

Supporting Information

Terminal Substituent Effects on Reactivity, Thermodynamics, and Stereoselectivity of the 8π - 6π Electrocyclization Cascades of 1,3,5,7-Tetraenes

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Table of Contents

Conformational analysis	S1
Influence of donor or acceptor substituents on the 8π - 6π electrocyclization cascade.....	S2
Discussion of the B3LYP/6-31G(d) study of the 8π - 6π electrocyclizations of tetraenes 1-10	S6
Cartesian coordinates, electronic energies, ZPE & thermal corrections, and transition state imaginary frequencies	S8
M06-2X/6-31+G(d,p).....	S8
B3LYP/6-31G(d).....	S61

Conformational analysis

The conformers of all tetraene substrates have been considered at the M06-2X/6-31+G(d,p) level of theory; for each reaction, the barrier is determined using the global minimum tetraene conformer. The 1,3,5-cyclooctatrienes as well as the resulting 6π electrocyclization transition states described in our manuscripts feature a twist-boat conformation. For the parent 1,3,5-cyclooctatriene, two enantiomeric twist-boat conformers exist.¹¹ For 1,3,5-cyclooctatrienes that possess a center of chirality, these two conformers as well as the related 6π electrocyclization transition state conformers are diastereomeric structures. In these cases, both conformers have been computed, and the lowest energy conformer of all stationary points are depicted and discussed in the manuscript. To illustrate these different conformations, *exo* and *endo* transition state conformers of 6π ring closure of **2COT** are shown below in Figure S1 below.

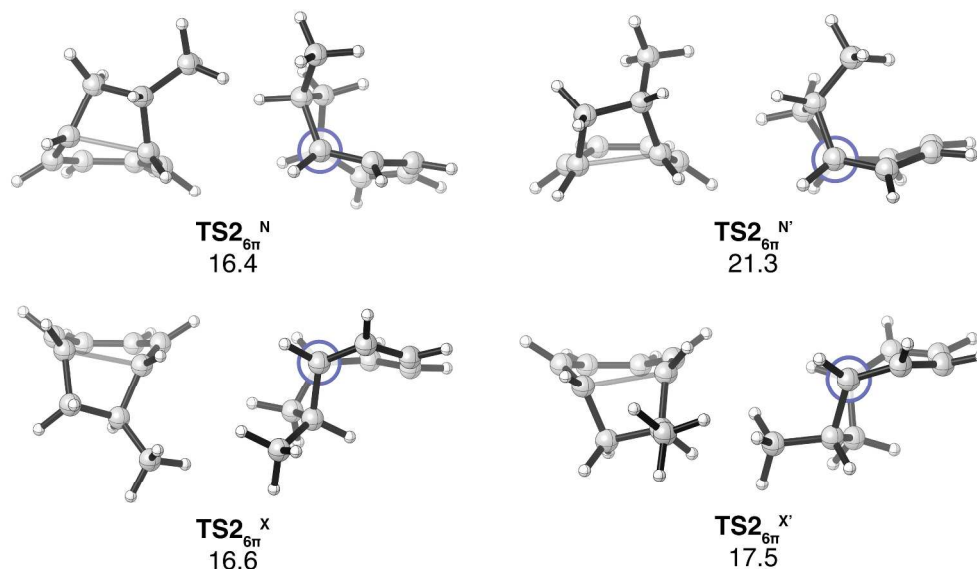


Figure S1. M06-2X/6-31+G(d,p) optimized structures of all *exo* and *endo* transition states of the 6π ring closures of **2COT**.

¹ For further details regarding the conformations of 1,3,5-cyclooctatriene, see: Anet, F.; Yavari, I. *Tetrahedron Lett.* **1975**, 48, 4221–4224.

Influence of donor or acceptor substituents on the 8π - 6π electrocyclization cascade

In the main text, we focus on the influence of alkyl substituents on the 8π - 6π electrocyclic reaction of tetraenes, considering the fact that a large majority of the natural products presented in Scheme 2 feature analogous substituents at the 7 and 8 positions of their bicyclo[4.2.0]2,4-octadiene skeletons (Scheme 2 of the main text). Here, we summarize the results for the 8π - 6π ring closures of fluorinated 1,3,5,7-tetraenes **2F** and **3F** as well as formylated tetraenes **2CHO** and **3CHO**. These substrates were chosen because they feature strong donor (fluorine) and acceptor (formyl) substituents.

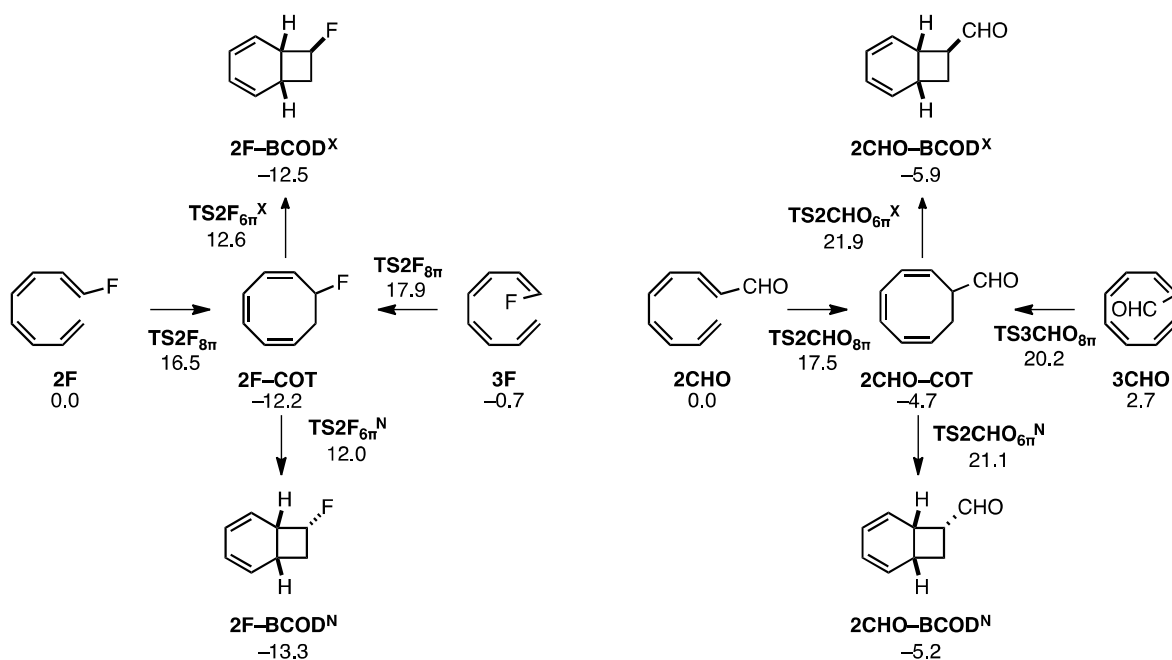


Figure S2. Summary of the M06-2X/6-31+G(d,p) computations of the 8π - 6π electrocyclization cascades of the 1-fluoro (**2F** and **3F**) and 1-formyl (**2CHO** and **3CHO**) substituted 1,3,5,7-octatetraenes.

Houk and coworkers performed an *ab initio* computational study of the influence of donor and acceptor substituents of the reactivity and torquoselectivity of tetraene ring closures by modeling the 8π ring closures of *cis* and *trans*-1-fluoro-1,3,5,7-octatetraenes and *cis* and *trans*-1-formyl-1,3,5,7-

octatetraenes.²² They found that both donor influence of both donors and acceptors only have a modest effect on the reactivity. However, the influences of classic donors and acceptors the 6π electrocyclizations step of these cascade reactions have yet to be modeled computationally. We expect that such effects are small as the terminal substituents of the tetraene precursors are no longer in conjugation with π system of the reacting cyclooctatrienes shown in Figure S2.

Shown below are the results of M06-2X/6-31+G(d,p) computations of the 8π - 6π cascades of the fluoro and formyl-substituted tetraenes. Neither the fluoro- nor the formyl substituent has a significant effect on the $\Delta G^\ddagger$ for 8π electrocyclization: these 8π ring closures have only slightly higher computed $\Delta G^\ddagger$ (ca 1 kcal mol⁻¹) than the analogous respectively, similar reactions of tetraenes **2** and **3**. The rate-determining step for the cascade reactions is the second (6π) electrocyclization. The $\Delta G^\ddagger$ values for the 8π - 6π ring closures of **2F** (and **3F**) and **2CHO** (and **3CHO**) are 24 kcal mol⁻¹ and 26 kcal mol⁻¹, respectively. These $\Delta G^\ddagger$ values are similar to the $\Delta G^\ddagger$ value (ca. 25 kcal mol⁻¹) of the reaction of the hydrocarbon substrate **2**.

Both the *endo* and the *exo* modes of the 6π ring closures of **2F-COT** are slightly more facile than the corresponding ring closure of **2COT**. The fluorine substituent, likely due to its smaller size, destabilizes both the intermediate and the 6π transition states to a lesser extent than does the methyl substituent of **2COT**. Also in contrast to the reaction of the methylated analogue of **2F**, a slight kinetic and thermodynamic preference is observed for the formation of *endo* diastereomer of the bicyclo[4.2.0]octadiene product.

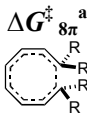
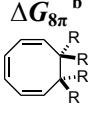
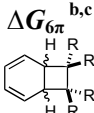
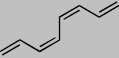
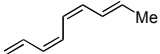
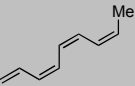
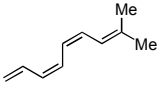
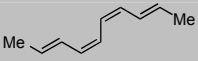
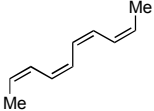
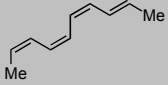
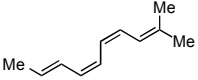
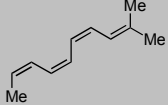
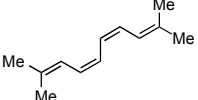
The 8π electrocyclization of **2CHO** is 5 kcal mol⁻¹ less exergonic than the analogous reaction of **2**. This is due to a difference in the stability of the tetraene precursors **2CHO** and **2**. The formyl substituent of tetraene **2CHO** is in conjugation with the π system of the tetraene, whereas the methyl group of **2** cannot interact with the π system in this way. This resonance effect also stabilizes the 8π

² Thomas, B. E.; Evanseck, J. D.; Houk, K. N. *J. Am. Chem. Soc.* **1993**, *115*, 4165–4169.

transition states to some extent. As a result of this stabilizing effect, transition states, and products that follow the 8π transition state shown in the diagram above are higher in relative energy than their analogs for the 1-methyl substrate **2**.

Discussion of the B3LYP/6-31G(d) study of the 8π - 6π electrocyclizations of tetraenes 1-10

Table S1. Summary of B3LYP/6-31G(d) computed activation and reaction free energies for cascade ring closures of tetraenes 1-10.

Tetraene					$\Delta\Delta G^{\ddagger}_{6\pi}$ ^d	
1		19	−4	23	−2	N/A
2		20	0	25	0	0
3		21	−2	22	−2 (<i>exo</i>)	0
4		24	3	27	2	N/A
5		21	6	27	3	N/A
6		16	0	21	−3	N/A
7		22	7	27	2 (<i>endo</i>)	4
8		27	13	30	7 (<i>exo</i>)	5
9		25	11	29	4 (<i>endo</i>)	5
10		33	20	40	11	N/A

All Gibbs free energies are reported in kcal mol⁻¹ and were calculated using the tetraene precursor as the point of reference. ^a $\Delta G_{8\pi}^{\ddagger}$ and $\Delta G_{6\pi}^{\ddagger}$ are the free energies of activation for 8π and 6π ring closure of the indicated tetraene, respectively. ^bThe reaction energies for the 8π and 6π electrocyclizations are, respectively, $\Delta G_{8\pi}$ and $\Delta G_{6\pi}$. ^cThe exo and endo designations indicate which of the two stereoproducts is more stable (where relevant). ^dFree energy difference between the endo and exo 6π ring closure transition states.

In comparison with M06-2X/6-31+G(d,p), the B3LYP/6-31G(d) level of theory performs poorly in two regards. The B3LYP/6-31G(d) model chemistry fails to accurately reproduce the thermodynamics of the electrocyclizations. The 8π – 6π electrocyclization cascades of **2**, **5**, **6**, and **7** are experimentally known to be exergonic. B3LYP/6-31G(d) computations erroneously predict the cascade reactions of **2**, **5**, **6**, and **7** are endergonic or thermoneutral. A similar argument can be made for **8**, which resembles, in terms of substitution pattern, naturally occurring trisubstituted tetraenes, although the kinetics and thermodynamics for the electrocyclization cascade of this substrate have not been studied experimentally. The failure of B3LYP to accurately reproduce the thermodynamics of π to σ transformations is documented.³ Secondly, the activation free energies of the 8π electrocyclic reaction of **2**, **5**, and **7** are slightly overestimated compared with experimental data.⁴ The B3LYP/6-31G(d) level of theory, despite its shortcomings, does predict a level of diastereoselectivity for the 6π electrocyclic reactions of **7COT**, **8COT**, and **9COT** in agreement with the M06-2X/6-31+G(d,p) computations.

³ Pieniazek, S. N.; Clemente, F. R.; Houk, K. N. *Angew. Chem. Int. Ed.* **2008**, *47*, 7746–7749.

⁴ The B3LYP/6-31G(d) model chemistry performs admirably in recapitulating experimental activation enthalpies of hydrocarbon pericyclic reactions; at this level of theory such values are slightly overestimated (MAD = 2 kcal mol⁻¹). See: Guner, V.; Khuong, K. S.; Leach, A. G.; Lee, P. S.; Bartberger, M. D.; Houk, K. N. *J. Phys. Chem. A* **2003**, *107*, 11445–11459.

