H	-7.988836	2.216785	1.250862

H_{7CC}

G = -2422,139796 u.a.

C	-1.181262	3.607887	3.186239
C	-1.270883	2.320060	2.614383
C	-2.518887	1.675514	2.466540
C	-3.665573	2.335633	2.916936
C	-3.591944	3.598110	3.493714
C	-2.358214	4.225258	3.620053
N	-0.088589	1.688625	2.106291
C	0.633906	0.881966	2.886622
C	0.189731	0.655724	4.312137
C	-2.643640	0.320831	1.785437
C	-3.504604	-0.672832	2.575578
C	0.143555	4.348594	3.290151
C	0.396894	4.925523	4.688954
C	1.801946	0.214118	2.471700
C	2.451864	0.210118	1.224774
C	3.710841	-0.616205	1.113917
N	2.029476	0.886679	0.152977
Zn	0.444133	2.025145	0.256518
O	-0.351881	3.202715	-0.884869
C	-0.187951	3.188953	-2.279501
C	-0.377469	4.591450	-2.862554
C	-1.674252	5.288724	-2.441602
C	-2.922275	4.510110	-2.819730
O	-4.114267	5.241864	-2.453668
C	-4.586434	6.091479	-3.381724
O	-5.642779	6.792668	-2.942710
C	-6.134571	6.621687	-1.601105
C	-7.090549	5.445267	-1.481977
C	-8.315314	5.566180	-2.388479
C	-9.261901	4.382519	-2.297548
O	-9.776978	4.199650	-0.960519
C	-10.852981	4.947659	-0.650400
O	-11.275689	4.723610	0.600161
C	-10.602656	3.758732	1.409861
C	2.753254	0.826167	-1.082300

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C	2.424302	-0.162329	-2.036723
C	3.079225	-0.137744	-3.271774
C	4.033936	0.828918	-3.564526
C	4.351457	1.791301	-2.613315
C	3.727335	1.810930	-1.362443
C	1.363057	-1.219562	-1.769431
C	1.874970	-2.644114	-2.023864
C	4.082628	2.898820	-0.359388
C	5.595754	3.025397	-0.137636
O	-4.149040	6.237928	-4.496269
O	-11.402638	5.732766	-1.381623
C	3.478127	4.248200	-0.777935
C	0.095826	-0.946421	-2.593763
C	-3.179505	0.490412	0.354611
C	0.228594	5.447854	2.218958
H	-0.813835	0.219705	4.339799
H	0.875174	-0.009319	4.839066
H	0.130686	1.603936	4.855228
H	3.944399	-1.108716	2.058663
H	3.610131	-1.379212	0.336056
H	4.559947	0.011404	0.825462
H	2.274004	-0.393813	3.233819
H	-2.306466	5.217732	4.059681
H	-4.494765	4.094816	3.838784
H	-4.633576	1.853672	2.808694
H	2.831892	-0.887071	-4.019264
H	4.528824	0.832675	-4.531807
H	5.097497	2.546289	-2.846706
H	1.114742	-3.378036	-1.735398
H	2.103267	-2.810591	-3.082096
H	2.784127	-2.858118	-1.452822
H	-0.680909	-1.685198	-2.367130
H	-0.309619	0.048840	-2.387328
H	0.306406	-0.999671	-3.667692
H	-3.489708	-1.655216	2.091421
H	-3.142676	-0.796529	3.601398
H	-4.551241	-0.354695	2.629745
H	-4.195341	0.901350	0.367019
H	-2.555423	1.176839	-0.226840
H	-3.212539	-0.473481	-0.165691
H	1.395364	5.373100	4.738136
H	-0.322789	5.710852	4.943727
H	0.334254	4.154565	5.463971
H	1.203156	5.947861	2.255337
H	0.086146	5.041098	1.212697
H	-0.543704	6.208380	2.381012
H	5.801951	3.748567	0.658651
H	6.044981	2.069155	0.149529
H	6.112148	3.377360	-1.037094
H	3.715033	5.023009	-0.040233
H	3.878050	4.572764	-1.745179
H	2.388816	4.190167	-0.870322
H	-5.295219	6.515427	-0.909930
H	-6.650972	7.562940	-1.389274
H	1.087197	-1.153507	-0.712068
H	-1.638375	-0.106664	1.711897
H	3.635182	2.622992	0.601126
H	0.942414	3.627852	3.086458
H	-0.919394	2.504496	-2.748871
H	0.805787	2.824338	-2.589545
H	0.464841	5.220323	-2.549168
H	-0.326266	4.521401	-3.958448
H	-1.667573	5.437577	-1.357439
H	-1.723526	6.274305	-2.918595
H	-2.992721	3.577291	-2.257206
H	-2.959057	4.303272	-3.893033
H	-11.141954	3.752010	2.357742
H	-10.637442	2.765619	0.954384
H	-9.559520	4.039755	1.577925
H	-6.542377	4.520528	-1.698945

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H	-7.407351	5.380596	-0.433539
H	-8.876085	6.480198	-2.160207
H	-7.993152	5.653522	-3.433061
H	-10.106061	4.507164	-2.980124
H	-8.748360	3.442195	-2.517550

3.2.2 Ring-opening polymerization of TMC

Study of the TMC ROP Initiation

A_{TMC}

G = -1962,087971 u.a.

C	-1.695989	0.317981	3.556844
C	0.187035	-1.158504	2.759062
C	-1.140288	-1.113067	3.531190
C	-4.142078	-2.671785	4.561909
C	-0.997145	-1.709256	4.927145
C	-0.380710	-0.958877	5.932331
C	-0.222258	-1.462253	7.218935
C	-0.683150	-2.738105	7.516785
C	-1.293809	-3.538270	6.545351
C	-1.448929	-3.015144	5.241860
N	-2.001816	-3.833494	4.207484
C	-3.255150	-3.630611	3.797669
C	-3.823848	-4.209369	2.650377
C	-3.253059	-5.038243	1.664360
C	0.991827	-4.198658	-0.250277
C	-0.501570	-4.467627	-0.491238
H	1.609096	-4.736010	-0.980567
H	-5.151884	-5.130037	0.637624
C	-4.086815	-5.221263	0.413786
C	-0.951161	-3.896190	-1.843908
C	-0.824379	-5.949262	-0.362679
C	-1.585635	-6.466194	0.709097
C	-1.857707	-7.853529	0.802372
C	-1.380545	-8.691865	-0.209496
C	-0.632098	-8.195956	-1.271597
C	-0.352703	-6.836757	-1.336173
H	-4.636644	-7.735426	1.331832
H	-4.668361	-9.108014	2.441431
C	-4.129417	-8.666159	1.595640
C	-2.652830	-8.443158	1.961254
C	-2.056590	-9.756714	2.484761
N	-2.044364	-5.592350	1.745970
Zn	-0.812061	-5.087556	3.229136
O	1.062887	-4.974283	3.092018
C	1.832176	-4.310098	4.054841
C	-1.799641	-4.922316	6.925252
C	-3.043002	-4.831829	7.824018
H	0.165634	-5.873657	6.962684
H	-3.412362	-5.833801	8.069806
H	-2.813090	-4.319577	8.765378
H	-3.858098	-4.285356	7.339796
H	1.894835	-4.860412	5.011057
H	-1.101523	-6.784572	7.788334
H	-2.089863	-5.432087	6.002079
H	1.467878	-3.301259	4.301852
H	2.867701	-4.183941	3.690684
O	-0.520200	-7.012573	4.395770
C	0.570912	-7.457124	4.068947
O	1.526543	-7.618353	4.982838
O	0.789373	-7.889124	2.834005
C	2.105208	-7.895380	2.232285
H	2.195257	-8.880157	1.765543
H	2.083418	-7.124910	1.460211
C	2.747391	-8.258269	4.568881
H	3.449856	-8.081891	5.384513
H	2.569022	-9.337621	4.482534

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H	-0.406700	-5.355720	8.560925
H	-0.566908	-3.125791	8.525648
H	0.255725	-0.859294	7.986500
H	-0.018330	0.039944	5.703606
H	-0.980454	1.026676	3.987650
H	-2.619824	0.387052	4.140451
H	-1.911650	0.657433	2.537930
H	0.066206	-0.713919	1.764325
H	0.966170	-0.595350	3.285467
H	0.540197	-2.185354	2.629735
H	-1.852786	-1.727922	2.973371
H	-3.932933	-1.636848	4.270196
H	-3.971495	-2.738927	5.638390
H	-5.194746	-2.871718	4.352372
H	-4.845538	-3.907064	2.449772
H	1.285748	-4.503455	0.759927
H	1.208549	-3.129455	-0.359024
H	-1.058223	-3.938208	0.288884
H	-0.800378	-2.811346	-1.867578
H	-2.009935	-4.096408	-2.037713
H	-0.377674	-4.322491	-2.674469
H	-3.831395	-4.429902	-0.301244
H	-3.902100	-6.174208	-0.082608
H	0.235268	-6.450321	-2.165093
H	-0.268635	-8.867425	-2.045349
H	-1.592795	-9.756415	-0.159939
H	-2.612196	-7.717769	2.779201
H	-0.988759	-9.656338	2.690188
H	-2.560069	-10.047963	3.412782
H	-2.191846	-10.580476	1.774204
H	-4.221844	-9.351718	0.744980
C	3.196871	-7.651545	3.257455
H	3.353764	-6.579430	3.397887
H	4.137661	-8.099822	2.922626
C	-0.717689	-5.776721	7.597861

$TS(A_{TMC} \rightarrow B_{TMC})$

G = -1962,076651 u.a.