Cartesian coordinates, electronic energies, ZPE & thermal corrections, and transition state imaginary frequencies

M06-2X/6-31+G(d,p)

1

C	4.01245	-0.13139	0.00062
C	2.68961	-0.34174	0.00004
H	4.42142	0.87586	0.00085
H	4.71899	-0.95396	0.00089
C	1.71719	0.74364	-0.00032
H	2.32139	-1.36466	-0.00018
C	0.37150	0.62448	-0.00052
C	-0.37149	-0.62447	-0.00048
H	2.13943	1.74732	-0.00040
H	-0.20521	1.54520	-0.00074
C	-1.71719	-0.74364	-0.00020
C	-2.68962	0.34175	0.00019
H	0.20521	-1.54520	-0.00069
H	-2.13943	-1.74731	-0.00024
C	-4.01245	0.13137	0.00050
H	-2.32141	1.36467	0.00024
H	-4.42141	-0.87587	0.00047
H	-4.71900	0.95394	0.00080

SCF energy: -310.659541 hartree

zero-point correction: +0.153822 hartree

enthalpy correction: +0.163704 hartree

free energy correction: +0.119260 hartree

quasiharmonic free energy correction: +0.120405 hartree

TS1_{8π}

C	1.78754	-0.71288	0.09340
C	0.83223	-1.37692	0.81795
C	1.72537	0.65629	-0.25800
C	0.69446	1.57764	-0.16708
C	-0.83223	-1.37692	-0.81795
C	-1.78754	-0.71288	-0.09340
C	-1.72537	0.65629	0.25800
C	-0.69446	1.57764	0.16708
H	-1.03676	2.59101	0.37531
H	1.03676	2.59101	-0.37531
H	-2.63161	-1.27716	0.29865
H	-2.64902	1.06676	0.66187
H	2.63161	-1.27716	-0.29865

H	2.64902	1.06676	-0.66187
H	0.13475	-0.81783	1.42663
H	0.95891	-2.42757	1.06066
H	-0.95891	-2.42757	-1.06066
H	-0.13475	-0.81783	-1.42663

SCF energy: -310.635846 hartree
 zero-point correction: +0.155243 hartree
 enthalpy correction: +0.163242 hartree
 free energy correction: +0.124345 hartree
 quasiharmonic free energy correction: +0.124345 hartree
 imaginary frequency: -357.5901

1COD

C	-1.38463	1.05301	-0.37553
C	-1.84773	-0.31424	0.04111
C	-0.22021	1.70156	-0.20609
C	1.08824	1.33511	0.36444
C	-0.78447	-1.20983	0.68072
C	0.26941	-1.63333	-0.30140
C	1.43352	-1.00012	-0.49526
C	1.83167	0.22547	0.19958
H	2.84950	0.25058	0.58645
H	1.57108	2.16033	0.88723
H	0.06857	-2.53510	-0.87820
H	2.16251	-1.43371	-1.17806
H	-2.17306	1.64540	-0.84006
H	-0.23295	2.74206	-0.53235
H	-2.27400	-0.82136	-0.83420
H	-2.68716	-0.17842	0.73798
H	-1.27625	-2.09974	1.08788
H	-0.32319	-0.67573	1.51801

SCF energy: -310.681322 hartree
 zero-point correction: +0.158094 hartree
 enthalpy correction: +0.165993 hartree
 free energy correction: +0.127255 hartree
 quasiharmonic free energy correction: +0.127255 hartree

TS1_{6π}

C	1.40823	0.97451	0.45416
C	0.31122	1.53997	-0.19635
C	1.82644	-0.36025	0.27956
H	2.16150	1.66445	0.82769
C	1.07316	-1.27609	-0.44345

H	2.87473	-0.56903	0.47809
C	-0.32123	-1.15880	-0.51004
C	-0.87000	0.91633	-0.65323
H	0.48124	2.55925	-0.54903
H	1.59282	-2.00600	-1.06176
C	-1.91310	0.29510	0.27630
H	-1.30054	1.41246	-1.52769
C	-1.13566	-0.90869	0.75343
H	-0.83808	-1.73604	-1.27758
H	-0.46516	-0.64997	1.57625
H	-1.73262	-1.77673	1.05444
H	-2.77123	-0.02021	-0.32615
H	-2.27702	0.98937	1.04345

SCF energy: -310.637441 hartree
 zero-point correction: +0.156872 hartree
 enthalpy correction: +0.163983 hartree
 free energy correction: +0.126888 hartree
 quasiharmonic free energy correction: +0.126888 hartree
 imaginary frequency: -593.5202

1BCOD

C	-0.98458	-1.34325	0.24992
C	-1.90889	-0.46257	-0.15738
C	-1.58178	0.96341	-0.31744
C	-0.40888	1.46985	0.08909
C	0.66914	0.62339	0.70531
C	0.42821	-0.89953	0.48447
H	0.85084	0.95061	1.73693
C	1.93783	0.50233	-0.18104
H	0.89989	-1.48304	1.28121
C	1.37229	-0.82045	-0.74866
H	-1.23769	-2.39196	0.38453
H	-2.92605	-0.78280	-0.36359
H	-2.33534	1.61709	-0.74766
H	-0.21365	2.53730	0.00052
H	2.83320	0.33957	0.42578
H	2.12853	1.31211	-0.89146
H	0.79392	-0.64946	-1.66099
H	2.06639	-1.64862	-0.91096

SCF energy: -310.682007 hartree
 zero-point correction: +0.158718 hartree
 enthalpy correction: +0.166052 hartree
 free energy correction: +0.128433 hartree
 quasiharmonic free energy correction: +0.128433 hartree

2

C	3.37105	0.32518	0.00036
C	2.06960	-0.00126	0.00013
H	3.63591	1.38244	0.00048
C	1.00802	0.99387	0.00009
H	1.79540	-1.05539	-0.00002
C	-0.32414	0.76522	-0.00018
C	-0.95907	-0.54152	-0.00054
H	1.34361	2.03000	0.00032
H	-0.97467	1.63523	-0.00013
C	-2.28945	-0.77799	-0.00051
C	-3.35125	0.21988	-0.00004
H	-0.30478	-1.40915	-0.00089
H	-2.62329	-1.81438	-0.00084
C	-4.65201	-0.10039	-0.00009
H	-3.07055	1.27027	0.00038
H	-4.97525	-1.13833	-0.00050
H	-5.42489	0.66019	0.00027
C	4.49766	-0.67340	0.00059
H	4.45123	-1.32210	-0.88012
H	5.47028	-0.17847	-0.00233
H	4.45451	-1.31794	0.88453

SCF energy: -349.957083 hartree

zero-point correction: +0.181728 hartree

enthalpy correction: +0.192562 hartree

free energy correction: +0.145456 hartree

quasiharmonic free energy correction: +0.146800 hartree

TS_{28π}

C	-1.00862	1.34396	0.20175
C	-1.32930	0.15962	-0.42278
C	0.28965	1.88996	0.28417
C	1.53298	1.35654	-0.02939
C	-0.29019	-1.20907	1.10946
C	0.55448	-1.84752	0.23481
C	1.67070	-1.23742	-0.37888
C	2.06625	0.09249	-0.41832
H	3.06902	0.20787	-0.82916
H	2.31641	2.11349	-0.00603
H	0.32505	-2.86760	-0.06804
H	2.34265	-1.91729	-0.89923
H	-1.80102	1.88150	0.72316
H	0.33029	2.91456	0.64933
H	-0.61841	-0.22357	-1.14637
H	-1.12522	-1.74275	1.55476
H	0.05314	-0.32501	1.62911

C	-2.74461	-0.32881	-0.55145
H	-3.18994	0.04015	-1.48295
H	-2.78822	-1.42088	-0.58167
H	-3.36178	0.02114	0.28081

SCF energy: -349.935781 hartree
 zero-point correction: +0.183432 hartree
 enthalpy correction: +0.192937 hartree
 free energy correction: +0.150636 hartree
 quasiharmonic free energy correction: +0.150636 hartree
 imaginary frequency: -362.9513

2COT

C	0.86547	1.07685	-0.67435
C	1.45955	-0.26014	-0.31515
C	-0.27076	1.69565	-0.31090
C	-1.45780	1.29998	0.46671
C	0.50980	-1.18013	0.45989
C	-0.66961	-1.62726	-0.35249
C	-1.87122	-1.03504	-0.34916
C	-2.19081	0.17241	0.41255
H	-3.13589	0.16825	0.95368
H	-1.86982	2.11306	1.06366
H	-0.53415	-2.51794	-0.96450
H	-2.68529	-1.48979	-0.91127
H	1.54454	1.68738	-1.27160
H	-0.34310	2.73249	-0.64193
H	1.72785	-0.76260	-1.25579
H	1.07607	-2.06051	0.78583
H	0.17166	-0.65560	1.36132
C	2.75811	-0.02762	0.47237
H	3.27467	-0.97432	0.65821
H	3.44094	0.63157	-0.07206
H	2.53614	0.43981	1.43756

SCF energy: -349.978758 hartree
 zero-point correction: +0.186351 hartree
 enthalpy correction: +0.195636 hartree
 free energy correction: +0.153751 hartree
 quasiharmonic free energy correction: +0.153918 hartree

TS_{6π}^x

C	1.98133	0.04680	-0.70566
C	1.51884	1.20006	-0.07005
C	1.62688	-1.26102	-0.31900

H	2.90180	0.14126	-1.27737
C	0.65307	-1.50457	0.64224
H	2.32837	-2.04968	-0.57967
C	-0.40644	-0.60780	0.82574
C	0.29949	1.41226	0.60662
H	2.28311	1.96739	0.06901
H	0.79933	-2.33238	1.33390
C	-1.06730	1.39391	-0.07465
H	0.38080	2.14996	1.40956
C	-1.19494	-0.08234	-0.37234
H	-0.99913	-0.70416	1.73853
H	-0.63445	-0.32620	-1.28068
H	-1.82790	1.69087	0.65789
H	-1.13754	2.07912	-0.92885
C	-2.60794	-0.64216	-0.47414
H	-3.14545	-0.19117	-1.31494
H	-2.59340	-1.72657	-0.62058
H	-3.17344	-0.42931	0.44051

SCF energy: -349.936760 hartree

zero-point correction: +0.184785 hartree

enthalpy correction: +0.193393 hartree

free energy correction: +0.152972 hartree

quasiharmonic free energy correction: +0.152972 hartree

imaginary frequency: -586.1981

TS2_{6π}^{X'}

C	1.85894	0.96533	0.38488
C	0.73105	1.54076	-0.20223
C	2.24326	-0.37692	0.19590
H	2.64597	1.64580	0.70195
C	1.43579	-1.28447	-0.47910
H	3.29798	-0.60189	0.33352
C	0.04098	-1.15970	-0.46447
C	-0.48875	0.92773	-0.55258
H	0.89225	2.55004	-0.58600
H	1.91147	-2.01956	-1.12622
C	-1.46618	0.33699	0.47354
H	-0.99166	1.41630	-1.39405
C	-0.69054	-0.90829	0.84933
H	-0.51254	-1.73964	-1.20252
H	0.03918	-0.70391	1.63655
H	-1.30544	-1.76187	1.16232
H	-1.63274	1.03481	1.30536
C	-2.81095	0.01975	-0.17423
H	-3.48486	-0.44563	0.55149
H	-3.29174	0.92805	-0.55142
H	-2.68948	-0.66955	-1.01721

SCF energy: -349.935736 hartree
 zero-point correction: +0.184933 hartree
 enthalpy correction: +0.193440 hartree
 free energy correction: +0.153276 hartree
 quasiharmonic free energy correction: +0.153276 hartree
 imaginary frequency: -586.3891

TS2_{6π}^N

C	1.29241	1.35404	-0.42829
C	0.23833	1.45681	0.48006
C	2.12344	0.22212	-0.54675
H	1.70163	2.28800	-0.80681
C	1.85313	-0.95833	0.13261
H	3.11888	0.39095	-0.94979
C	0.53666	-1.31717	0.45040
C	-0.56904	0.43451	1.02519
H	0.15400	2.43737	0.95258
H	2.68737	-1.53548	0.52764
C	-1.55593	-0.40023	0.20032
H	-0.94132	0.67704	2.02563
C	-0.56508	-1.22123	-0.59391
H	0.39667	-2.10676	1.18933
H	-0.20477	-0.66351	-1.46391
H	-0.92175	-2.20011	-0.93464
H	-2.07423	-1.06419	0.90392
C	-2.58490	0.41419	-0.57403
H	-3.26927	-0.24322	-1.12080
H	-3.17976	1.04295	0.09673
H	-2.08160	1.06865	-1.29342

SCF energy: -349.937278 hartree
 zero-point correction: +0.184889 hartree
 enthalpy correction: +0.193433 hartree
 free energy correction: +0.153140 hartree
 quasiharmonic free energy correction: +0.153140 hartree
 imaginary frequency: -583.6402

C	1.73631	0.24595	0.76613
C	1.13664	1.40952	0.28103
C	1.61275	-1.00794	0.14170
H	2.59284	0.36830	1.42536
C	0.78993	-1.20795	-0.96329
H	2.40053	-1.72908	0.34732
C	-0.38601	-0.48098	-1.17664
C	-0.06583	1.53196	-0.43592
H	1.77725	2.29293	0.31118
H	1.16784	-1.85125	-1.75744
C	-1.44745	1.15259	0.10514

H	-0.08539	2.40949	-1.08681
C	-1.50116	-0.34976	-0.12187
H	-0.76219	-0.47693	-2.20041
H	-2.44227	-0.65535	-0.59567
H	-2.20502	1.67036	-0.49054
H	-1.58316	1.46381	1.14879
C	-1.35373	-1.18100	1.14887
H	-1.27828	-2.24787	0.92119
H	-0.47402	-0.89561	1.72945
H	-2.23684	-1.02315	1.77679

SCF energy: -349.929557 hartree
 zero-point correction: +0.184755 hartree
 enthalpy correction: +0.193480 hartree
 free energy correction: +0.151827 hartree
 quasiharmonic free energy correction: +0.153198 hartree
 imaginary frequency:

2BCOD^x

C	0.73081	-1.49649	0.43033
C	1.87257	-1.16909	-0.19083
C	2.17299	0.22795	-0.54305
C	1.40593	1.24410	-0.12253
C	0.17018	1.03694	0.70690
C	-0.30076	-0.44652	0.71209
H	0.29770	1.51775	1.68482
C	-1.14318	1.39959	-0.03565
H	-0.86228	-0.67232	1.62617
C	-1.29656	-0.08877	-0.43063
H	0.52517	-2.52791	0.70606
H	2.60918	-1.92975	-0.43279
H	3.06378	0.42788	-1.13191
H	1.68080	2.27091	-0.35825
H	-1.92566	1.70873	0.66636
H	-1.07699	2.13275	-0.84554
H	-0.80402	-0.26840	-1.39339
C	-2.67842	-0.71391	-0.41157
H	-3.31662	-0.28761	-1.19261
H	-2.62633	-1.79561	-0.57350
H	-3.16601	-0.53923	0.55426

SCF energy: -349.981312 hartree
 zero-point correction: +0.186671 hartree
 enthalpy correction: +0.195501 hartree
 free energy correction: +0.154484 hartree
 quasiharmonic free energy correction: +0.154538 hartree\
 imaginary frequency: -593.4637

2BCOD^N

C	1.77760	-1.01296	-0.03138
C	2.26167	0.18613	-0.38317
C	1.44789	1.40358	-0.24269
C	0.25665	1.39319	0.37317
C	-0.34735	0.14400	0.94956
C	0.36322	-1.14719	0.44596
H	-0.45167	0.26039	2.03638
C	-1.63756	-0.34762	0.22327
H	0.26888	-1.95155	1.18208
C	-0.74704	-1.27859	-0.63240
H	2.39062	-1.90672	-0.11787
H	3.27371	0.28478	-0.76488
H	1.85361	2.33757	-0.62155
H	-0.29367	2.32337	0.50365
H	-2.22470	-0.94716	0.92909
H	-0.43880	-0.77848	-1.55735
H	-1.11981	-2.27889	-0.86874
C	-2.53498	0.64988	-0.48620
H	-3.33005	0.13142	-1.03166
H	-3.00761	1.34031	0.22071
H	-1.96106	1.24247	-1.20651

SCF energy: -349.980888 hartree

zero-point correction: +0.186917 hartree

enthalpy correction: +0.195642 hartree

free energy correction: +0.154927 hartree

quasiharmonic free energy correction: +0.154927 hartree

3

C	-3.39882	0.59532	0.00042
C	-2.05667	0.67059	0.00024
H	-3.95808	1.52782	0.00064
C	-1.17920	-0.49057	-0.00005
H	-1.60180	1.65713	0.00033
C	0.17358	-0.48081	-0.00032
C	1.01485	0.70324	-0.00046
H	-1.66853	-1.46214	-0.00004
H	0.67432	-1.44505	-0.00047
C	2.36617	0.71415	-0.00035
C	3.24818	-0.44568	-0.00000
H	0.51414	1.66738	-0.00067
H	2.86772	1.68063	-0.00049
C	4.58381	-0.34312	0.00006
H	2.79872	-1.43562	0.00021
H	5.07287	0.62776	-0.00013
H	5.22155	-1.22013	0.00032
C	-4.19979	-0.68055	0.00035
H	-3.98125	-1.29184	0.88267
H	-5.27044	-0.46988	0.00074
H	-3.98181	-1.29139	-0.88243

SCF energy: -349.957020 hartree

zero-point correction: +0.181888 hartree

enthalpy correction: +0.192659 hartree

free energy correction: +0.145242 hartree

quasiharmonic free energy correction: +0.147278 hartree

TS3_{8π}

C	1.77405	0.29876	-0.41939
C	1.44172	-0.91269	0.15260
C	1.09601	1.53259	-0.30662
C	-0.20957	1.87379	0.02801
C	-0.33584	-1.23451	-1.30309
C	-1.38097	-1.23777	-0.41325
C	-1.92259	-0.08863	0.20581
C	-1.43637	1.20647	0.30435
H	-2.17838	1.89924	0.69945
H	-0.33822	2.95407	0.08857
H	-1.81612	-2.19337	-0.12562
H	-2.89106	-0.23748	0.68096
H	2.62552	0.30261	-1.10016
H	1.69643	2.39062	-0.60601
H	2.05308	-1.76474	-0.14364
H	-0.02355	-2.15982	-1.77800
H	-0.07775	-0.31852	-1.81594

C	0.80115	-1.04315	1.50358
H	1.60623	-1.11532	2.24499
H	0.18701	-0.18013	1.75807
H	0.19129	-1.94629	1.58543

SCF energy: -349.932063 hartree

zero-point correction: +0.183543 hartree

enthalpy correction: +0.192911 hartree

free energy correction: +0.151058 hartree

quasiharmonic free energy correction: +0.151058 hartree

imaginary frequency: -385.0629

4

C	2.95702	-0.10680	-0.00000
C	1.61746	-0.25851	0.00011
C	0.62911	0.80832	0.00024
H	1.24132	-1.27909	0.00023
C	-0.71555	0.65575	0.00021
C	-1.43208	-0.60768	-0.00007
H	1.00276	1.82835	0.00049
H	-1.31293	1.56314	0.00040
C	-2.77524	-0.75798	-0.00015
C	-3.77118	0.30557	0.00002
H	-0.83643	-1.51625	-0.00025
H	-3.17504	-1.77080	-0.00038
C	-5.08983	0.06902	-0.00007
H	-3.42409	1.33593	0.00025
H	-5.47869	-0.94619	-0.00030
H	-5.81263	0.87736	0.00007
C	3.86609	-1.30569	0.00012
H	3.30465	-2.24265	0.00072
H	4.52032	-1.29478	-0.88005
H	4.52099	-1.29409	0.87978
C	3.67765	1.21339	-0.00033
H	4.32848	1.28469	-0.87977
H	3.01272	2.07654	-0.00106
H	4.32789	1.28559	0.87946

SCF energy: -389.258950 hartree

zero-point correction: +0.210322 hartree

enthalpy correction: +0.223219 hartree

free energy correction: +0.171349 hartree

quasiharmonic free energy correction: +0.173206 hartree

TS4_{8π}

C	0.87065	1.35780	-0.36008
C	1.35834	0.19324	0.21524
C	-0.42968	1.89675	-0.30134
C	-1.68438	1.36201	-0.01473
C	0.17769	-1.11952	-1.25550
C	-0.66730	-1.79012	-0.40259
C	-1.82923	-1.23465	0.17272
C	-2.25361	0.08568	0.24423
H	-3.28160	0.17592	0.59320
H	-2.44981	2.13691	0.01227
H	-0.41669	-2.80903	-0.11201
H	-2.51078	-1.95106	0.62853
H	1.56419	1.90830	-0.99867
H	-0.47772	2.94065	-0.60854

H	1.01492	-1.64142	-1.71022
H	-0.19080	-0.25021	-1.78234
C	0.84794	-0.27123	1.55269
H	-0.17784	0.03801	1.74508
H	0.91749	-1.35728	1.66193
H	1.48869	0.18366	2.31951
C	2.78497	-0.21484	-0.07418
H	3.09938	0.08957	-1.07572
H	3.46367	0.24436	0.65582
H	2.90455	-1.29910	0.01241

SCF energy: -389.232486 hartree

zero-point correction: +0.211520 hartree

enthalpy correction: +0.222277 hartree

free energy correction: +0.177638 hartree

quasiharmonic free energy correction: +0.177638 hartree

imaginary frequency: -393.2575

4COT

C	0.56630	1.18683	-0.59848
C	1.28136	0.02022	0.03981
C	-0.68360	1.66913	-0.49543
C	-1.91095	1.22277	0.18488
C	0.33959	-0.89834	0.83765
C	-0.65039	-1.65110	-0.00273
C	-1.90735	-1.25220	-0.24104
C	-2.47905	0.00373	0.24299
H	-3.48462	-0.05341	0.65739
H	-2.50759	2.04777	0.57312
H	-0.32948	-2.60948	-0.40776
H	-2.57661	-1.91613	-0.78583
H	1.24176	1.79979	-1.19963
H	-0.83907	2.62129	-1.00444
H	0.96324	-1.61878	1.38250
H	-0.19010	-0.29331	1.58255
C	2.33501	0.60252	0.99964
H	2.94697	-0.19983	1.42672
H	3.00235	1.29463	0.47518
H	1.85485	1.14731	1.81859
C	2.00150	-0.78185	-1.05577
H	2.73188	-0.15555	-1.57939
H	2.53887	-1.62902	-0.61308
H	1.29303	-1.16553	-1.79504

SCF energy: -389.277560 hartree

zero-point correction: +0.214332 hartree

enthalpy correction: +0.224889 hartree

free energy correction: +0.180513 hartree

quasiharmonic free energy correction: +0.180756 hartree

TS4_{6π}

C	-2.46270	-0.04532	0.38677
C	-1.89737	-1.23935	-0.04297
C	-1.86420	1.20053	0.11431
H	-3.50952	-0.02625	0.67954
C	-0.75521	1.36538	-0.71660
H	-2.49182	2.07496	0.27114
C	0.30188	0.46624	-0.96422
C	-0.51107	-1.37280	-0.19228
H	-2.56011	-2.03158	-0.38723
H	-0.81325	2.23549	-1.37322
C	0.42698	-0.89474	0.90658
H	-0.15967	-2.23052	-0.76494
C	1.32511	0.02881	0.10343
H	0.75399	0.59719	-1.95391
H	0.94573	-1.71818	1.41471
H	-0.14328	-0.33495	1.65411
C	1.90894	1.20621	0.88269
H	2.44339	1.89134	0.21468
H	1.11509	1.76902	1.38299
H	2.61615	0.84928	1.64050
C	2.45481	-0.75314	-0.57089
H	3.15122	-1.13558	0.18289
H	2.07227	-1.60231	-1.14606
H	3.01676	-0.10882	-1.25619

SCF energy: -389.236416 hartree

zero-point correction: +0.212669 hartree

enthalpy correction: +0.222533 hartree

free energy correction: +0.179681 hartree

quasiharmonic free energy correction: +0.179681 hartree

imaginary frequency: -580.5568

4BCOD

C	1.86842	-1.22931	0.09987
C	2.59702	-0.11050	0.21065
C	2.00733	1.20918	-0.06100
C	0.76626	1.34398	-0.55037
C	-0.12614	0.17155	-0.83747
C	0.40922	-1.16246	-0.23626
H	-0.37510	0.15767	-1.90816
C	-1.38134	0.04248	0.09356
H	0.11770	-2.01837	-0.85189
C	-0.58027	-0.97822	0.94650

H	2.31615	-2.20304	0.28373
H	3.64572	-0.15858	0.48909
H	2.61968	2.08968	0.11275
H	0.38054	2.33501	-0.78274
H	-0.08286	-0.48996	1.79120
H	-1.11911	-1.86198	1.30396
C	-2.53769	-0.62502	-0.64636
H	-3.33082	-0.90777	0.05488
H	-2.96699	0.05668	-1.38924
H	-2.21175	-1.53051	-1.16966
C	-1.86038	1.29023	0.82064
H	-2.28551	2.01976	0.12114
H	-2.64044	1.02634	1.54382
H	-1.04184	1.77364	1.36260

SCF energy: -389.280523 hartree

zero-point correction: +0.214708 hartree

enthalpy correction: +0.224799 hartree

free energy correction: +0.181344 hartree

quasiharmonic free energy correction: +0.181432 hartree

5

C	3.99769	0.41346	-0.00012
C	2.71322	0.02615	-0.00114
H	4.21774	1.48195	0.00330
C	1.60248	0.96726	0.00212
H	2.49217	-1.03986	-0.00498
C	0.28444	0.66841	0.00405
C	-0.28442	-0.66841	0.00434
H	1.88343	2.01944	0.00302
H	-0.41073	1.50345	0.00593
C	-1.60246	-0.96725	0.00258
C	-2.71322	-0.02615	-0.00074
H	0.41075	-1.50344	0.00645
H	-1.88342	-2.01943	0.00367
C	-3.99769	-0.41350	-0.00077
H	-2.49217	1.03986	-0.00343
H	-4.21768	-1.48200	0.00168
C	5.17178	-0.51548	-0.00402
H	4.84983	-1.56008	-0.00707
H	5.80246	-0.34760	-0.88400
H	5.80413	-0.35313	0.87577
C	-5.17181	0.51548	-0.00400
H	-5.80336	0.35316	0.87641
H	-4.84988	1.56009	-0.00710
H	-5.80324	0.34771	-0.88339

SCF energy: -389.260334 hartree

zero-point correction: +0.210161 hartree

enthalpy correction: +0.223186 hartree

free energy correction: +0.170701 hartree

quasiharmonic free energy correction: +0.172988 hartree

5COT

C	0.10244	1.58887	-0.61043
C	1.18759	0.55312	-0.44926
C	-1.13909	1.70110	-0.10794
C	-2.02248	0.81008	0.66220
C	0.71293	-0.75506	0.20618
C	-0.30958	-1.44424	-0.65677
C	-1.63815	-1.36286	-0.50894
C	-2.30258	-0.49082	0.45925
H	-3.12592	-0.92190	1.02668
H	-2.63754	1.33212	1.39445
H	0.08866	-2.10785	-1.42617
H	-2.27786	-1.99562	-1.12216
H	0.44764	2.46468	-1.16209
H	-1.61501	2.66430	-0.29748