C	-1.651974	0.287959	3.737374
C	0.356819	-0.972505	2.899948
C	-0.997731	-1.097041	3.612908
C	-4.069246	-2.528340	4.499664
C	-0.867035	-1.787193	4.966037
C	-0.196236	-1.121308	5.996912
C	-0.053966	-1.690498	7.256442
C	-0.591926	-2.947593	7.502933
C	-1.261338	-3.664683	6.506554
C	-1.393123	-3.077014	5.225809
N	-1.997729	-3.827009	4.167762
C	-3.234920	-3.547988	3.754765
C	-3.849486	-4.112175	2.620943
C	-3.349170	-5.000136	1.650414
C	0.925856	-4.315754	-0.209550
C	-0.572268	-4.518101	-0.481915
H	1.534154	-4.834810	-0.959668
H	-5.205327	-4.765997	0.569711
C	-4.232038	-5.243455	0.447911
C	-0.970309	-3.902125	-1.830628
C	-0.951371	-5.988630	-0.383587
C	-1.744254	-6.491178	0.673447
C	-2.069553	-7.866344	0.739980
C	-1.588735	-8.711886	-0.264808
C	-0.805139	-8.231648	-1.306741
C	-0.491834	-6.878838	-1.358713
H	-4.811418	-8.389413	0.741361
H	-4.827186	-9.455180	2.153286
C	-4.209751	-9.094891	1.323101
C	-2.917185	-8.458869	1.858300
C	-2.127579	-9.483862	2.685196

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N	-2.163412	-5.605930	1.718446
Zn	-0.983727	-5.276365	3.269522
O	1.024463	-5.355186	3.175814
C	1.881977	-4.396899	3.752996
C	-1.874849	-5.016767	6.842136
C	-3.174510	-4.837863	7.643440
H	0.015464	-6.089510	7.021503
H	-3.629007	-5.811202	7.859403
H	-2.980246	-4.338152	8.599563
H	-3.910105	-4.238350	7.098485
H	2.587772	-4.886786	4.436288
H	-1.370912	-6.927388	7.723011
H	-2.130466	-5.509231	5.899730
H	1.342590	-3.641525	4.337737
H	2.461022	-3.882553	2.971480
O	-0.405756	-6.894380	4.350736
C	0.806897	-6.996686	4.008025
O	1.744382	-6.988986	4.994584
O	1.075812	-7.825976	2.965998
C	2.372893	-7.759362	2.358937
H	2.474025	-8.715586	1.840354
H	2.362024	-6.953401	1.621020
C	2.887205	-7.824748	4.774047
H	3.583390	-7.584120	5.580061
H	2.584679	-8.874912	4.874758
H	-0.656306	-5.562258	8.582424
H	-0.491579	-3.385959	8.491966
H	0.468607	-1.153915	8.043850
H	0.220614	-0.135243	5.807032
H	-1.002038	0.992462	4.267772
H	-2.600338	0.246058	4.281447
H	-1.846472	0.708478	2.744623
H	0.236113	-0.471729	1.932720
H	1.063667	-0.383101	3.494801
H	0.807284	-1.951377	2.719301
H	-1.641198	-1.713133	2.977668
H	-3.974035	-1.542765	4.031686
H	-3.762605	-2.428974	5.541880
H	-5.124981	-2.806920	4.460858
H	-4.856915	-3.757828	2.434712
H	1.195322	-4.701399	0.778602
H	1.185325	-3.251437	-0.250557
H	-1.122312	-3.982292	0.298134
H	-0.764423	-2.826019	-1.833943
H	-2.035151	-4.042858	-2.042607
H	-0.408117	-4.344528	-2.660315
H	-3.759349	-4.840289	-0.454079
H	-4.380157	-6.311007	0.269608
H	0.120929	-6.502958	-2.174403
H	-0.441689	-8.908307	-2.075761
H	-1.832527	-9.770615	-0.224736
H	-3.198461	-7.643029	2.531300
H	-1.230995	-9.034493	3.115178
H	-2.748098	-9.865563	3.504040
H	-1.826855	-10.340879	2.071172
H	-3.994458	-9.953388	0.676908
C	3.478561	-7.558505	3.401722
H	3.865161	-6.535920	3.370148
H	4.320611	-8.234124	3.217905
C	-0.907646	-5.944628	7.586281

B_{TMC}

G = -1962,089234 u.a.

C	-0.606331	0.034072	3.490463
C	1.376518	-1.532879	3.538066
C	-0.145304	-1.415001	3.706390
C	-3.956950	-2.230012	4.140537
C	-0.595943	-1.958082	5.054519
C	-0.099839	-1.375845	6.225321

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C	-0.464968	-1.848125	7.479457
C	-1.340797	-2.923028	7.579537
C	-1.873571	-3.535392	6.441744
C	-1.496792	-3.038616	5.172726
N	-1.988203	-3.687192	3.991314
C	-3.175694	-3.345080	3.486202
C	-3.789005	-3.980565	2.390082
C	-3.354198	-5.058545	1.598746
C	0.356729	-4.523340	-0.841601
C	-1.105363	-4.985721	-0.911665
H	0.991031	-5.132043	-1.496190
H	-5.291262	-5.081879	0.649672
C	-4.305721	-5.532834	0.525166
C	-1.663411	-4.793315	-2.328862
C	-1.247051	-6.418388	-0.414651
C	-1.794137	-6.729532	0.852390
C	-1.897937	-8.070525	1.286084
C	-1.430722	-9.082174	0.440568
C	-0.878567	-8.790971	-0.800346
C	-0.794171	-7.467997	-1.219027
H	-4.516957	-8.811121	1.808459
H	-4.239724	-9.518683	3.408708
C	-3.773919	-9.309788	2.439408
C	-2.513928	-8.450700	2.625159
C	-1.500475	-9.151802	3.541340
N	-2.175974	-5.672431	1.740429
Zn	-0.987890	-5.183736	3.221217
O	2.089269	-4.915491	4.732886
C	2.192676	-5.410150	6.057468
C	-2.804201	-4.730211	6.601083
C	-3.942359	-4.465528	7.596264
H	-1.237893	-6.223325	6.268866
H	-4.642772	-5.307668	7.602536
H	-3.569193	-4.347057	8.619146
H	-4.504261	-3.560269	7.343539
H	2.956325	-6.192705	6.130989
H	-2.683582	-6.851486	7.085821
H	-3.263986	-4.929835	5.627634
H	1.233102	-5.805323	6.406644
H	2.479129	-4.560224	6.680408
O	0.329719	-6.224135	4.035491
C	1.589544	-5.834250	3.799672
O	2.489234	-6.918527	3.778823
O	1.622404	-5.146808	2.551723
C	2.912793	-5.199552	1.938341
H	2.892860	-4.492379	1.106198
H	3.662236	-4.863120	2.662746
C	2.527013	-7.566528	2.513977
H	3.092086	-8.490439	2.660322
H	1.511325	-7.834348	2.199605
H	-1.528232	-5.845159	7.973201
H	-1.615632	-3.297286	8.562185
H	-0.065066	-1.383607	8.376823
H	0.591641	-0.540567	6.148927
H	-0.165126	0.706799	4.234321
H	-1.694386	0.133032	3.560026
H	-0.300130	0.389612	2.500283
H	1.672060	-1.221081	2.529771
H	1.904518	-0.886794	4.248724
H	1.713678	-2.559650	3.700280
H	-0.612586	-2.028846	2.929267
H	-3.324383	-1.357450	4.320609
H	-4.332267	-2.550298	5.118309
H	-4.808714	-1.933639	3.526576
H	-4.763995	-3.588268	2.126908
H	0.741326	-4.607592	0.177628
H	0.448682	-3.479016	-1.161257
H	-1.677228	-4.337308	-0.240820
H	-1.645371	-3.732736	-2.601826
H	-2.695845	-5.147421	-2.415854

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H	-1.069153	-5.330227	-3.076082
H	-3.933308	-5.272685	-0.470497
H	-4.406263	-6.621476	0.547932
H	-0.364284	-7.243646	-2.191728
H	-0.519084	-9.591455	-1.441343
H	-1.503801	-10.117380	0.763980
H	-2.823878	-7.525373	3.122511
H	-0.637009	-8.510194	3.738712
H	-1.966987	-9.401565	4.501015
H	-1.144211	-10.087910	3.096302
H	-3.536531	-10.272271	1.973097
C	3.189770	-6.635987	1.484824
H	4.271652	-6.802273	1.430245
H	2.772553	-6.823492	0.489508
C	-2.015320	-5.986808	7.001643

TS(B_{TMC}→C_{TMC})

G = -1962,078512 u.a.