H	1.55655	0.30363	-1.45658
H	0.24294	-0.49071	1.16262
C	2.35035	1.20673	0.31687
H	3.25291	0.59141	0.28326
H	2.59611	2.18270	-0.11236
H	2.07223	1.36248	1.36538
C	1.87459	-1.71917	0.47592
H	2.45103	-1.89666	-0.44077
H	2.55668	-1.33166	1.23644
H	1.49538	-2.68343	0.82626

SCF energy: -389.274722 hartree

zero-point correction: +0.214611 hartree

enthalpy correction: +0.225208 hartree

free energy correction: +0.180587 hartree

quasiharmonic free energy correction: +0.180796 hartree

TS5_{8π}

C	0.07169	1.74025	-0.28505
C	0.72470	0.93757	0.63225
C	-1.28376	1.61602	-0.63430
C	-2.22266	0.63708	-0.31290
C	0.72475	-0.93754	-0.63228
C	0.07171	-1.74028	0.28496
C	-1.28372	-1.61606	0.63425
C	-2.22264	-0.63711	0.31295
H	-3.23409	-0.93785	0.58494
H	-3.23413	0.93781	-0.58482
H	0.65536	-2.48796	0.82293
H	-1.67881	-2.42530	1.24545
H	0.65532	2.48792	-0.82305
H	-1.67888	2.42525	-1.24549
H	0.10344	0.41714	1.35218
H	0.10354	-0.41711	-1.35224
C	2.14541	1.19352	1.04632
H	2.17007	1.84583	1.92697
H	2.65905	0.26584	1.31640
H	2.71193	1.68388	0.24894
C	2.14550	-1.19347	-1.04625
H	2.17022	-1.84566	-1.92699
H	2.65918	-0.26576	-1.31615
H	2.71191	-1.68394	-0.24887

SCF energy: -389.236898 hartree

zero-point correction: +0.211774 hartree

enthalpy correction: +0.222673 hartree

free energy correction: +0.177405 hartree

quasiharmonic free energy correction: +0.177405 hartree

imaginary frequency: -379.4390

TS5_{6π}

C	-2.19796	0.54972	-0.59286
C	-1.55780	1.36322	0.33378
C	-1.91573	-0.82682	-0.69468
H	-3.12061	0.89117	-1.05554
C	-1.10664	-1.52612	0.20209
H	-2.62106	-1.41646	-1.27600
C	-0.02201	-1.05618	0.97332
C	-0.25738	1.07098	0.76352
H	-2.12940	2.15480	0.81510
H	-1.48516	-2.51673	0.46150
C	0.83624	0.73021	-0.24175
H	0.10560	1.58079	1.65896
C	1.30224	-0.56856	0.37993
H	0.10230	-1.60680	1.91098
H	1.96043	-0.32193	1.22548
H	0.36246	0.51811	-1.20789
C	2.00348	-1.57330	-0.52609
H	2.22035	-2.50516	0.00642
H	1.36622	-1.81398	-1.38359
H	2.95095	-1.16773	-0.89762
C	1.88542	1.82131	-0.41288
H	2.67477	1.49828	-1.10016
H	1.44159	2.73777	-0.81339
H	2.35233	2.06103	0.54947

SCF energy: -389.237035 hartree

zero-point correction: +0.212779 hartree

enthalpy correction: +0.222867 hartree

free energy correction: +0.179238 hartree

quasiharmonic free energy correction: +0.179372 hartree

imaginary frequency: -573.4947

5BCOD

C	1.44731	-1.44128	0.15145
C	2.34781	-0.63749	-0.43151
C	2.14062	0.81775	-0.49051
C	1.12812	1.41684	0.15357
C	0.11911	0.65432	0.96480
C	0.16720	-0.87702	0.68733
H	0.18655	0.96901	2.01433
C	-1.32611	0.65806	0.38093
H	-0.18420	-1.44126	1.55914
C	-1.00760	-0.68730	-0.31368
H	1.61775	-2.51344	0.21204

H	3.26010	-1.04482	-0.85757
H	2.85920	1.41519	-1.04478
H	1.03874	2.50159	0.13171
H	-2.03342	0.47665	1.20158
H	-0.58917	-0.48531	-1.30897
C	-2.08887	-1.74841	-0.39310
H	-2.91727	-1.42087	-1.03069
H	-1.69932	-2.68461	-0.80624
H	-2.49347	-1.96006	0.60325
C	-1.80399	1.81842	-0.47322
H	-2.78953	1.60147	-0.89875
H	-1.88761	2.74216	0.10927
H	-1.11006	2.00087	-1.30068

SCF energy: -389.280360 hartree

zero-point correction: +0.214816 hartree

enthalpy correction: +0.225105 hartree

free energy correction: +0.180942 hartree

quasiharmonic free energy correction: +0.181129 hartree

6

C	3.96253	-0.69426	0.00021
C	2.61821	-0.69808	0.00009
H	4.47171	-1.65502	0.00036
C	1.80310	0.50756	-0.00009
H	2.11166	-1.65915	0.00014
C	0.45127	0.56852	-0.00025
C	-0.45127	-0.56852	-0.00036
H	2.34275	1.45212	-0.00009
H	0.00195	1.55773	-0.00034
C	-1.80310	-0.50757	-0.00025
C	-2.61822	0.69808	0.00005
H	-0.00195	-1.55773	-0.00054
H	-2.34275	-1.45212	-0.00035
C	-3.96253	0.69426	0.00019
H	-2.11166	1.65915	0.00021
H	-4.47171	1.65502	0.00050
C	-4.82973	-0.53758	0.00010
H	-4.64431	-1.15924	0.88282
H	-5.88784	-0.27080	-0.00035
H	-4.64363	-1.15959	-0.88222
C	4.82973	0.53758	0.00019
H	4.64372	1.15961	0.88252
H	5.88784	0.27080	0.00056
H	4.64423	1.15921	-0.88252

SCF energy: -389.254501 hartree

zero-point correction: +0.210121 hartree

enthalpy correction: +0.221710 hartree

free energy correction: +0.171971 hartree

quasiharmonic free energy correction: +0.174517 hartree

TS6_{8π}

C	-1.68127	-0.49075	0.43393
C	-1.04348	-1.27116	-0.50933
C	-1.61090	0.90902	0.60894
C	-0.65921	1.86077	0.26225
C	1.04238	-1.27203	0.50931
C	1.68084	-0.49215	-0.43394
C	1.61170	0.90768	-0.60893
C	0.66081	1.86023	-0.26222
H	0.99626	2.87304	-0.48185
H	-0.99379	2.87386	0.48192
H	2.29310	-1.01404	-1.16904
H	2.43765	1.31830	-1.18923
H	-2.29397	-1.01211	1.16902
H	-2.43651	1.32034	1.18925
H	-1.20848	-2.34501	-0.42127

H	1.20647	-2.34601	0.42122
C	-0.75520	-0.80025	-1.90787
H	-0.47726	0.25283	-1.94575
H	0.03202	-1.39056	-2.38259
H	-1.67101	-0.92676	-2.49819
C	0.75450	-0.80093	1.90786
H	0.47722	0.25232	1.94579
H	-0.03305	-1.39075	2.38264
H	1.67028	-0.92802	2.49811

SCF energy: -389.227374 hartree

zero-point correction: +0.212039 hartree

enthalpy correction: +0.222686 hartree

free energy correction: +0.178301 hartree

quasiharmonic free energy correction: +0.178301 hartree

imaginary frequency: -396.7635

7

C	-4.06414	0.42552	-0.00051
C	-2.73335	0.61522	-0.00043
H	-4.70178	1.30629	-0.00089
C	-1.75857	-0.46559	0.00023
H	-2.36441	1.63713	-0.00084
C	-0.41180	-0.33657	0.00055
C	0.32526	0.91473	0.00044
H	-2.16130	-1.47615	0.00054
H	0.17134	-1.25355	0.00104
C	1.67145	1.03726	0.00025
C	2.64967	-0.04076	-0.00005
H	-0.25441	1.83342	0.00061
H	2.08812	2.04350	0.00034
C	3.97353	0.17705	-0.00009
H	2.29228	-1.06905	-0.00034
H	4.32989	1.20809	0.00010
C	-4.75178	-0.91501	0.00002
H	-4.48287	-1.50374	0.88386
H	-5.83674	-0.79791	-0.00202
H	-4.47978	-1.50611	-0.88126
C	5.01747	-0.89596	-0.00037
H	4.56327	-1.89019	-0.00065
H	5.66496	-0.81331	-0.88023
H	5.66493	-0.81380	0.87953

SCF energy: -389.257438 hartree

zero-point correction: +0.210287 hartree

enthalpy correction: +0.222501 hartree

free energy correction: +0.172015 hartree

quasiharmonic free energy correction: +0.173866 hartree

TS7_{8π}

C	-0.88645	1.42316	0.17216
C	-1.28703	0.38019	-0.63436
C	0.43203	1.90617	0.29568
C	1.64746	1.37010	-0.11217
C	-0.48522	-1.36411	0.63003
C	0.39001	-1.77805	-0.35723
C	1.59764	-1.16987	-0.75739
C	2.10300	0.11885	-0.60667
H	3.12553	0.19641	-0.97526
H	2.46570	2.08424	-0.02862
H	0.08272	-2.63352	-0.95931
H	2.23599	-1.81192	-1.36276
H	-1.64209	1.90780	0.79175
H	0.51733	2.87422	0.78722

H	-0.61619	0.09761	-1.43738
H	-1.41910	-1.92212	0.70435
C	-2.73961	0.03522	-0.82393
H	-3.17706	0.65129	-1.61842
H	-2.87024	-1.01069	-1.11452
H	-3.31024	0.21336	0.09267
C	-0.04047	-0.73224	1.91702
H	0.88181	-0.16349	1.80540
H	-0.80833	-0.07960	2.34085
H	0.14599	-1.54005	2.63525

SCF energy: -389.231471 hartree
 zero-point correction: +0.211704 hartree
 enthalpy correction: +0.222607 hartree
 free energy correction: +0.177333 hartree
 quasiharmonic free energy correction: +0.177333 hartree
 imaginary frequency: -394.0202

7COT

C	-0.70745	1.39496	-0.53807
C	-1.40311	0.05625	-0.57700
C	0.47661	1.85184	-0.08958
C	1.66608	1.23781	0.51368
C	-0.62669	-1.15371	-0.01683
C	0.60059	-1.43478	-0.85172
C	1.83907	-0.94680	-0.70736
C	2.27516	0.06777	0.25023
H	3.23200	-0.11186	0.73835
H	2.17780	1.89686	1.21426
H	0.44786	-2.14807	-1.66127
H	2.61873	-1.34404	-1.35685
H	-1.36157	2.18196	-0.91843
H	0.58101	2.93521	-0.15417
H	-1.58960	-0.15921	-1.63938
H	-1.28818	-2.01465	-0.18296
C	-2.77769	0.20327	0.09683
H	-3.37978	0.96434	-0.40844
H	-3.32888	-0.74230	0.06344
H	-2.66989	0.50320	1.14352
C	-0.40498	-1.07241	1.50208
H	-1.33708	-1.30522	2.02490
H	0.34971	-1.79795	1.81796
H	-0.07774	-0.08335	1.82552

SCF energy: -389.268841 hartree
 zero-point correction: +0.214896 hartree
 enthalpy correction: +0.225566 hartree
 free energy correction: +0.180840 hartree
 quasiharmonic free energy correction: +0.180966 hartree

TS7_{6π}^X

C	2.22767	0.51974	-0.63955
C	1.34870	1.50466	-0.18362
C	2.28498	-0.78481	-0.11298
H	3.11920	0.86315	-1.15951
C	1.35749	-1.24625	0.81544
H	3.22781	-1.31324	-0.23106
C	0.04692	-0.75626	0.82694
C	0.06231	1.35279	0.36914
H	1.80025	2.49390	-0.08584
H	1.70529	-1.89993	1.61358
C	-1.15053	0.80930	-0.39832
H	-0.20042	2.14896	1.07388
C	-0.74751	-0.65491	-0.47326
H	-0.55546	-0.96798	1.71259
H	-0.04068	-0.77829	-1.30008
H	-1.24293	1.29165	-1.38173
C	-1.84968	-1.70033	-0.60337
H	-1.41942	-2.70582	-0.63533
H	-2.42793	-1.54821	-1.52121
H	-2.54280	-1.65856	0.24338
C	-2.43538	1.06615	0.38511
H	-3.30491	0.65859	-0.13859
H	-2.59406	2.14146	0.51425
H	-2.39376	0.61381	1.38244

SCF energy: -389.234298 hartree

zero-point correction: +0.213114 hartree

enthalpy correction: +0.223014 hartree

free energy correction: +0.179915 hartree

quasiharmonic free energy correction: +0.179931 hartree

imaginary frequency: -576.5579

TS7_{6π}^N

C	1.45126	1.16445	0.81473
C	0.44593	1.71120	0.01648
C	2.16300	-0.00329	0.48802
H	1.92783	1.83266	1.52859
C	1.83084	-0.78321	-0.61323
H	3.14722	-0.11440	0.93691
C	0.52500	-0.86813	-1.11073
C	-0.41746	1.07039	-0.89426
H	0.47280	2.80106	-0.04209
H	2.64713	-1.21901	-1.18823

C	-1.51276	0.05423	-0.55263
H	-0.71939	1.73669	-1.70901
C	-0.69986	-1.20126	-0.24669
H	0.42740	-1.22505	-2.13694
H	-1.17590	-2.09583	-0.66949
H	-2.05157	-0.12758	-1.49061
C	-2.51443	0.54943	0.48579
H	-2.98717	1.47762	0.14837
H	-3.30314	-0.19131	0.65695
H	-2.01642	0.75581	1.43794
C	-0.46103	-1.50253	1.23035
H	-1.40957	-1.79418	1.69250
H	0.24166	-2.33265	1.34287
H	-0.06382	-0.65141	1.78528