H	1.696308	3.587567	-1.697338
C	1.944342	2.558945	-1.416414
H	2.371820	2.061926	-2.294216
H	1.003598	2.050081	-1.179061
C	2.927857	2.497514	-0.237100
H	0.611415	2.150697	1.086371
C	1.185943	2.966208	1.518300
C	3.221055	1.035487	0.131367
H	3.596206	0.493724	-0.744675
H	2.311670	0.526184	0.470992
H	3.966907	0.968739	0.925417
H	3.870828	2.947113	-0.564311
C	0.673585	3.659862	2.608044
C	2.426198	3.292196	0.961217
C	3.163302	4.351870	1.538004
C	1.406348	4.703912	3.160053
C	2.654053	5.068456	2.645163
H	1.002802	5.252148	4.007908
N	4.466581	4.672914	1.035757
C	4.597310	5.513267	0.011554
C	3.364280	6.125828	-0.612996
H	2.634157	6.417407	0.144788
H	3.624354	6.997675	-1.215657
H	2.869937	5.398168	-1.265050
C	3.407132	6.229908	3.278810
H	4.353521	6.341435	2.740206
C	3.746443	5.949879	4.749144
H	4.317212	6.783562	5.174766
H	4.345478	5.039533	4.834267
H	2.840223	5.829967	5.353857
C	2.636329	7.551251	3.139323
H	3.219684	8.380606	3.554900
H	2.416788	7.786612	2.093110
H	1.682305	7.516483	3.677363
C	5.826091	5.871362	-0.577027
H	5.740542	6.541074	-1.424813
C	7.141592	5.488397	-0.268124
H	7.876952	6.924356	-1.701391
C	8.203885	6.001898	-1.217430
H	9.159436	6.176805	-0.721009
H	8.378943	5.259349	-2.004043
N	7.491751	4.699472	0.753552
C	8.874734	4.425383	0.994878
C	9.519951	3.358965	0.329169
C	10.864209	3.105768	0.624984
C	11.563157	3.879497	1.541539
C	10.914429	4.920526	2.197531
H	10.425409	7.013134	4.100433
C	9.568863	5.208321	1.951934
H	8.776265	7.240336	4.670173
H	9.499221	5.621580	4.678672

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C	9.428929	6.557470	4.116331
C	8.877292	6.341312	2.701614
H	8.458025	8.468016	2.512399
C	8.927962	7.669055	1.927941
H	8.403569	7.608657	0.972112
H	9.965293	7.962381	1.730503
H	11.463908	5.515257	2.920790
H	12.608951	3.670406	1.750213
H	11.370975	2.286456	0.121529
H	10.513075	1.953574	-1.960863
C	9.540440	2.451905	-2.038971
H	9.718994	3.458549	-2.429813
Zn	6.075360	3.831186	1.838281
H	7.811770	2.894882	-0.854245
C	8.809571	2.476507	-0.687937
H	8.950606	1.899652	-2.778483
C	8.622525	1.047780	-0.155234
H	8.008528	1.041664	0.748672
H	8.122371	0.425136	-0.905636
H	9.589460	0.582980	0.070531
O	6.148014	1.812878	2.088350
C	5.717672	1.725020	3.285263
O	5.985182	3.462534	3.829247
O	6.395371	1.037307	4.236453
O	4.388034	1.591896	3.433078
C	3.863306	1.552184	4.756197
H	2.779560	1.581214	4.641056
H	4.164083	0.637092	5.273741
H	4.197465	2.427810	5.319081
C	7.822431	1.196233	4.209735
H	8.220353	0.742956	3.297390
H	8.158611	0.608184	5.066915
C	7.040496	3.532086	4.763235
H	6.672115	3.191212	5.743550
H	7.353683	4.576807	4.884717
H	7.819799	6.063131	2.793979
H	-0.295027	3.391540	3.021812
C	8.230700	2.670633	4.338559
H	9.039633	2.770447	5.072107
H	8.619941	3.044520	3.386536

C_{TMC}

G = -1962,088219 u.a.

H	1.559924	3.720761	-1.591368
C	1.869608	2.689474	-1.395488
H	2.273968	2.272942	-2.324629
H	0.966351	2.120124	-1.150117
C	2.913381	2.597138	-0.270454
H	0.652179	2.155035	1.106290
C	1.229535	2.955919	1.561373
C	3.257588	1.126096	0.003103
H	3.571144	0.632867	-0.924371
H	2.387963	0.582982	0.390643
H	4.066982	1.040952	0.729045
H	3.829598	3.081818	-0.621023
C	0.737138	3.592347	2.694839
C	2.450600	3.322741	0.987499
C	3.195355	4.360775	1.597197
C	1.466861	4.627607	3.267317
C	2.696089	5.032313	2.737512
H	1.072645	5.143067	4.139656
N	4.493156	4.702697	1.097156
C	4.613574	5.484948	0.026347
C	3.379784	6.077625	-0.617665
H	2.600516	6.284057	0.118317
H	3.630544	7.000952	-1.143836
H	2.958821	5.381663	-1.350679
C	3.420160	6.212965	3.369511
H	4.368075	6.342214	2.837671

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C	3.756193	5.967767	4.846039
H	4.267099	6.842272	5.265669
H	4.421943	5.105940	4.942409
H	2.852600	5.799281	5.443575
C	2.614385	7.509896	3.194725
H	3.171819	8.363486	3.596486
H	2.396926	7.715071	2.141507
H	1.657229	7.459636	3.726239
C	5.834707	5.809895	-0.595203
H	5.737892	6.436643	-1.474334
C	7.153026	5.438014	-0.284817
H	7.862998	6.779063	-1.817635
C	8.204083	5.895936	-1.273793
H	9.157785	6.119045	-0.792753
H	8.387656	5.104707	-2.008877
N	7.513552	4.718918	0.782606
C	8.899141	4.466478	1.032747
C	9.560141	3.389695	0.398708
C	10.905429	3.157352	0.708182
C	11.589888	3.959067	1.610434
C	10.926800	5.011282	2.233864
H	10.475584	7.302430	3.908307
C	9.581776	5.284247	1.970342
H	8.851864	7.502200	4.559858
H	9.652148	5.926674	4.662065
C	9.505983	6.805048	4.026487
C	8.881889	6.443191	2.673187
H	8.348077	8.525764	2.346852
C	8.820507	7.704784	1.795935
H	8.242145	7.546122	0.883899
H	9.828858	8.027441	1.512156
H	11.467166	5.629719	2.943474
H	12.635889	3.765060	1.832493
H	11.423668	2.331037	0.228243
H	10.585495	1.924432	-1.842191
C	9.609352	2.411819	-1.942244
H	9.783684	3.407919	-2.360507
Zn	6.123190	4.054189	2.041092
H	7.864843	2.864815	-0.780839
C	8.868388	2.468444	-0.597340
H	9.030213	1.833542	-2.670363
C	8.702855	1.051780	-0.026816
H	8.090373	1.059756	0.877480
H	8.211139	0.401523	-0.759227
H	9.676597	0.608048	0.211270
O	6.080432	1.704112	2.090539
C	5.540734	1.442388	3.162854
O	6.146041	3.842589	3.911299
O	6.153480	1.000047	4.248872
O	4.226889	1.504144	3.291422
C	3.648357	1.445724	4.601350
H	2.587359	1.636041	4.446300
H	3.802362	0.462217	5.052121
H	4.085986	2.223931	5.228874
C	7.599283	1.050749	4.269479
H	7.982102	0.373103	3.500114
H	7.831052	0.630545	5.250863
C	7.286004	3.583560	4.671319
H	6.977240	3.318370	5.699132
H	7.923302	4.478529	4.771312
H	7.847697	6.127823	2.863265
H	-0.217702	3.293576	3.119963
C	8.176297	2.456777	4.123297
H	9.139426	2.463871	4.650853
H	8.402638	2.667798	3.073428

$TS(C_{TMC} \rightarrow D_{TMC})$

G = -1962,085977 u.a.