SCF energy: -389.228531 hartree

zero-point correction: +0.213351 hartree

enthalpy correction: +0.223230 hartree

free energy correction: +0.180084 hartree

quasiharmonic free energy correction: +0.180418 hartree

imaginary frequency: -580.2701

7BCOD^x

C	1.38983	1.29725	0.62023
C	2.44816	0.72859	0.02568
C	2.37927	-0.64444	-0.49833
C	1.32060	-1.43564	-0.27171
C	0.11357	-0.97490	0.49299
C	0.08282	0.56834	0.69612
H	-0.01527	-1.59094	1.39411
C	-1.17313	-0.85092	-0.37400
H	-0.46491	0.83616	1.60679
C	-0.86028	0.66609	-0.53682
H	1.45612	2.30482	1.02357
H	3.38691	1.26717	-0.06623
H	3.23241	-1.02513	-1.05284
H	1.31943	-2.46351	-0.63088
H	-1.15369	-1.41963	-1.31171
H	-0.24125	0.80496	-1.43075
C	-2.44434	-1.17050	0.40066
H	-3.33863	-0.87556	-0.15781
H	-2.50940	-2.24458	0.60159
H	-2.46533	-0.65201	1.36613
C	-1.98641	1.68373	-0.52028
H	-1.58427	2.70209	-0.53093
H	-2.63658	1.57215	-1.39469
H	-2.60608	1.57843	0.37635

SCF energy: -389.279268 hartree
 zero-point correction: +0.215044 hartree
 enthalpy correction: +0.225222 hartree
 free energy correction: +0.181392 hartree
 quasiharmonic free energy correction: +0.181503 hartree

7BCOD^N

C	1.74866	-0.93944	-0.42709
C	2.31341	-0.00697	0.35223
C	1.63237	1.26687	0.63545
C	0.48000	1.59845	0.03651
C	-0.18242	0.71552	-0.98412
C	0.38532	-0.73164	-1.01580
H	-0.19153	1.24530	-1.94607
C	-1.56522	0.12091	-0.58341
H	0.34735	-1.13903	-2.03119
C	-0.86629	-1.22321	-0.21101
H	2.26628	-1.87443	-0.62917
H	3.29400	-0.17377	0.78894
H	2.09711	1.95185	1.33918
H	0.01586	2.56079	0.24546
H	-2.15782	-0.02600	-1.49376
H	-1.34877	-2.10767	-0.64194
C	-2.41210	0.83484	0.45643
H	-2.74713	1.80862	0.08347
H	-3.30285	0.24780	0.70323
H	-1.85194	1.00646	1.38098
C	-0.64313	-1.45683	1.27769
H	-1.60151	-1.59360	1.78959
H	-0.04273	-2.35682	1.44056
H	-0.11991	-0.62048	1.74947

SCF energy: -389.277406 hartree
 zero-point correction: +0.215415 hartree
 enthalpy correction: +0.225423 hartree
 free energy correction: +0.182144 hartree
 quasiharmonic free energy correction: +0.182178 hartree

8

C	-3.57981	0.01612	0.00009
C	-2.25160	0.24645	0.00060
C	-1.20050	-0.75886	0.00053
H	-1.93659	1.28758	0.00117
C	0.13218	-0.52330	0.00023
C	0.77307	0.78004	-0.00038
H	0.78392	-1.39276	0.00041
C	2.10600	1.00533	-0.00049
C	3.16325	0.00456	0.00006
H	2.44486	2.04033	-0.00105
C	4.46720	0.32032	-0.00023
H	4.74585	1.37506	-0.00090
C	5.58826	-0.67211	0.00024
H	6.22832	-0.54149	0.87977
H	5.20897	-1.69731	0.00134
H	6.22758	-0.54313	-0.88008
C	-4.55859	1.15893	0.00032
H	-4.05364	2.12754	0.00092
H	-5.21121	1.10965	-0.87982
H	-5.21170	1.10884	0.88005
C	-4.22088	-1.34461	-0.00084
H	-4.86568	-1.45486	-0.88077
H	-3.50542	-2.16641	-0.00109
H	-4.86629	-1.45583	0.87852
H	-1.51108	-1.79981	0.00088
H	0.12668	1.65315	-0.00085
H	2.88396	-1.04768	0.00075

SCF energy: -428.559267 hartree

zero-point correction: +0.238566 hartree

enthalpy correction: +0.253011 hartree

free energy correction: +0.197268 hartree

quasiharmonic free energy correction: +0.199734 hartree

TS8_{8π}

C	-0.23423	-1.57959	-0.63167
C	-0.92884	-0.88026	0.35743
C	1.14133	-1.59941	-0.89751
C	2.21227	-0.77360	-0.53164
C	-0.55692	1.12143	-0.65236
C	0.21022	1.74367	0.32088
C	1.56251	1.48561	0.57996
C	2.39616	0.46182	0.12627
H	3.16613	-1.19412	-0.84874
H	2.05489	2.20968	1.22712
H	-0.84422	-2.14707	-1.33710

H	-0.01270	0.62921	-1.44970
C	-1.90896	1.66749	-1.02365
H	-1.79066	2.49473	-1.73344
H	-2.53946	0.91614	-1.50508
H	-2.43812	2.05495	-0.14719
C	-2.43406	-1.01325	0.38888
H	-2.85432	-1.18344	-0.60560
H	-2.71584	-1.86012	1.02711
H	-2.90257	-0.12082	0.81563
C	-0.32279	-0.71194	1.72737
H	0.76267	-0.64119	1.70876
H	-0.72624	0.16313	2.24580
H	-0.59057	-1.60189	2.31162
H	-0.27580	2.49127	0.94927
H	3.44769	0.65384	0.33559
H	1.43907	-2.39613	-1.57770

SCF energy: -428.531522 hartree

zero-point correction: +0.240114 hartree

enthalpy correction: +0.252148 hartree

free energy correction: +0.204855 hartree

quasiharmonic free energy correction: +0.204855 hartree

imaginary frequency: -411.5178

8COT

C	0.38177	1.75649	0.32024
C	-0.93959	1.04762	0.15430
C	1.68573	1.41874	0.33267
C	2.44257	0.16834	0.23269
C	-0.96690	-0.49706	0.31145
C	-0.30535	-1.17307	-0.87334
C	0.99061	-1.39966	-1.13142
C	2.17353	-1.00422	-0.37176
H	-1.00366	-1.55393	-1.61953
H	-1.57597	1.44340	0.96333
C	-2.43602	-0.96499	0.33655
H	-2.48070	-2.03669	0.55616
H	-2.99764	-0.43677	1.11451
H	-2.93969	-0.80372	-0.62042
C	-0.35891	-0.90197	1.66448
H	-0.38104	-1.99085	1.77310
H	0.66891	-0.56872	1.79128
H	-0.95856	-0.46666	2.47218
C	-1.56300	1.52480	-1.17102
H	-2.61125	1.22732	-1.25518
H	-1.52295	2.61574	-1.24264
H	-1.00729	1.11505	-2.01975
H	2.34846	2.26638	0.50411

H	2.97676	-1.73976	-0.36644
H	0.21690	2.82698	0.45655
H	3.43065	0.24179	0.68476
H	1.21043	-1.98967	-2.02117

SCF energy: -428.564792 hartree
 zero-point correction: +0.242997 hartree
 enthalpy correction: +0.255028 hartree
 free energy correction: +0.207146 hartree
 quasiharmonic free energy correction: +0.208039 hartree

TS8_{6π}^x

C	2.52697	0.46362	0.35691
C	1.80056	1.29449	-0.48909
C	2.20204	-0.89611	0.52383
C	1.23673	-1.56458	-0.23203
H	2.96019	-1.51202	1.00244
C	0.06471	-1.05192	-0.82225
C	0.43964	1.07065	-0.72699
H	2.33932	2.04526	-1.06475
C	-0.51264	0.81193	0.43431
C	-1.13851	-0.49609	-0.03647
H	-0.23809	-1.60231	-1.72019
H	0.09676	0.59558	1.31965
C	-2.30195	-0.27332	-1.00636
H	-2.61801	-1.22921	-1.43818
H	-3.16301	0.16100	-0.48861
H	-2.02617	0.39126	-1.83178
C	-1.58820	-1.42520	1.09107
H	-1.91508	-2.39358	0.69532
H	-0.76802	-1.60387	1.79312
H	-2.42896	-0.98280	1.63895
C	-1.43903	1.98180	0.74728
H	-2.15754	1.71418	1.53027
H	-0.86187	2.84263	1.09779
H	-2.00317	2.29325	-0.13801
H	-0.00798	1.59220	-1.57518
H	1.52902	-2.57062	-0.53886
H	3.52064	0.76742	0.67680

SCF energy: -428.535404 hartree
 zero-point correction: +0.240943 hartree
 enthalpy correction: +0.252208 hartree
 free energy correction: +0.206482 hartree
 quasiharmonic free energy correction: +0.206549 hartree
 imaginary frequency: -567.2281

TS8_{6π}^N

C	-2.17799	0.60557	0.56354
C	-1.45300	1.43514	-0.29340
C	-2.21176	-0.79443	0.45118
C	-1.42152	-1.48052	-0.46468
H	-3.07416	-1.29655	0.88330
C	-0.17922	-1.00950	-0.90481
C	-0.28312	1.15781	-1.02590
H	-1.98087	2.34876	-0.57385
C	1.10823	0.85761	-0.46165
C	0.97644	-0.58714	0.02421
H	0.18083	-1.43557	-1.84376
C	0.69563	-0.72049	1.52264
H	-0.11981	-0.08564	1.86918
H	0.44387	-1.75614	1.77004
H	1.59773	-0.44610	2.07981
C	2.22059	-1.42431	-0.29324
H	2.45506	-1.39568	-1.36265
H	3.08842	-1.03928	0.25486
H	2.07277	-2.47055	-0.00298
C	1.62359	1.91219	0.51287
H	2.63294	1.66512	0.86119
H	1.66365	2.89302	0.02804
H	0.96381	1.99550	1.38159
H	1.78123	0.83960	-1.32941
H	-0.22851	1.74758	-1.94640
H	-2.99743	1.06338	1.11312
H	-1.86669	-2.33901	-0.96665

SCF energy: -428.528375 hartree

zero-point correction: +0.241137 hartree

enthalpy correction: +0.252373 hartree

free energy correction: +0.206560 hartree

quasiharmonic free energy correction: +0.206951 hartree

imaginary frequency: -573.1288

8BCOD^X

C	1.36952	-1.50487	-0.27682
C	2.36742	-0.82467	0.30451
C	2.34827	0.64519	0.38110
C	1.39591	1.36998	-0.22267
C	0.30547	0.74258	-1.04551
C	0.18052	-0.79423	-0.84969
C	-1.14627	0.89152	-0.50348
H	-0.13554	-1.27938	-1.78042
C	-1.08217	-0.56634	0.05736

H	1.40023	-2.59112	-0.32526
H	3.21654	-1.35036	0.73197
H	3.14190	1.14054	0.93354
H	1.42492	2.45704	-0.17139
H	-1.83723	0.90432	-1.35622
C	-1.48573	2.04088	0.43028
C	-0.78899	-0.63504	1.55423
C	-2.28724	-1.43585	-0.27740
H	-2.50976	-1.40780	-1.34954
H	-3.17674	-1.08901	0.26241
H	-2.11004	-2.47985	0.00631
H	0.09096	-0.05017	1.83334
H	-0.61072	-1.67145	1.85945
H	-1.64703	-0.25826	2.12243
H	-0.80103	2.08120	1.28323
H	-2.50549	1.93995	0.81712
H	-1.42266	3.00014	-0.09446
H	0.42144	1.07935	-2.08407

SCF energy: -428.578109 hartree

zero-point correction: +0.243115 hartree

enthalpy correction: +0.254553 hartree

free energy correction: +0.208433 hartree

quasiharmonic free energy correction: +0.208520 hartree

8BCOD^N

C	-1.75928	1.35558	-0.29799
C	-2.67850	0.50940	0.18693
C	-2.39033	-0.92645	0.32583
C	-1.25735	-1.47114	-0.14132
C	-0.18732	-0.66456	-0.81818
C	-0.38346	0.87020	-0.63940
C	1.16409	-0.54394	-0.03463
H	0.02478	1.42409	-1.49266
C	0.65801	0.82576	0.51201
H	-1.98702	2.41213	-0.41856
H	-3.66388	0.86629	0.47235
H	-3.14291	-1.55749	0.79078
H	-1.10259	-2.54611	-0.06563
C	1.62216	1.98477	0.68854
H	2.13521	2.22406	-0.24891
H	2.38477	1.75578	1.44158
H	1.08997	2.88347	1.01729
H	-0.06045	-1.02284	-1.84994
C	2.33396	-0.40619	-1.00585
H	2.53333	-1.36830	-1.49094
H	3.24590	-0.09608	-0.48301
H	2.13113	0.32733	-1.79381

C	1.47744	-1.59366	1.02193
H	2.36841	-1.30076	1.58996
H	1.67933	-2.57076	0.56712
H	0.64775	-1.71000	1.72621
H	0.11972	0.64051	1.45102

SCF energy: -428.579442 hartree

zero-point correction: +0.242520 hartree

enthalpy correction: +0.254099 hartree

free energy correction: +0.207502 hartree

quasiharmonic free energy correction: +0.207741 hartree

9

C	3.53574	0.19062	0.00016
C	2.18965	0.26422	0.00080
C	1.26394	-0.85743	0.00084
H	1.75531	1.26145	0.00145
C	-0.08753	-0.78180	0.00031
C	-0.87546	0.43799	-0.00075
H	-0.63065	-1.72257	0.00065
C	-2.22633	0.51605	-0.00097
C	-3.15300	-0.60706	-0.00024
H	-2.66077	1.51191	-0.00181
C	-4.49510	-0.52127	0.00027
C	4.37399	1.44015	0.00033
H	3.75915	2.34301	0.00079
H	5.02841	1.46677	0.88008
H	5.02791	1.46734	-0.87978
C	4.33178	-1.08558	-0.00090
H	4.98679	-1.11964	0.87772
H	3.71777	-1.98568	0.00009
H	4.98412	-1.11982	-0.88150
H	1.69536	-1.85442	0.00144
H	-0.33100	1.37819	-0.00150
H	-2.72306	-1.60508	-0.00012
H	-5.05320	-1.45612	0.00074
C	-5.33223	0.72263	0.00029
H	-5.98456	0.74324	0.88014
H	-4.73876	1.63765	-0.00030
H	-5.98550	0.74265	-0.87888

SCF energy: -428.557102 hartree

zero-point correction: +0.238669 hartree

enthalpy correction: +0.253209 hartree

free energy correction: +0.196584 hartree

quasiharmonic free energy correction: +0.199732 hartree

TS9_{8π}

C	0.59178	-1.71394	-0.43420
C	-0.29563	-1.45992	0.59545
C	1.79336	-1.04340	-0.74130
C	2.25799	0.23494	-0.44881
C	-1.35731	0.36550	-0.33278
C	-0.82049	1.29616	0.54423
C	0.47815	1.84165	0.58794
C	1.71908	1.41621	0.12017
H	3.28804	0.38398	-0.77026
H	0.53732	2.76480	1.16417

H	0.32004	-2.50708	-1.13055
C	-2.79915	-0.04688	-0.12967
H	-3.46983	0.68161	-0.60324
H	-2.99989	-1.01786	-0.59230
H	-3.05768	-0.10866	0.93136
H	-1.19124	-2.08155	0.60452
C	0.13881	-0.99283	1.95716
H	0.96613	-0.28512	1.91272
H	-0.68545	-0.53805	2.51293
H	0.47808	-1.87078	2.52048
H	2.48937	2.17338	0.26082
H	2.46193	-1.60762	-1.39083
H	-1.48294	1.64787	1.33735
C	-0.90745	0.32836	-1.77096
H	0.14514	0.57952	-1.89203
H	-1.09619	-0.64551	-2.23089
H	-1.49765	1.07589	-2.31765

SCF energy: -428.527592 hartree

zero-point correction: +0.239972 hartree

enthalpy correction: +0.252047 hartree

free energy correction: +0.204791 hartree

quasiharmonic free energy correction: +0.204791 hartree

imaginary frequency: -406.0158

10

C	4.03310	-0.08651	0.00049
C	2.69513	-0.25113	0.00039
C	1.69467	0.80458	-0.00084
H	2.32929	-1.27553	0.00150
C	0.35162	0.63515	-0.00151
C	-0.35161	-0.63512	-0.00165
H	-0.25494	1.53643	-0.00220
C	-1.69467	-0.80456	-0.00101
C	-2.69513	0.25114	0.00035
H	-2.05639	-1.82890	-0.00147
C	-4.03310	0.08650	0.00051
C	-4.95462	1.27601	0.00206
H	-5.60917	1.25746	0.88198
H	-4.40259	2.21862	0.00324
H	-5.60922	1.25970	-0.87787
C	4.95460	-1.27603	0.00211
H	4.40256	-2.21863	0.00328
H	5.60929	-1.25974	-0.87775
H	5.60906	-1.25748	0.88211
C	4.74021	1.24110	-0.00085
H	5.39092	1.31880	-0.87993
H	4.06568	2.09682	-0.00300
H	5.38900	1.32165	0.87940
H	2.05640	1.82892	-0.00109
H	0.25495	-1.53640	-0.00253
H	-2.32931	1.27554	0.00141
C	-4.74019	-1.24112	-0.00072
H	-5.39079	-1.31898	-0.87987
H	-4.06564	-2.09682	-0.00262
H	-5.38909	-1.32151	0.87947

SCF energy: -467.858191 hartree

zero-point correction: +0.266685 hartree

enthalpy correction: +0.282679 hartree

free energy correction: +0.222879 hartree

quasiharmonic free energy correction: +0.226212 hartree

10COT

C	0.03602	1.67529	-0.23216
C	-1.05952	0.62438	-0.16042
C	1.36038	1.75863	-0.00220
C	2.42088	0.81761	0.37148
C	-0.57276	-0.81399	0.22653
C	0.40298	-1.32834	-0.82147
C	1.73779	-1.23458	-0.87939
C	2.61414	-0.45755	-0.00831

H	-0.06420	-1.91840	-1.61058
C	-1.73943	-1.82690	0.21727
H	-1.36002	-2.80445	0.53389
H	-2.53333	-1.54216	0.91230
H	-2.17560	-1.95149	-0.77768
C	-0.00306	-0.83476	1.66031
H	0.61408	-1.72638	1.80574
H	0.60302	0.03901	1.89694
H	-0.82666	-0.87563	2.37998
C	-1.74995	0.61665	-1.54072
H	-2.67700	0.03653	-1.51543
H	-2.01261	1.63789	-1.83534
H	-1.09329	0.20685	-2.31297
H	1.74783	2.77464	-0.08400
H	3.54985	-0.93066	0.28528
H	-0.40684	2.64025	-0.48980
H	3.21283	1.27233	0.96538
H	2.24275	-1.79889	-1.66333
C	-2.07997	1.16825	0.86378
H	-2.41557	2.16461	0.55763
H	-2.96686	0.53081	0.92187
H	-1.64337	1.25684	1.86188

SCF energy: -467.859315 hartree

zero-point correction: +0.271216 hartree

enthalpy correction: +0.284302 hartree

free energy correction: +0.234923 hartree

quasiharmonic free energy correction: +0.235386 hartree

TS10_{8π}

C	0.04295	-1.58323	-0.70521
C	-0.77925	-1.10389	0.31696
C	1.42749	-1.46945	-0.87796
C	2.39757	-0.60064	-0.36689
C	-0.77925	1.10389	-0.31696
C	0.04295	1.58323	0.70521
C	1.42749	1.46944	0.87796
C	2.39757	0.60064	0.36689
H	3.40704	-0.90564	-0.63947
H	1.83052	2.17122	1.60763
H	-0.46433	-2.12648	-1.50485
C	-2.24023	1.49239	-0.23295
H	-2.36238	2.52124	-0.59521
H	-2.86706	0.85484	-0.86180
H	-2.61844	1.45097	0.79269
C	-2.24023	-1.49239	0.23295
H	-2.61844	-1.45096	-0.79269
H	-2.36238	-2.52123	0.59521

H	-2.86706	-0.85484	0.86180
C	-0.26369	-1.05852	1.73472
H	0.79321	-0.80593	1.79543
H	-0.83303	-0.35518	2.34996
H	-0.39462	-2.06058	2.16446
H	3.40704	0.90564	0.63947
H	1.83052	-2.17122	-1.60763
H	-0.46433	2.12648	1.50485
C	-0.26369	1.05852	-1.73472
H	0.79321	0.80593	-1.79543
H	-0.83303	0.35518	-2.34996
H	-0.39462	2.06058	-2.16446

SCF energy: -467.825831 hartree

zero-point correction: +0.268534 hartree

enthalpy correction: +0.281692 hartree

free energy correction: +0.232472 hartree

quasiharmonic free energy correction: +0.232472 hartree

imaginary frequency: -426.3436

TS10_{6π}

C	-2.34506	-0.85572	0.41149
C	-1.34834	-1.63679	-0.18010
C	-2.58136	0.48673	0.08058
C	-1.75654	1.18791	-0.79562
H	-3.57683	0.87213	0.28805
C	-0.39703	0.90892	-0.95867
C	-0.12467	-1.24730	-0.75059
H	-1.66722	-2.65650	-0.40507
C	1.10672	-0.63139	-0.05634
C	0.62692	0.81899	0.18895
H	0.04808	1.27954	-1.88443
C	1.69783	1.90367	-0.00187
H	1.25444	2.89071	0.16900
H	2.51407	1.77304	0.71828
H	2.12635	1.89975	-1.00720
C	0.04225	1.03911	1.58943
H	-0.44776	2.01580	1.64007
H	-0.68618	0.28633	1.88658
H	0.85735	1.02853	2.32057
C	2.26456	-0.69350	-1.06281
H	3.17409	-0.24946	-0.64789
H	2.48230	-1.73897	-1.30560
H	2.02309	-0.17912	-1.99864
H	0.18079	-1.92838	-1.55330
H	-2.23805	1.87463	-1.49125
H	-3.16715	-1.38643	0.88654
C	1.51970	-1.42663	1.18585
H	1.78906	-2.44974	0.90088

H	2.39391	-0.96887	1.66525
H	0.70987	-1.48699	1.91635

SCF energy: -467.824286 hartree
 zero-point correction: +0.269595 hartree
 enthalpy correction: +0.281850 hartree
 free energy correction: +0.234331 hartree
 quasiharmonic free energy correction: +0.234591 hartree
 imaginary frequency: -561.7964

10BCOD

C	-1.74245	1.25259	-0.61108
C	-2.71142	0.49312	-0.08124
C	-2.48185	-0.92445	0.24156
C	-1.33700	-1.54374	-0.07904
C	-0.22859	-0.85247	-0.82114
C	-0.37749	0.69268	-0.87714
C	1.13318	-0.66739	-0.07488
H	0.00817	1.08823	-1.82388
C	0.73039	0.83113	0.22517
H	-1.92953	2.29906	-0.84183
H	-3.69209	0.91403	0.12171
H	-3.27552	-1.47179	0.74248
H	-1.20724	-2.60023	0.14908
C	0.15889	1.03177	1.62946
C	1.78542	1.90251	-0.03160
H	2.19979	1.84821	-1.04187
H	2.61440	1.81424	0.68126
H	1.34539	2.89824	0.09559
H	-0.64715	0.33173	1.86002
H	-0.24489	2.04463	1.72866
H	0.94852	0.90874	2.37920
C	2.28705	-0.78828	-1.07103
H	2.41245	-1.83648	-1.36430
H	3.23070	-0.44401	-0.63361
H	2.10502	-0.21079	-1.98336
H	-0.10744	-1.34724	-1.79585
C	1.41084	-1.56577	1.12463
H	1.56520	-2.60039	0.79702
H	2.32239	-1.24297	1.64151
H	0.58996	-1.56338	1.84619

SCF energy: -467.875807 hartree
 zero-point correction: +0.271382 hartree
 enthalpy correction: +0.283977 hartree
 free energy correction: +0.235804 hartree
 quasiharmonic free energy correction: +0.235815 hartree

2F

C	-3.38705	0.26327	0.00000
C	-2.09552	-0.06312	0.00000
H	-3.79397	1.26953	0.00001
C	-1.05924	0.95758	0.00002
H	-1.83845	-1.11777	-0.00002
C	0.27445	0.74665	0.00004
C	0.92651	-0.55166	0.00006
H	-1.41024	1.98788	0.00002
H	0.91168	1.62612	0.00005
C	2.25993	-0.76741	0.00003
C	3.30721	0.24590	-0.00003
H	0.28485	-1.42875	0.00010
H	2.60901	-1.79870	0.00005
C	4.61165	-0.05805	-0.00005
H	3.01276	1.29245	-0.00007
H	4.94788	-1.09180	-0.00001
H	5.37488	0.71216	-0.00009
F	-4.34733	-0.67666	-0.00005

SCF energy: -409.869557 hartree

zero-point correction: +0.146333 hartree

enthalpy correction: +0.156132 hartree

free energy correction: +0.111950 hartree

quasiharmonic free energy correction: +0.112256 hartree

TS2F_{8π}

C	-1.15830	1.24160	0.15531
C	-1.35043	0.03373	-0.45922
C	0.09249	1.87549	0.29720
C	1.38559	1.45267	0.02326
C	-0.23974	-1.26312	1.07857
C	0.67163	-1.81868	0.21534
C	1.74219	-1.11051	-0.37346
C	2.02920	0.24720	-0.38127
H	3.02526	0.45356	-0.77192
H	2.10082	2.27154	0.08766
H	0.52939	-2.84876	-0.10572
H	2.47343	-1.72375	-0.89619
H	-2.02934	1.70366	0.61303
H	0.03183	2.89417	0.67308
H	-0.69662	-0.37720	-1.21517
H	-1.04686	-1.86371	1.48761
H	0.01764	-0.35927	1.61493
F	-2.60459	-0.45562	-0.53574

SCF energy: -409.846218 hartree

zero-point correction: +0.147618 hartree
 enthalpy correction: +0.156398 hartree
 free energy correction: +0.115289 hartree
 quasiharmonic free energy correction: +0.115289 hartree
 imaginary frequency: -380.2156

TS2F_{6π}^X

C	1.94602	0.16974	-0.66661
C	1.40495	1.27788	-0.01354
C	1.66488	-1.16868	-0.32150
H	2.87004	0.33217	-1.21665
C	0.69438	-1.50490	0.61422
H	2.41580	-1.90478	-0.59694
C	-0.41573	-0.67508	0.80087
C	0.15449	1.40088	0.62467
H	2.11948	2.08180	0.17221
H	0.87100	-2.35021	1.27569
C	-1.18756	1.31196	-0.09948
H	0.15737	2.10863	1.45612
C	-1.17349	-0.15439	-0.40216
H	-1.04824	-0.81927	1.67685
H	-0.64954	-0.40181	-1.32947
H	-1.99391	1.51375	0.61214
H	-1.28372	1.99618	-0.94839
F	-2.44289	-0.72232	-0.48004