C	-0.963364	-1.691452	2.941696

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H	-1.151330	-0.646631	3.208441
H	-1.623310	-2.304478	3.559147
H	0.074583	-1.918379	3.192074
C	-1.215685	-1.917980	1.468548
H	-3.824486	-5.604614	4.006434
C	-3.011737	-5.375220	3.308187
C	-0.074474	-1.881748	0.642710
H	-2.532856	-6.322366	3.035805
H	-2.276273	-4.767411	3.845216
H	0.852437	-1.669326	1.161956
H	-2.557643	0.843518	3.891196
H	-2.631707	2.270493	2.840944
H	-4.080651	1.704537	3.672250
C	-3.173256	1.371951	3.156204
C	-3.510868	0.499243	1.935614
C	-4.104953	-0.841406	2.350779
H	-2.578654	0.303454	1.396435
C	-5.236581	-0.847463	3.172106
H	-6.691991	-2.011225	4.250340
C	-5.815644	-2.033468	3.607679
H	-5.671072	0.100888	3.477119
H	-3.977136	2.234977	0.720216
C	-4.432523	1.272448	0.981341
H	-5.399245	1.480811	1.453829
H	-4.617600	0.718056	0.059609
C	-5.255815	-3.247000	3.226906
H	-5.696945	-4.175652	3.580523
C	-3.560808	-2.085838	1.952780
C	-4.128330	-3.300654	2.401770
N	-2.458768	-2.130207	1.035764
C	-3.535004	-4.658912	2.053521
H	-2.674649	-4.488962	1.397608
H	-0.961673	-0.154149	-2.503921
C	-4.528656	-5.542563	1.287100
H	-5.428835	-5.739675	1.880573
Zn	-2.778586	-2.631544	-0.851394
H	-4.818950	-5.064790	0.346963
H	-4.071612	-6.511020	1.052937
N	-0.954288	-2.399743	-1.554930
C	0.057344	-2.091023	-0.738046
H	2.180991	-1.754454	-0.534547
C	1.449288	-1.975859	-1.312641
H	1.488171	-1.181274	-2.063492
H	1.743731	-2.899691	-1.819151
C	-0.714044	-2.726787	-2.928314
C	-0.824388	-1.731742	-3.926059
C	-0.751199	-2.126847	-5.266480
H	-0.844213	-1.374294	-6.045567
H	-0.518133	-3.742210	-6.669167
C	-0.560158	-3.456339	-5.621560
C	-0.394618	-4.415110	-4.627849
H	-1.579641	-6.630097	-3.017268
H	-0.209980	-5.448656	-4.909165
C	-1.364477	-6.124681	-2.068934
H	-2.276157	-5.616273	-1.742328
C	-0.450986	-4.074883	-3.273356
C	-0.192197	-5.144700	-2.217678
H	-0.072684	-4.638500	-1.254565
H	-1.126269	-6.895036	-1.326792
C	1.111210	-5.910130	-2.492182
H	1.337615	-6.582106	-1.657310
H	1.961527	-5.232908	-2.622303
H	1.039028	-6.526139	-3.394983
H	0.176182	1.589391	-3.801591
C	0.227233	0.549709	-4.142669
H	1.187897	0.134487	-3.821753
H	0.227757	0.562554	-5.238240
C	-0.965725	-0.251351	-3.594378
C	-2.280780	0.353876	-4.105540
H	-2.377755	0.231679	-5.190634

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H	-2.306761	1.428369	-3.892186
H	-3.152553	-0.094424	-3.623497
O	-4.257831	-3.548314	-1.469301
O	-4.846444	-0.568831	-1.966956
C	-5.796204	-1.275341	-1.690427
O	-6.313664	-1.298349	-0.465560
C	-7.279709	-2.302582	-0.138080
H	-7.453859	-2.188876	0.931422
H	-8.208107	-2.149416	-0.694948
H	-6.872690	-3.292532	-0.350907
O	-6.470981	-2.044008	-2.546340
C	-5.889910	-2.206374	-3.854033
H	-6.654312	-2.776156	-4.388744
H	-5.356206	-4.657284	-2.775703
C	-4.440391	-4.041353	-2.769308
H	-3.620398	-4.708854	-3.076757
H	-5.791322	-1.222369	-4.323699
C	-4.561412	-2.956015	-3.843973
H	-3.727047	-2.259748	-3.722810
H	-4.440346	-3.412469	-4.835564

D_{TMC}

G = -1962,102449 u.a.

C	0.022371	-4.087381	-3.298981
C	-0.148236	-2.770854	-2.815580
C	-0.043643	-1.659888	-3.682589
C	0.222369	-1.894267	-5.034930
C	0.385722	-3.184148	-5.526186
C	0.287598	-4.266480	-4.659998
N	-0.522248	-2.560694	-1.448632
C	0.407331	-2.412179	-0.499823
C	1.863483	-2.470784	-0.894916
C	-0.244724	-0.233548	-3.190823
C	-1.600087	0.321160	-3.655853
C	-0.107871	-5.303189	-2.392393
C	1.096056	-6.249116	-2.500163
Zn	-2.419126	-2.451471	-1.008874
O	-3.983755	-2.477476	-1.941645
C	-4.125056	-2.901322	-3.273321
C	-5.428002	-2.358640	-3.859650
C	-6.632315	-2.817639	-3.057950
O	-7.856363	-2.230912	-3.555502
C	-8.422255	-2.861121	-4.596171
O	-9.535859	-2.239357	-5.013185
C	-9.961983	-1.049151	-4.350168
N	-2.298814	-2.160235	0.921981
C	-3.508112	-2.034388	1.681420
C	-4.106107	-0.764286	1.831458
C	-5.314468	-0.676440	2.528884
C	-5.924204	-1.805159	3.062990
C	-5.331939	-3.050947	2.892711
C	-4.124819	-3.193228	2.202428
C	-3.502949	0.486443	1.209844
C	-4.315646	0.915287	-0.022507
C	-3.543948	-4.581121	1.976781
C	-4.349950	-5.324153	0.899028
C	-3.369720	1.643237	2.208969
C	-1.111789	-2.085049	1.525621
C	0.124778	-2.199526	0.860314
C	-1.063415	-1.858505	3.017975
C	-3.454360	-5.410916	3.263667
C	-1.416044	-6.058562	-2.670987
C	0.898309	0.700504	-3.610804
O	-8.021914	-3.869330	-5.124191
H	-1.548634	-0.913359	3.281314
H	-1.609666	-2.645006	3.547497
H	-0.035386	-1.838050	3.381959
H	-4.444670	-5.644175	3.669256
H	-2.952996	-6.364321	3.065333

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H	-2.891029	-4.889000	4.044125
H	0.995415	-2.106496	1.497946
H	-2.795330	1.350817	3.094114
H	-2.859665	2.492152	1.740968
H	-4.346624	2.000407	2.552179
H	-2.493583	0.234381	0.867885
H	-6.863205	-1.715678	3.602442
H	-5.788644	0.294186	2.647960
H	-3.850324	1.778580	-0.511912
H	-5.333649	1.202333	0.264766
H	-4.393908	0.103126	-0.752217
H	-5.820356	-3.934044	3.296005
H	-2.524121	-4.457523	1.598081
H	-0.258754	-0.258816	-2.096308
H	-5.378603	-5.498039	1.234445
H	-4.400989	-4.746710	-0.029735
H	-3.899284	-6.298420	0.678425
H	2.513437	-2.313733	-0.033126
H	2.090192	-1.711304	-1.649656
H	2.106034	-3.438472	-1.344870
H	0.297630	-1.050470	-5.715720
H	0.588034	-3.345541	-6.581432
H	-1.440103	-6.437104	-3.698734
H	0.412979	-5.273662	-5.048911
H	-2.289122	-5.412129	-2.538289
H	-0.150456	-4.944790	-1.358814
H	-1.520942	-6.914353	-1.994978
H	1.008400	-7.058605	-1.767600
H	2.040434	-5.726979	-2.315602
H	1.163012	-6.712166	-3.490433
H	0.765004	1.689258	-3.158914
H	1.873290	0.314112	-3.296655
H	0.932348	0.841322	-4.696428
H	-1.655192	0.353876	-4.749699
H	-1.750212	1.339980	-3.281477
H	-2.431612	-0.295356	-3.299485
H	-10.872063	-0.740891	-4.866651
H	-10.178240	-1.237860	-3.295175
H	-9.207021	-0.261755	-4.423918
H	-6.557729	-2.480584	-2.023930
H	-4.145127	-4.004547	-3.340851
H	-3.293785	-2.570527	-3.917551
H	-6.731756	-3.906585	-3.086562
H	-5.530858	-2.699256	-4.896617
H	-5.394536	-1.262361	-3.861446

Study of Propagation step of the TMC ROP reaction

E_{TMC}

G = -2343,578799 u.a.