SCF energy: -409.855116 hartree
 zero-point correction: +0.149142 hartree
 enthalpy correction: +0.157024 hartree
 free energy correction: +0.117820 hartree
 quasiharmonic free energy correction: +0.117820 hartree
 imaginary frequency: -567.1512

TS2F_{6π}^N

C	-1.60246	0.69351	-0.61747
C	-0.70100	1.60623	-0.07195
C	-1.78890	-0.61375	-0.13338
H	-2.42142	1.10549	-1.20248
C	-0.99348	-1.15433	0.86931
H	-2.74713	-1.07850	-0.35208
C	0.33368	-0.75227	1.04527
C	0.51639	1.35182	0.59031
H	-1.08516	2.62505	0.00519
H	-1.46487	-1.79547	1.61189
C	1.74333	0.70678	-0.05703

H	0.77429	2.12755	1.31569
C	1.32246	-0.73292	-0.11981
H	0.81416	-0.99714	1.99264
H	2.11550	-1.48035	-0.00467
H	2.59411	0.80685	0.62374
H	2.02252	1.14253	-1.02296
F	0.71310	-1.00961	-1.33316

SCF energy: -409.845826 hartree
zero-point correction: +0.148913 hartree
enthalpy correction: +0.156828 hartree
free energy correction: +0.117536 hartree
quasiharmonic free energy correction: +0.117630 hartree
imaginary frequency: -599.5886

2F-BCOD^X

C	0.77258	-1.48754	0.40807
C	1.90211	-1.08252	-0.18857
C	2.13197	0.33551	-0.50904
C	1.30431	1.30212	-0.08663
C	0.06584	1.01215	0.71295
C	-0.31904	-0.50079	0.68932
H	0.14245	1.47904	1.70112
C	-1.26075	1.31495	-0.04004
H	-0.90712	-0.76630	1.57300
C	-1.29100	-0.15787	-0.45584
H	0.61845	-2.53223	0.66322
H	2.68449	-1.79568	-0.43054
H	3.02315	0.59440	-1.07343
H	1.53147	2.34645	-0.29232
H	-2.07451	1.52412	0.65962
H	-1.24484	2.06786	-0.83184
H	-0.85742	-0.34726	-1.44252
F	-2.52802	-0.77627	-0.41196

SCF energy: -409.897994 hartree
zero-point correction: +0.151121 hartree
enthalpy correction: +0.159218 hartree
free energy correction: +0.119402 hartree
quasiharmonic free energy correction: +0.119457 hartree

2F-BCOD^N

C	1.70762	-1.06637	0.02669
C	2.24657	0.10733	-0.32865
C	1.46738	1.35273	-0.25602

C	0.25909	1.40202	0.32098
C	-0.39059	0.19036	0.92927
C	0.27020	-1.13985	0.44716
H	-0.51765	0.33283	2.00924
C	-1.65425	-0.27309	0.18001
H	0.11186	-1.94132	1.17400
C	-0.80374	-1.20754	-0.67973
H	2.29145	-1.98234	-0.00504
H	3.27746	0.16293	-0.66532
H	1.90974	2.25871	-0.65997
H	-0.27986	2.34293	0.39207
H	-2.35185	-0.80440	0.83487
H	-0.45028	-0.67498	-1.56723
H	-1.21453	-2.17922	-0.95971
F	-2.37667	0.69904	-0.48791

SCF energy: -409.897019 hartree

zero-point correction: +0.151332 hartree

enthalpy correction: +0.159358 hartree

free energy correction: +0.119775 hartree

quasiharmonic free energy correction: +0.119775 hartree

3F

C	-3.38705	0.26327	-0.00002
C	-2.09552	-0.06312	-0.00002
H	-3.79397	1.26953	0.00001
C	-1.05924	0.95758	0.00002
H	-1.83845	-1.11777	-0.00004
C	0.27445	0.74665	0.00004
C	0.92651	-0.55166	0.00005
H	-1.41024	1.98788	0.00002
H	0.91168	1.62612	0.00006
C	2.25993	-0.76741	0.00002
C	3.30721	0.24590	-0.00002
H	0.28485	-1.42875	0.00007
H	2.60902	-1.79870	0.00004
C	4.61165	-0.05805	-0.00004
H	3.01276	1.29245	-0.00005
H	4.94788	-1.09181	-0.00001
H	5.37488	0.71215	-0.00007
F	-4.34733	-0.67667	-0.00002

SCF energy: -409.869557 hartree

zero-point correction: +0.146333 hartree

enthalpy correction: +0.156132 hartree

free energy correction: +0.111950 hartree

quasiharmonic free energy correction: +0.112256 hartree

TS3F_{8π}

C	1.76956	-0.43567	-0.25616
C	0.92105	-1.30691	0.38059
C	1.61075	0.95765	-0.34701
C	0.51484	1.78100	-0.11201
C	-0.70708	-1.18718	-1.20187
C	-1.69365	-0.73554	-0.35897
C	-1.78029	0.57321	0.16204
C	-0.86582	1.61677	0.17464
H	-1.31601	2.55805	0.48778
H	0.78316	2.83590	-0.15782
H	-2.44514	-1.44267	-0.01305
H	-2.73514	0.81666	0.62511
H	2.58967	-0.89348	-0.80406
H	2.49631	1.48788	-0.69101
H	1.08178	-2.37878	0.41315
H	-0.75094	-2.19914	-1.59394
H	-0.12891	-0.47430	-1.77503
F	0.20101	-0.87668	1.42904

SCF energy: -409.844743 hartree
zero-point correction: +0.147790 hartree
enthalpy correction: +0.156365 hartree
free energy correction: +0.116018 hartree
quasiharmonic free energy correction: +0.116018 hartree
imaginary frequency: -413.6633

2CHO

C	2.89413	0.44032	0.00000
C	1.58902	0.10660	0.00000
H	3.22842	1.47528	-0.00000
C	0.51100	1.07529	0.00000
H	1.33521	-0.95301	0.00000
C	-0.81287	0.79404	-0.00000
C	-1.40831	-0.52906	-0.00000
H	0.81341	2.12005	0.00000
H	-1.49239	1.64182	-0.00000
C	-2.73449	-0.79002	-0.00000
C	-3.82015	0.18142	-0.00000
H	-0.73669	-1.38266	-0.00001
H	-3.04529	-1.83355	-0.00001
C	-5.10938	-0.18136	0.00001
H	-3.57160	1.23951	-0.00001
H	-5.39851	-1.22920	0.00001
H	-5.90658	0.55357	0.00001
C	3.93119	-0.59842	0.00000
O	5.12242	-0.37265	0.00000
H	3.55383	-1.64341	0.00000

SCF energy: -423.948561 hartree

zero-point correction: +0.163784 hartree

enthalpy correction: +0.174686 hartree

free energy correction: +0.127668 hartree

quasiharmonic free energy correction: +0.128464 hartree

TS2CHO_{8π}

C	-0.35551	1.61601	0.23416
C	-0.98363	0.49108	-0.26545
C	1.02503	1.86017	0.17633
C	2.07862	1.02661	-0.19171
C	-0.20512	-1.02694	1.25242
C	0.42052	-1.86862	0.36230
C	1.59238	-1.54722	-0.34975
C	2.27538	-0.34499	-0.50802
H	3.24372	-0.49184	-0.98473
H	3.01253	1.57934	-0.28944
H	-0.04487	-2.82467	0.13435
H	2.05656	-2.38441	-0.86747
H	-0.96528	2.34597	0.76764
H	1.33201	2.86505	0.45767
H	-0.51195	-0.09794	-1.04177
H	-1.09843	-1.35686	1.77488
H	0.35168	-0.21575	1.70314
C	-2.44583	0.35506	-0.13514

O	-3.10760	-0.48313	-0.70790
H	-2.92613	1.07920	0.55819

SCF energy: -423.924283 hartree
 zero-point correction: +0.165083 hartree
 enthalpy correction: +0.175008 hartree
 free energy correction: +0.131039 hartree
 quasiharmonic free energy correction: +0.131107 hartree
 imaginary frequency: - 357.8850

2CHO-COT

C	0.66305	1.53138	0.89759
C	1.43115	0.25284	1.07040
C	-0.41987	1.85920	0.17532
C	-1.31852	1.10293	-0.70914
C	0.85283	-1.00329	0.41688
C	-0.47235	-1.43114	0.99104
C	-1.67398	-1.04763	0.54178
C	-1.90031	-0.10030	-0.55191
H	-2.64921	-0.38844	-1.28804
H	-1.63648	1.67388	-1.58080
H	-0.43306	-2.13135	1.82255
H	-2.56090	-1.49400	0.98900
H	1.13101	2.36553	1.41972
H	-0.66995	2.91981	0.18940
H	1.54336	0.06035	2.14377
H	2.44319	0.42335	0.68084
H	1.56519	-1.81952	0.61846
C	0.86650	-0.91138	-1.10439
O	1.61341	-0.18884	-1.71637
H	0.18850	-1.61451	-1.62943

SCF energy: -423.961745 hartree
 zero-point correction: +0.167549 hartree
 enthalpy correction: +0.177270 hartree
 free energy correction: +0.134146 hartree
 quasiharmonic free energy correction: +0.134149 hartree

TS2CHO_{8π}^X

C	2.12013	-0.28723	-0.88443
C	1.93046	0.98481	-0.34080
C	1.65532	-1.47733	-0.29109
H	2.94072	-0.39629	-1.58954
C	0.81632	-1.46376	0.81578
H	2.19151	-2.38796	-0.54480
C	-0.06319	-0.39473	1.02248

C	0.87894	1.45849	0.47087
H	2.80606	1.63263	-0.41251
H	0.94838	-2.22186	1.58516
C	-0.56589	1.58737	-0.00461
H	1.18877	2.25884	1.14801
C	-0.92573	0.11823	-0.12752
H	-0.52602	-0.29824	2.00703
H	-0.59853	-0.30364	-1.08030
H	-1.15792	2.05029	0.79465
H	-0.68335	2.19502	-0.90887
C	-2.39512	-0.16710	0.05884
O	-3.12791	-0.59442	-0.79843
H	-2.79386	0.07403	1.07154

SCF energy: -423.918006 hartree

zero-point correction: +0.165915 hartree

enthalpy correction: +0.175155 hartree

free energy correction: +0.132190 hartree

quasiharmonic free energy correction: +0.132833 hartree

imaginary frequency: -595.3691

TS2CHO_{8π}^N

C	1.51199	1.41663	-0.41035
C	0.49362	1.42557	0.54365
C	2.40215	0.34142	-0.60080
H	1.84785	2.38554	-0.77180
C	2.23053	-0.87653	0.04457
H	3.36826	0.58407	-1.03576
C	0.95133	-1.32015	0.40074
C	-0.22166	0.33588	1.09415
H	0.37587	2.38073	1.05862
H	3.11185	-1.41543	0.38676
C	-1.19873	-0.52230	0.28462
H	-0.56341	0.52024	2.11581
C	-0.19803	-1.24505	-0.59534
H	0.88277	-2.14613	1.10867
H	0.09193	-0.62834	-1.45164
H	-0.51737	-2.22465	-0.96509
H	-1.71336	-1.21758	0.95435
C	-2.23981	0.30133	-0.43815
O	-3.43084	0.19781	-0.27217
H	-1.82599	1.03830	-1.16114

SCF energy: -423.919744 hartree

zero-point correction: +0.166174 hartree

enthalpy correction: +0.175346 hartree

free energy correction: +0.132546 hartree

quasiharmonic free energy correction: +0.133266 hartree

imaginary frequency: -594.0189

2CHO-BCOD^X

C	0.79558	-1.47714	0.60951
C	1.90555	-1.43463	-0.13917
C	2.40318	-0.16537	-0.69424
C	1.87572	1.01580	-0.34374
C	0.72593	1.13326	0.61770
C	0.00703	-0.22521	0.84691
H	1.04451	1.67863	1.51452
C	-0.57602	1.65191	-0.04199
H	-0.48471	-0.24056	1.82659
C	-1.02999	0.18319	-0.25251
H	0.43656	-2.41404	1.02650
H	2.46791	-2.34061	-0.34408
H	3.24215	-0.20180	-1.38301
H	2.29172	1.94157	-0.73681
H	-1.21449	2.16888	0.68305
H	-0.48136	2.26609	-0.94101
H	-0.75159	-0.21117	-1.23278
C	-2.46285	-0.13411	0.04639
O	-3.19779	-0.77491	-0.66562
H	-2.83319	0.26604	1.01887

SCF energy: -423.964348 hartree

zero-point correction: +0.167974 hartree

enthalpy correction: +0.177393 hartree

free energy correction: +0.133911 hartree

quasiharmonic free energy correction: +0.134771 hartree

2CHO-BCOD^N

C	2.20403	-0.82691	-0.08844
C	2.52231	0.43385	-0.41086
C	1.56843	1.53600	-0.20846
C	0.40382	1.35964	0.43128
C	-0.02306	0.02206	0.97327
C	0.83180	-1.15461	0.41818
H	-0.13239	0.08659	2.06228
C	-1.26662	-0.60738	0.25949
H	0.86102	-1.98046	1.13521
C	-0.28006	-1.40243	-0.63426
H	2.92314	-1.63211	-0.21438
H	3.50394	0.67181	-0.80946
H	1.84845	2.52611	-0.55648
H	-0.24958	2.20991	0.61889

H	-1.83183	-1.24548	0.94332
H	-0.06037	-0.85427	-1.55741
H	-0.54272	-2.43369	-0.87880
C	-2.21323	0.32191	-0.44343
O	-3.37924	0.45681	-0.15542
H	-1.77029	0.90427	-1.28045