O	-2.580203	-1.788093	4.323332
C	-1.818144	-2.362011	3.399182
O	-0.702821	-1.785160	2.983694
C	-0.237426	-0.512115	3.483924
C	-1.382568	0.309482	4.026174
C	-2.182399	-0.555668	4.971700
O	-2.159064	-3.440499	2.931447
Zn	-1.906551	-3.900224	0.776191
O	-2.540776	-2.216981	0.232064
C	-3.804630	-1.771118	0.617479
C	-3.883085	-0.250302	0.458347
C	-5.238688	0.355151	0.774378
O	-5.750472	-0.043628	2.072568
C	-5.197660	0.538860	3.136614
O	-5.697195	0.071796	4.289147
C	-6.690472	-0.959483	4.254576
N	-2.932544	-5.565942	0.327091
C	-2.308510	-6.656933	-0.107888

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C	-0.911149	-6.776862	-0.237903
C	0.113112	-5.847550	0.013789
C	1.498928	-6.266881	-0.430992
C	-4.356699	-5.469902	0.259910
C	-5.126274	-5.653417	1.431869
C	-6.510140	-5.464980	1.359040
C	-7.128552	-5.091858	0.172080
C	-6.361333	-4.920953	-0.974610
C	-4.976547	-5.113018	-0.962650
C	-4.497918	-6.094786	2.746289
C	-4.890157	-5.190297	3.921179
C	-4.189770	-4.925122	-2.254702
C	-4.051258	-3.441115	-2.626218
C	-3.114750	-7.857165	-0.555287
C	-4.795993	-5.720876	-3.420206
C	-4.846167	-7.558374	3.061417
N	-0.067695	-4.638429	0.550967
C	1.067566	-3.827757	0.865462
C	1.564720	-2.900788	-0.076327
C	2.652377	-2.098625	0.286947
C	3.250411	-2.212270	1.535431
C	2.747558	-3.125924	2.456644
C	1.647757	-3.933809	2.154139
C	0.954359	-2.745658	-1.461638
C	2.004474	-2.888437	-2.573047
C	1.097777	-4.898641	3.198356
C	1.139104	-4.329504	4.622297
C	0.197460	-1.414957	-1.593816
C	1.815898	-6.257830	3.176671
O	-4.343000	1.396945	3.125017
H	0.866990	-0.565719	-1.410989
H	1.569569	-7.352227	-0.525467
H	1.681361	-6.778650	2.226434
H	1.424048	-6.908753	3.966628
H	-4.598137	-4.154500	3.734362
H	-4.360235	-7.878372	3.990146
H	-5.927267	-7.687972	3.187729
H	-4.522486	-8.235193	2.264949
H	-4.382048	-5.519247	4.834510
H	-3.412182	-6.026515	2.628808
H	0.512837	-0.726765	4.253124
H	0.260856	-0.046805	2.632576
H	-3.119543	-0.083698	5.267258
H	-1.610192	-0.826219	5.867124
H	-5.967978	-5.223864	4.118175
H	-7.113049	-5.616129	2.251004
H	-8.204720	-4.943391	0.137657
H	-6.847712	-4.634936	-1.903712
H	-5.771998	-5.323300	-3.719616
H	-4.935465	-6.776987	-3.166705
H	-4.141592	-5.664747	-4.296984
H	-3.503951	-3.336940	-3.570652
H	-5.036259	-2.978606	-2.760823
H	-3.506353	-2.891666	-1.851915
H	-3.177489	-5.306383	-2.089881
H	-3.402267	-7.750214	-1.607156
H	-4.036754	-7.961479	0.019404
H	-2.526654	-8.772689	-0.463110
H	-0.574804	-7.725103	-0.641809
H	-0.643047	-1.364524	-0.894724
H	-0.203378	-1.308166	-2.608664
H	0.223342	-3.550511	-1.591857
H	1.519646	-2.880723	-3.555331
H	2.572658	-3.819933	-2.481706
H	2.723189	-2.061539	-2.559189
H	1.705224	-5.830882	-1.415657
H	2.281273	-5.913348	0.242084
H	3.042758	-1.379327	-0.428789
H	4.105595	-1.591870	1.791543
H	3.216524	-3.207331	3.433478

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H	0.047342	-5.074663	2.945003
H	0.709079	-3.325230	4.667705
H	0.569742	-4.975339	5.299095
H	2.160774	-4.275411	5.015353
H	2.891812	-6.133681	3.346678
H	-2.033415	0.671859	3.226179
H	-0.997403	1.184545	4.558993
H	-4.041845	-2.024338	1.666063
H	-4.611203	-2.230391	0.014314
H	-3.111433	0.220407	1.075385
H	-3.644108	0.004353	-0.582332
H	-6.006328	-0.005836	0.085133
H	-5.205706	1.447918	0.741016
H	-7.589987	-0.618549	3.736065
H	-6.920191	-1.171363	5.299255
H	-6.307469	-1.857076	3.764499

TS(E_{TMC}→F_{TMC})

G = -2343,563192 u.a.

O	-2.913717	-2.057922	4.016437
C	-1.881539	-2.592738	3.299303
O	-0.717107	-1.895173	3.378987
C	-0.788640	-0.471374	3.219173
C	-1.883795	0.146859	4.104134
C	-2.554896	-0.971809	4.882827
O	-1.773590	-3.857703	3.280765
Zn	-1.710689	-4.211276	1.302128
O	-2.343959	-2.294292	1.562476
C	-3.662273	-1.854993	1.286229
C	-3.665952	-0.468756	0.645911
C	-5.060337	0.080030	0.389343
O	-5.880974	0.100708	1.578899
C	-5.613431	1.076180	2.460704
O	-6.401327	1.008219	3.539996
C	-7.384544	-0.027199	3.628569
N	-2.856678	-5.579112	0.441872
C	-2.286031	-6.641471	-0.133137
C	-0.903247	-6.801952	-0.323050
C	0.169760	-5.929283	-0.049521
C	1.513814	-6.348432	-0.601732
C	-4.276382	-5.414903	0.412963
C	-5.029596	-5.630894	1.590858
C	-6.404813	-5.378185	1.557870
C	-7.031392	-4.917371	0.406745
C	-6.281667	-4.715797	-0.746440
C	-4.905959	-4.963999	-0.774231
C	-4.401020	-6.179635	2.864020
C	-4.772641	-5.369048	4.111384
C	-4.137415	-4.723708	-2.069169
C	-3.950944	-3.225177	-2.348827
C	-3.155561	-7.759830	-0.665675
C	-4.798870	-5.408219	-3.274554
C	-4.766846	-7.660435	3.056347
N	0.059957	-4.779569	0.613656
C	1.223845	-3.981018	0.860299
C	1.604457	-2.991114	-0.073047
C	2.723782	-2.201944	0.208215
C	3.460353	-2.383313	1.372442
C	3.069652	-3.355602	2.285129
C	1.948899	-4.161105	2.061193
C	0.816849	-2.742423	-1.350773
C	1.703314	-2.756345	-2.603459
C	1.562251	-5.203879	3.101873
C	1.415202	-4.592152	4.501429
C	0.029194	-1.427108	-1.254911
C	2.560586	-6.371924	3.132072
O	-4.772184	1.934334	2.335786
H	0.705886	-0.572114	-1.143490
H	1.537654	-7.421865	-0.798315

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H	2.633671	-6.877587	2.164577
H	2.253725	-7.116792	3.874802
H	-4.476267	-4.323073	4.009276
H	-4.281557	-8.060932	3.953257
H	-5.849136	-7.786717	3.176248
H	-4.453615	-8.272332	2.204803
H	-4.251140	-5.774851	4.984621
H	-3.314658	-6.118098	2.752705
H	0.209364	-0.121185	3.488141
H	-0.962317	-0.262314	2.160272
H	-3.489644	-0.646555	5.343129
H	-1.892805	-1.356119	5.668192
H	-5.847189	-5.413698	4.323535
H	-6.994640	-5.550714	2.454113
H	-8.100730	-4.723446	0.404742
H	-6.775615	-4.361043	-1.647532
H	-5.756047	-4.941815	-3.531576
H	-4.991621	-6.468915	-3.085865
H	-4.153759	-5.330565	-4.156399
H	-3.406532	-3.073173	-3.287650
H	-4.918678	-2.718296	-2.437654
H	-3.384345	-2.738668	-1.550009
H	-3.137562	-5.151797	-1.954905
H	-3.465238	-7.552769	-1.695734
H	-4.064234	-7.881758	-0.073212
H	-2.602212	-8.701219	-0.670811
H	-0.620506	-7.724642	-0.816772
H	-0.645822	-1.437950	-0.394003
H	-0.566492	-1.265458	-2.161005
H	0.087797	-3.552673	-1.453547
H	1.088865	-2.666069	-3.506038
H	2.283736	-3.681378	-2.679323
H	2.412391	-1.921406	-2.608147
H	1.699176	-5.830101	-1.549844
H	2.333821	-6.085385	0.068162
H	3.024200	-1.434447	-0.500696
H	4.333645	-1.766940	1.569238
H	3.643928	-3.492514	3.197661
H	0.584199	-5.604923	2.820363
H	0.704327	-3.764149	4.490164
H	1.049307	-5.349330	5.203632
H	2.374027	-4.225873	4.886439
H	3.564835	-6.026253	3.403040
H	-2.626803	0.675702	3.500485
H	-1.464672	0.874578	4.807060
H	-4.232291	-1.826929	2.222355
H	-4.171801	-2.570974	0.628322
H	-3.117353	0.236362	1.276824
H	-3.142126	-0.501866	-0.317709
H	-5.622057	-0.558813	-0.297228
H	-5.010077	1.094214	-0.016453
H	-8.105171	0.042504	2.809817
H	-7.887906	0.136213	4.582028
H	-6.919137	-1.015836	3.615364

F_{TMC}

G = -2343,578076 u.a.

O	-2.452716	-0.527754	2.261975
C	-2.647342	-1.616473	1.385725
O	-1.846961	-1.459241	0.221422
C	-1.658675	-0.085408	-0.128127
C	-0.776653	0.585332	0.930272
C	-1.100797	-0.082723	2.275377
O	-2.337231	-2.783085	1.967747
Zn	-1.725696	-4.128847	0.831288
O	-3.972795	-1.540375	0.931297
C	-4.968651	-1.572311	1.950081
C	-5.614782	-0.201389	2.112166
C	-6.699777	-0.172850	3.173640

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O	-6.158982	-0.453508	4.482658
C	-5.743802	0.620419	5.180773
O	-5.198024	0.274425	6.352902
C	-5.067770	-1.108513	6.687413
N	-2.736205	-5.515031	-0.105527
C	-2.123773	-6.637122	-0.493578
C	-0.754931	-6.904701	-0.307682
C	0.257865	-6.127074	0.282694
C	1.634660	-6.746024	0.341943
C	-4.153556	-5.373718	-0.275405
C	-5.021445	-5.845264	0.736003
C	-6.396243	-5.648876	0.576945
C	-6.910262	-5.010695	-0.546287
C	-6.043702	-4.548018	-1.528484
C	-4.659428	-4.711289	-1.414923
C	-4.502028	-6.519382	1.998566
C	-4.590760	-5.565984	3.200822
C	-3.754073	-4.159950	-2.506250
C	-3.895726	-2.635266	-2.625113
C	-2.939016	-7.725950	-1.150475
C	-4.007812	-4.835988	-3.861773
C	-5.217734	-7.842725	2.301586
N	0.074330	-4.901125	0.780109
C	1.177300	-4.158473	1.314278
C	2.032606	-3.446976	0.440582
C	3.044330	-2.658973	0.996508
C	3.221667	-2.571516	2.372469
C	2.380956	-3.284633	3.217622
C	1.351351	-4.086899	2.714712
C	1.864480	-3.482577	-1.072650
C	3.177240	-3.787514	-1.807793
C	0.472097	-4.860498	3.686785
C	-0.324093	-3.920848	4.604328
C	1.252051	-2.170946	-1.584743
C	1.290583	-5.866567	4.510170
O	-5.844857	1.771689	4.836828
H	1.916223	-1.323844	-1.378058
H	1.596574	-7.808610	0.097652
H	1.849542	-6.556958	3.870175
H	0.630702	-6.460677	5.151763
H	-4.045842	-4.635338	3.015798
H	-4.748589	-8.339096	3.157910
H	-6.271842	-7.687057	2.554873
H	-5.181237	-8.530821	1.450627
H	-4.174078	-6.038090	4.098039
H	-3.443379	-6.751448	1.842914
H	-1.203386	-0.077703	-1.120839
H	-2.637879	0.401146	-0.191288
H	-1.015503	0.611610	3.114547
H	-0.432333	-0.931506	2.461495
H	-5.634216	-5.306916	3.414014
H	-7.076100	-6.001995	1.347901
H	-7.982786	-4.872065	-0.653421
H	-6.446644	-4.041704	-2.401891
H	-5.025362	-4.643066	-4.219075
H	-3.876031	-5.921578	-3.810377
H	-3.314276	-4.449475	-4.616706
H	-3.178345	-2.242834	-3.354927
H	-4.898887	-2.358000	-2.968670
H	-3.720976	-2.145869	-1.663881
H	-2.719836	-4.375492	-2.218081
H	-3.547266	-7.325674	-1.965477
H	-3.635697	-8.169079	-0.431150
H	-2.297164	-8.517004	-1.540663
H	-0.430251	-7.873137	-0.668445
H	0.292078	-1.974228	-1.100905
H	1.091723	-2.215382	-2.668025
H	1.158212	-4.282692	-1.315174
H	2.989833	-3.914848	-2.879387
H	3.652577	-4.701158	-1.436214

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H	3.902297	-2.973646	-1.700340
H	2.311525	-6.256758	-0.365615
H	2.076179	-6.623673	1.334667
H	3.702787	-2.099333	0.337456
H	4.014097	-1.951944	2.783539
H	2.524500	-3.220400	4.293220
H	-0.247989	-5.436625	3.095764
H	-0.962945	-3.248645	4.024654
H	-0.961697	-4.501703	5.280671
H	0.344962	-3.313307	5.224125
H	2.012281	-5.359217	5.159640
H	-0.987742	1.660217	0.956255
H	0.286348	0.459653	0.697873
H	-4.530595	-1.909083	2.894059
H	-5.716460	-2.314495	1.644133
H	-4.845474	0.536822	2.356765
H	-6.062684	0.101719	1.157316
H	-7.446518	-0.956734	3.012043
H	-7.194082	0.800682	3.204596
H	-6.043287	-1.600035	6.730084
H	-4.601351	-1.122628	7.673250
H	-4.431864	-1.630111	5.967485

$TS(F_{TMC} \rightarrow G_{TMC})$

G = -2343,568597 u.a.

C	1.713346	3.557462	-1.728332
C	2.059736	2.241301	-1.329426
C	2.694401	1.356774	-2.231061
C	2.967761	1.810376	-3.526455
C	2.617819	3.090062	-3.936060
C	1.993370	3.951295	-3.040082
N	1.801693	1.840708	0.019590
Zn	3.160087	2.120250	1.445867
O	4.392306	3.671203	1.825600
C	4.632727	4.820004	1.047707
C	5.025878	4.471110	-0.389311
C	6.252870	3.544845	-0.426226
O	6.656382	3.150676	0.894521
C	5.750863	2.413026	1.581598
O	6.158840	2.182806	2.841002
C	6.869799	3.215722	3.529198
C	3.075120	-0.068476	-1.854499
C	4.598067	-0.266966	-1.841246
C	1.042457	4.529308	-0.764206
C	-0.490842	4.432251	-0.820557
C	0.668951	1.193405	0.314054
C	-0.284475	0.800156	-0.794920
C	0.282717	0.789431	1.602247
C	0.959745	0.862424	2.834869
C	0.228556	0.281428	4.023875
N	2.179052	1.372252	3.000269
C	2.793796	1.335439	4.295247
C	3.509073	0.185475	4.701725
C	4.146670	0.205562	5.946050
C	4.089265	1.319835	6.775146
C	3.375863	2.440355	6.365040
C	2.715952	2.471620	5.132755
C	3.621809	-1.061550	3.834524
C	5.053583	-1.254268	3.312476
C	1.927150	3.714800	4.746656
C	0.770303	3.978439	5.722177
C	3.149834	-2.324087	4.572016
C	2.835601	4.947223	4.636224
C	1.468976	5.986972	-0.978721
O	5.066146	1.498094	1.026548
C	2.413618	-1.097288	-2.785173
H	2.139751	-2.212629	4.979463
H	3.147525	-3.182356	3.891102
H	3.813051	-2.573508	5.407595

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H	4.704993	-0.669943	6.267887
H	5.109394	-2.145073	2.675887
H	5.755399	-1.394657	4.142742
H	5.382006	-0.391834	2.728935
H	2.972235	-0.924167	2.964212
H	3.335153	3.308512	7.017372
H	0.343867	0.909687	4.909762
H	-0.833819	0.159469	3.806331
H	0.638501	-0.701413	4.278889
H	1.492887	3.537848	3.757403
H	2.254064	5.824417	4.328285
H	3.619946	4.772223	3.894728
H	3.305193	5.182532	5.597954
H	0.183323	4.844753	5.396588
H	0.092924	3.121387	5.791237
H	1.140576	4.189579	6.731356
H	-0.689091	0.311723	1.650003
H	-1.308979	0.742562	-0.421171
H	-0.249529	1.484829	-1.643063
H	-0.014462	-0.194464	-1.167390
H	1.050433	6.403789	-1.901604
H	1.101746	6.607830	-0.154738
H	2.556503	6.094018	-1.027410
H	-0.944324	5.158753	-0.136997
H	-0.850226	3.441342	-0.535476
H	-0.855262	4.647994	-1.831485
H	1.726844	4.952532	-3.365522
H	2.831571	3.418344	-4.949734
H	3.458529	1.140762	-4.228163
H	2.811991	-1.029722	-3.803665
H	1.329876	-0.959576	-2.848092
H	2.712652	-0.252528	-0.838231
H	2.607784	-2.113743	-2.425963
H	5.072939	0.377595	-1.097978
H	4.842277	-1.305379	-1.590261
H	5.031946	-0.053939	-2.825168
H	6.064321	2.650394	-1.025375
H	7.134922	4.051859	-0.823215
H	5.442619	5.401854	1.515516
H	3.740855	5.461252	1.045608
H	1.347351	4.237477	0.248188
H	4.603936	1.325871	7.731321
H	5.234163	5.394835	-0.942709
H	4.178100	3.990285	-0.886473
C	7.201486	2.679612	4.910419
C	7.989921	3.662081	5.758012
O	7.249435	4.876446	6.003443
C	6.458444	4.865569	7.092955
O	5.792343	6.017235	7.239546
C	6.003612	7.080000	6.306779
O	6.341003	3.954574	7.874273
H	6.229519	4.101541	3.587655
H	7.779462	3.474241	2.975745
H	6.282992	2.396009	5.432341
H	7.802995	1.768419	4.804915
H	8.899487	3.996918	5.250249
H	8.252271	3.214482	6.719130
H	7.052077	7.388412	6.290932
H	5.379893	7.900915	6.662020
H	5.695886	6.788836	5.299567

G_{TMC}

G = -2343,574646 u.a.

C	1.635762	3.573690	-1.784781
C	2.016596	2.274665	-1.358464
C	2.679329	1.391090	-2.241496
C	2.941550	1.824440	-3.546479
C	2.559144	3.085302	-3.981626
C	1.912060	3.947855	-3.102582

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N	1.766655	1.895744	-0.001829
Zn	3.003549	2.450379	1.465004
O	3.975363	4.030262	1.783579
C	4.382660	4.923651	0.795892
C	4.990755	4.258128	-0.448854
C	6.385721	3.669449	-0.252638
O	6.678351	3.280674	1.109246
C	5.960543	2.308692	1.649984
O	6.255392	2.096987	2.923242
C	7.060037	3.059771	3.632458
C	3.117502	-0.009537	-1.834685
C	4.647844	-0.142352	-1.822479
C	0.939536	4.547334	-0.839819
C	-0.574024	4.292061	-0.748832
C	0.679780	1.173638	0.289861
C	-0.235262	0.704613	-0.822003
C	0.303417	0.770829	1.580814
C	0.969892	0.891822	2.815173
C	0.262100	0.268509	3.998027
N	2.152473	1.480289	2.983563
C	2.786151	1.440776	4.267867
C	3.484666	0.278976	4.675707
C	4.138667	0.296893	5.911546
C	4.111435	1.417468	6.734126
C	3.411251	2.546642	6.324948
C	2.736732	2.582888	5.100510
C	3.554413	-0.985708	3.827886
C	4.966370	-1.220398	3.271228
C	1.929628	3.821694	4.737914
C	0.726843	3.987573	5.680428
C	3.085099	-2.226650	4.604197
C	2.790327	5.091246	4.718171
C	1.180820	6.019395	-1.194824
O	5.157165	1.593868	1.059114
C	2.507362	-1.087705	-2.744573
H	2.102952	-2.081635	5.065024
H	3.022619	-3.092064	3.935259
H	3.785165	-2.486234	5.405922
H	4.682393	-0.587467	6.234429
H	4.989339	-2.135151	2.667307
H	5.691989	-1.340166	4.084042
H	5.287896	-0.386325	2.645565
H	2.886657	-0.854460	2.970883
H	3.383831	3.415908	6.976583
H	0.452382	0.820988	4.919906
H	-0.814237	0.226609	3.819368
H	0.613383	-0.756237	4.157329
H	1.538762	3.679565	3.725563
H	2.170587	5.961765	4.472897
H	3.567475	5.001988	3.954323
H	3.252044	5.280312	5.693960
H	0.120777	4.850215	5.381023
H	0.079785	3.104533	5.673938
H	1.051837	4.151523	6.713957
H	-0.640064	0.239187	1.629781
H	-1.249231	0.552066	-0.446431
H	-0.265831	1.400977	-1.661201
H	0.120641	-0.256657	-1.208189
H	0.636650	6.315737	-2.099035
H	0.821855	6.659101	-0.382158
H	2.241346	6.236620	-1.353116
H	-1.044260	5.034634	-0.094458
H	-0.801908	3.305199	-0.341764
H	-1.040874	4.371749	-1.737318
H	1.622982	4.935077	-3.449222
H	2.766295	3.399745	-5.001100
H	3.452418	1.154497	-4.233499
H	2.911635	-1.027761	-3.761244
H	1.419642	-0.998765	-2.820951
H	2.765384	-0.187158	-0.813784

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H	2.741199	-2.086231	-2.359501
H	5.098669	0.548461	-1.107116
H	4.938218	-1.159628	-1.536388
H	5.067572	0.055008	-2.815720
H	6.557177	2.808028	-0.904994
H	7.159732	4.414833	-0.449265
H	5.129769	5.617680	1.223895
H	3.549951	5.560539	0.449649
H	1.357510	4.377549	0.160847
H	4.635384	1.420338	7.685323
H	5.063544	4.993243	-1.261460
H	4.301598	3.484681	-0.801444
C	7.306687	2.498818	5.019432
C	8.104223	3.448951	5.897106
O	7.396447	4.684643	6.118320
C	6.592736	4.707771	7.201374
O	5.950361	5.872753	7.323791
C	6.167480	6.908192	6.360731
O	6.453137	3.809987	7.994294
H	6.509693	4.003457	3.667708
H	7.999017	3.220545	3.092922
H	6.353884	2.264527	5.502886
H	7.865516	1.558651	4.938244
H	9.043467	3.750025	5.422990
H	8.315600	2.988174	6.864343
H	7.221294	7.194920	6.320859
H	5.565448	7.749306	6.705426
H	5.835128	6.597504	5.367393

$TS(G_{TMC} \rightarrow H_{TMC})$

G = -2343,572007 u.a.

C	-1.008202	-1.677077	2.946728
C	-1.241379	-0.332198	3.324574
C	-2.155169	-0.018325	4.356461
C	-2.755834	-1.072347	5.053880
C	-2.482903	-2.398126	4.739953
C	-1.628526	-2.691008	3.682160
N	-0.476753	0.703697	2.699355
C	-0.903119	1.260272	1.560763
C	-2.256137	0.865184	1.017086
C	-2.539981	1.415955	4.697580
C	-2.128591	1.822198	6.119952
C	-0.144147	-2.039782	1.743514
C	-0.882564	-2.980818	0.779205
Zn	1.325286	1.113637	3.412366
O	2.468653	0.148150	4.509515
C	2.097778	-0.909008	5.348354
C	1.013901	-0.554976	6.373130
C	1.492572	0.269481	7.563718
O	2.605686	1.135987	7.267246
C	2.384233	2.141977	6.423107
O	3.489992	2.836817	6.164422
C	4.761048	2.325920	6.602801
N	1.883256	2.467658	2.075715
C	3.157732	3.115994	2.199574
C	3.233327	4.452776	2.657673
C	4.498971	5.023922	2.824763
C	5.662073	4.314363	2.549718
C	5.570348	3.007312	2.086070
C	4.331330	2.387872	1.896356
C	2.003763	5.297521	2.971231
C	1.865458	5.567187	4.476531
C	4.294157	0.974308	1.332007
C	4.990105	-0.032504	2.258249
C	2.010079	6.626833	2.199286
C	1.122817	2.710622	1.008262
C	-0.163735	2.174798	0.798451
C	1.632625	3.623219	-0.084350
C	4.891215	0.925187	-0.083082

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C	1.209691	-2.641827	2.143588
C	-4.048093	1.644677	4.502263
O	1.304549	2.466413	5.965959
H	1.463705	4.671951	0.179377
H	2.706570	3.500108	-0.239087
H	1.109852	3.426221	-1.022063
H	5.953737	1.191599	-0.076869
H	4.804932	-0.084697	-0.499557
H	4.380611	1.615156	-0.762768
H	-0.648155	2.506760	-0.112072
H	2.164004	6.485825	1.124685
H	1.059175	7.152070	2.340934
H	2.803995	7.291999	2.556029
H	1.117073	4.734604	2.662694
H	6.637468	4.768258	2.697681
H	4.571759	6.048223	3.181236
H	0.979636	6.183973	4.668968
H	2.737772	6.110485	4.857819
H	1.766926	4.637724	5.040051
H	6.482855	2.460946	1.863863
H	3.244230	0.673666	1.250319
H	-2.008797	2.074781	4.003053
H	6.044708	0.226415	2.404507
H	4.487575	-0.066359	3.229657
H	4.954659	-1.036489	1.818957
H	-3.039673	1.036745	1.760116
H	-2.282067	-0.202047	0.775543
H	-2.498779	1.430230	0.116026
H	-3.452113	-0.845862	5.857591
H	-2.951758	-3.201322	5.302153
H	1.076847	-3.544986	2.750112
H	-1.445461	-3.728998	3.415975
H	1.810657	-1.931219	2.717956
H	0.066500	-1.115464	1.196709
H	1.781410	-2.920599	1.251168
H	-0.299058	-3.116081	-0.137866
H	-1.866131	-2.588926	0.500635
H	-1.035586	-3.973291	1.216783
H	-4.293195	2.703017	4.642786
H	-4.385887	1.349956	3.503521
H	-4.636196	1.072006	5.227985
H	-2.569102	1.151842	6.867192
H	-2.481262	2.836455	6.337972
H	-1.043013	1.820546	6.242267
H	1.897813	-0.375961	8.347112
H	2.997976	-1.257096	5.884584
H	1.728780	-1.777092	4.779264
H	0.682479	0.869847	7.990028
H	0.205283	-0.038673	5.848474
H	0.575520	-1.477923	6.775101
C	5.808979	3.351025	6.212604
C	7.213788	2.933774	6.612537
O	7.612547	1.712314	5.957826
C	8.221848	1.862729	4.765312
O	8.527250	0.686903	4.207489
C	8.203035	-0.526970	4.891773
O	8.487910	2.913170	4.235636
H	4.937223	1.362596	6.117181
H	4.741041	2.169770	7.686974
H	5.770723	3.532348	5.134502
H	5.584659	4.304403	6.706378
H	7.281441	2.706549	7.680831
H	7.932388	3.716578	6.360370
H	8.697905	-0.574424	5.865063
H	8.571432	-1.325406	4.247191
H	7.123438	-0.626836	5.026275

H_{TMC}

G = -2343,600701 u.a.

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C	2.990565	4.253269	2.683310
C	3.040799	2.960670	2.117602
C	4.270647	2.285622	1.954761
C	5.443543	2.938151	2.344818
C	5.411884	4.217534	2.887001
C	4.192439	4.861697	3.057321
N	1.819021	2.291642	1.777492
C	1.315992	2.390340	0.545931
C	2.052139	3.220211	-0.478758
C	4.336862	0.858008	1.433225
C	5.399989	0.661729	0.345359
C	1.671488	4.964168	2.944671
C	1.649903	6.400571	2.406189
Zn	0.910804	1.228018	3.142822
O	1.444165	1.084418	4.878754
C	0.908243	0.188672	5.818491
C	1.160342	0.699970	7.236483
C	2.643229	0.869125	7.515677
O	2.876639	1.448108	8.817840
C	2.864114	0.593175	9.839689
O	2.713568	-0.608081	9.782827
N	-0.610518	0.580596	2.104450
C	-0.763921	0.936624	0.825616
C	0.127245	1.764601	0.121463
C	-1.568388	-0.264513	2.752473
C	-2.630318	0.321460	3.477642
C	-3.489685	-0.517946	4.192775
C	-3.317133	-1.897151	4.193859
C	-2.275223	-2.459755	3.466166
C	-1.387583	-1.665504	2.734240
C	-2.836761	1.828629	3.522599
C	-4.278772	2.236008	3.191447
C	-0.244807	-2.319924	1.971393
C	0.841590	-2.825265	2.932703
C	-1.968064	0.427607	0.069993
C	-0.723989	-3.452870	1.053263
C	-2.407830	2.401045	4.882332
O	3.054535	1.297874	10.965829
C	3.076364	0.514109	12.165734
C	3.213091	1.484739	13.324807
C	3.231326	0.789730	14.676205
O	4.336213	-0.125721	14.791589
C	5.483779	0.412472	15.223142
O	5.661668	1.566792	15.542726
O	6.404102	-0.556420	15.246155
C	7.693348	-0.132853	15.694183
C	4.557560	-0.120733	2.598199
C	1.338803	4.934317	4.445263
H	2.196626	4.243001	-0.118136
H	3.051526	2.811689	-0.660080
H	1.510676	3.252190	-1.425157
H	6.414384	0.800324	0.734353
H	5.344825	-0.355136	-0.058008
H	5.264629	1.362621	-0.484832
H	-0.143127	1.952786	-0.910436
H	1.888171	6.437599	1.338038
H	0.657559	6.842866	2.545852
H	2.367288	7.042696	2.928351
H	0.885789	4.409172	2.421384
H	6.334819	4.707395	3.185188
H	4.170198	5.854912	3.497907
H	0.361143	5.392361	4.634252
H	2.086729	5.492387	5.019829
H	1.322053	3.910116	4.831494
H	6.397847	2.431293	2.229938
H	3.366129	0.622213	0.984793
H	-2.189369	2.274759	2.760546
H	5.531439	0.052110	3.069972
H	3.793318	0.000037	3.372949
H	4.534246	-1.158122	2.245525

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H	-2.894400	0.730375	0.568012
H	-1.974026	-0.666476	0.041179
H	-1.980668	0.804415	-0.953524
H	-4.305581	-0.081323	4.762822
H	-3.993303	-2.531938	4.759906
H	0.444476	-3.592204	3.606856
H	-2.143762	-3.538556	3.469487
H	1.237591	-2.015218	3.553066
H	0.211669	-1.554502	1.335370
H	1.676314	-3.266024	2.376477
H	0.108924	-3.830711	0.450640
H	-1.510208	-3.116734	0.369473
H	-1.122207	-4.298743	1.623900
H	-4.361028	3.326967	3.139343
H	-4.604835	1.825911	2.230150
H	-4.985788	1.893452	3.954606
H	-3.014881	1.981880	5.692553
H	-2.529744	3.489770	4.900215
H	-1.359361	2.174970	5.101383
H	3.165697	-0.090488	7.455471
H	1.369560	-0.811299	5.720622
H	-0.176913	0.038380	5.695129
H	3.087554	1.573712	6.812582
H	0.659348	1.666702	7.367245
H	0.731901	-0.006296	7.957638
H	3.911421	-0.192090	12.129569
H	2.152694	-0.072030	12.235032
H	4.123763	2.081726	13.210972
H	2.369808	2.185733	13.311962
H	2.345048	0.164598	14.818017
H	3.290065	1.524490	15.482718
H	8.092126	0.649917	15.043869
H	8.323174	-1.021211	15.650331
H	7.642780	0.248423	16.717324