SCF energy: -423.963542 hartree

zero-point correction: +0.168190 hartree

enthalpy correction: +0.177550 hartree

free energy correction: +0.134248 hartree

quasiharmonic free energy correction: +0.135091 hartree

3CHO

C	3.01324	0.95796	0.00002
C	1.66251	0.87430	0.00003
H	3.47368	1.94237	0.00003
C	0.87094	-0.33996	0.00005
H	1.12343	1.81920	0.00005
C	-0.48497	-0.37106	0.00003
C	-1.38440	0.76697	-0.00005
H	1.41488	-1.27694	0.00008
H	-0.94419	-1.35601	0.00006
C	-2.73464	0.69530	-0.00005
C	-3.55048	-0.51160	0.00003
H	-0.94528	1.76020	-0.00012
H	-3.29167	1.63100	-0.00012
C	-4.88936	-0.47373	0.00001
H	-3.05166	-1.47716	0.00011
H	-5.42504	0.47217	-0.00007
H	-5.48356	-1.38071	0.00007
C	3.95962	-0.17219	0.00002
O	3.66589	-1.35181	-0.00011
H	5.02762	0.12445	0.00018

SCF energy: -423.943813 hartree

zero-point correction: +0.164144 hartree

enthalpy correction: +0.175883 hartree

free energy correction: +0.125501 hartree

quasiharmonic free energy correction: +0.128047 hartree

TS3CHO_{8π}

C	0.04872	-1.86935	0.48623
C	1.15956	-1.06305	0.33911
C	-1.25398	-1.65684	-0.01621
C	-1.94430	-0.53706	-0.47161
C	0.38723	0.69729	1.65075
C	0.22976	1.71657	0.74590
C	-0.84789	1.81839	-0.16230
C	-1.76713	0.87343	-0.58601
H	-2.56569	1.31252	-1.18156
H	-2.92488	-0.81881	-0.85384
H	0.99360	2.48845	0.68984
H	-0.97673	2.79939	-0.61571
H	0.16057	-2.75281	1.11331
H	-1.87502	-2.55054	0.00562
H	2.07730	-1.31983	0.86388
H	1.21155	0.71598	2.35644
H	-0.45882	0.07079	1.90115
C	1.37614	-0.26742	-0.88859

O	2.43878	0.24872	-1.15990
H	0.51917	-0.20660	-1.58352

SCF energy: -423.919289 hartree

zero-point correction: +0.164991 hartree

enthalpy correction: +0.174931 hartree

free energy correction: +0.130953 hartree

quasiharmonic free energy correction: +0.131420 hartree

imaginary frequency: -365.8702

B3LYP/6-31G(d)

1

C	4.01245	-0.13139	0.00062
C	2.68961	-0.34174	0.00004
H	4.42142	0.87586	0.00085
H	4.71899	-0.95396	0.00089
C	1.71719	0.74364	-0.00032
H	2.32139	-1.36466	-0.00018
C	0.37150	0.62448	-0.00052
C	-0.37149	-0.62447	-0.00048
H	2.13943	1.74732	-0.00040
H	-0.20521	1.54520	-0.00074
C	-1.71719	-0.74364	-0.00020
C	-2.68962	0.34175	0.00019
H	0.20521	-1.54520	-0.00069
H	-2.13943	-1.74731	-0.00024
C	-4.01245	0.13137	0.00050
H	-2.32141	1.36467	0.00024
H	-4.42141	-0.87587	0.00047
H	-4.71900	0.95394	0.00080

SCF energy: -310.799273 hartree

zero-point correction: +0.153306 hartree

enthalpy correction: +0.163039 hartree

free energy correction: +0.119466 hartree

quasiharmonic free energy correction: +0.120133 hartree

TS1_{8π}

C	1.78754	-0.71288	0.09340
C	0.83223	-1.37692	0.81795
C	1.72537	0.65629	-0.25800
C	0.69446	1.57764	-0.16708
C	-0.83223	-1.37692	-0.81795
C	-1.78754	-0.71288	-0.09340
C	-1.72537	0.65629	0.25800
C	-0.69446	1.57764	0.16708
H	-1.03676	2.59101	0.37531
H	1.03676	2.59101	-0.37531
H	-2.63161	-1.27716	0.29865
H	-2.64902	1.06676	0.66187
H	2.63161	-1.27716	-0.29865
H	2.64902	1.06676	-0.66187
H	0.13475	-0.81783	1.42663
H	0.95891	-2.42757	1.06066
H	-0.95891	-2.42757	-1.06066
H	-0.13475	-0.81783	-1.42663

SCF energy: -310.773667 hartree
 zero-point correction: +0.154518 hartree
 enthalpy correction: +0.162548 hartree
 free energy correction: +0.124198 hartree
 quasiharmonic free energy correction: +0.124198 hartree
 imaginary frequency: -299.391

1COT

C	-1.38463	1.05301	-0.37553
C	-1.84773	-0.31424	0.04111
C	-0.22021	1.70156	-0.20609
C	1.08824	1.33511	0.36444
C	-0.78447	-1.20983	0.68072
C	0.26941	-1.63333	-0.30140
C	1.43352	-1.00012	-0.49526
C	1.83167	0.22547	0.19958
H	2.84950	0.25058	0.58645
H	1.57108	2.16033	0.88723
H	0.06857	-2.53510	-0.87820
H	2.16251	-1.43371	-1.17806
H	-2.17306	1.64540	-0.84006
H	-0.23295	2.74206	-0.53235
H	-2.27400	-0.82136	-0.83420
H	-2.68716	-0.17842	0.73798
H	-1.27625	-2.09974	1.08788
H	-0.32319	-0.67573	1.51801

SCF energy: -310.811850 hartree
 zero-point correction: +0.157477 hartree
 enthalpy correction: +0.165397 hartree
 free energy correction: +0.126534 hartree
 quasiharmonic free energy correction: +0.126534 hartree

TS1_{6π}

C	1.40823	0.97451	0.45416
C	0.31122	1.53997	-0.19635
C	1.82644	-0.36025	0.27956
H	2.16150	1.66445	0.82769
C	1.07316	-1.27609	-0.44345
H	2.87473	-0.56903	0.47809
C	-0.32123	-1.15880	-0.51004
C	-0.87000	0.91633	-0.65323
H	0.48124	2.55925	-0.54903
H	1.59282	-2.00600	-1.06176

C	-1.91310	0.29510	0.27630
H	-1.30054	1.41246	-1.52769
C	-1.13566	-0.90869	0.75343
H	-0.83808	-1.73604	-1.27758
H	-0.46516	-0.64997	1.57625
H	-1.73262	-1.77673	1.05444
H	-2.77123	-0.02021	-0.32615
H	-2.27702	0.98937	1.04345

SCF energy: -310.769115 hartree

zero-point correction: +0.155969 hartree

enthalpy correction: +0.163148 hartree

free energy correction: +0.125869 hartree

quasiharmonic free energy correction: +0.125869 hartree

imaginary frequency: -557.3462

1BCOD

C	-0.98458	-1.34325	0.24992
C	-1.90889	-0.46257	-0.15738
C	-1.58178	0.96341	-0.31744
C	-0.40888	1.46985	0.08909
C	0.66914	0.62339	0.70531
C	0.42821	-0.89953	0.48447
H	0.85084	0.95061	1.73693
C	1.93783	0.50233	-0.18104
H	0.89989	-1.48304	1.28121
C	1.37229	-0.82045	-0.74866
H	-1.23769	-2.39196	0.38453
H	-2.92605	-0.78280	-0.36359
H	-2.33534	1.61709	-0.74766
H	-0.21365	2.53730	0.00052
H	2.83320	0.33957	0.42578
H	2.12853	1.31211	-0.89146
H	0.79392	-0.64946	-1.66099
H	2.06639	-1.64862	-0.91096

SCF energy: -310.809304 hartree

zero-point correction: +0.157862 hartree

enthalpy correction: +0.165300 hartree

free energy correction: +0.127261 hartree

quasiharmonic free energy correction: +0.127329 hartree

2

C	3.37105	0.32518	0.00036
C	2.06960	-0.00126	0.00013
H	3.63591	1.38244	0.00048
C	1.00802	0.99387	0.00009
H	1.79540	-1.05539	-0.00002
C	-0.32414	0.76522	-0.00018
C	-0.95907	-0.54152	-0.00054
H	1.34361	2.03000	0.00032
H	-0.97467	1.63523	-0.00013
C	-2.28945	-0.77799	-0.00051
C	-3.35125	0.21988	-0.00004
H	-0.30478	-1.40915	-0.00089
H	-2.62329	-1.81438	-0.00084
C	-4.65201	-0.10039	-0.00009
H	-3.07055	1.27027	0.00038
H	-4.97525	-1.13833	-0.00050
H	-5.42489	0.66019	0.00027
C	4.49766	-0.67340	0.00059
H	4.45123	-1.32210	-0.88012
H	5.47028	-0.17847	-0.00233
H	4.45451	-1.31794	0.88453

SCF energy: -350.119593 hartree

zero-point correction: +0.181492 hartree

enthalpy correction: +0.192772 hartree

free energy correction: +0.145325 hartree

quasiharmonic free energy correction: +0.146290 hartree

TS2_{8π}

C	-1.00862	1.34396	0.20175
C	-1.32930	0.15962	-0.42278
C	0.28965	1.88996	0.28417
C	1.53298	1.35654	-0.02939
C	-0.29019	-1.20907	1.10946
C	0.55448	-1.84752	0.23481
C	1.67070	-1.23742	-0.37888
C	2.06625	0.09249	-0.41832
H	3.06902	0.20787	-0.82916
H	2.31641	2.11349	-0.00603
H	0.32505	-2.86760	-0.06804
H	2.34265	-1.91729	-0.89923
H	-1.80102	1.88150	0.72316
H	0.33029	2.91456	0.64933
H	-0.61841	-0.22357	-1.14637
H	-1.12522	-1.74275	1.55476
H	0.05314	-0.32501	1.62911

C	-2.74461	-0.32881	-0.55145
H	-3.18994	0.04015	-1.48295
H	-2.78822	-1.42088	-0.58167
H	-3.36178	0.02114	0.28081

SCF energy: -350.091842 hartree
 zero-point correction: +0.182724 hartree
 enthalpy correction: +0.192269 hartree
 free energy correction: +0.149814 hartree
 quasiharmonic free energy correction: +0.149814 hartree
 imaginary frequency: -337.6589

2COT

C	0.86547	1.07685	-0.67435
C	1.45955	-0.26014	-0.31515
C	-0.27076	1.69565	-0.31090
C	-1.45780	1.29998	0.46671
C	0.50980	-1.18013	0.45989
C	-0.66961	-1.62726	-0.35249
C	-1.87122	-1.03504	-0.34916
C	-2.19081	0.17241	0.41255
H	-3.13589	0.16825	0.95368
H	-1.86982	2.11306	1.06366
H	-0.53415	-2.51794	-0.96450
H	-2.68529	-1.48979	-0.91127
H	1.54454	1.68738	-1.27160
H	-0.34310	2.73249	-0.64193
H	1.72785	-0.76260	-1.25579
H	1.07607	-2.06051	0.78583
H	0.17166	-0.65560	1.36132
C	2.75811	-0.02762	0.47237
H	3.27467	-0.97432	0.65821
H	3.44094	0.63157	-0.07206
H	2.53614	0.43981	1.43756

SCF energy: -350.125873 hartree
 zero-point correction: +0.185677 hartree
 enthalpy correction: +0.194994 hartree
 free energy correction: +0.152976 hartree
 quasiharmonic free energy correction: +0.153195 hartree

TS_{6π}^x

C	1.98133	0.04680	-0.70566
C	1.51884	1.20006	-0.07005
C	1.62688	-1.26102	-0.31900

H	2.90180	0.14126	-1.27737
C	0.65307	-1.50457	0.64224
H	2.32837	-2.04968	-0.57967
C	-0.40644	-0.60780	0.82574
C	0.29949	1.41226	0.60662
H	2.28311	1.96739	0.06901
H	0.79933	-2.33238	1.33390
C	-1.06730	1.39391	-0.07465
H	0.38080	2.14996	1.40956
C	-1.19494	-0.08234	-0.37234
H	-0.99913	-0.70416	1.73853
H	-0.63445	-0.32620	-1.28068
H	-1.82790	1.69087	0.65789
H	-1.13754	2.07912	-0.92885
C	-2.60794	-0.64216	-0.47414
H	-3.14545	-0.19117	-1.31494
H	-2.59340	-1.72657	-0.62058
H	-3.17344	-0.42931	0.44051

SCF energy: -350.085869 hartree

zero-point correction: +0.184007 hartree

enthalpy correction: +0.192658 hartree

free energy correction: +0.152117 hartree

quasiharmonic free energy correction: +0.152117 hartree

imaginary frequency: -552.7210

TS2_{6π}^N

C	1.29241	1.35404	-0.42829
C	0.23833	1.45681	0.48006
C	2.12344	0.22212	-0.54675
H	1.70163	2.28800	-0.80681
C	1.85313	-0.95833	0.13261
H	3.11888	0.39095	-0.94979
C	0.53666	-1.31717	0.45040
C	-0.56904	0.43451	1.02519
H	0.15400	2.43737	0.95258
H	2.68737	-1.53548	0.52764
C	-1.55593	-0.40023	0.20032
H	-0.94132	0.67704	2.02563
C	-0.56508	-1.22123	-0.59391
H	0.39667	-2.10676	1.18933
H	-0.20477	-0.66351	-1.46391
H	-0.92175	-2.20011	-0.93464
H	-2.07423	-1.06419	0.90392
C	-2.58490	0.41419	-0.57403
H	-3.26927	-0.24322	-1.12080
H	-3.17976	1.04295	0.09673
H	-2.08160	1.06865	-1.29342

SCF energy: -350.086135 hartree
 zero-point correction: +0.184104 hartree
 enthalpy correction: +0.192707 hartree
 free energy correction: +0.152265 hartree
 quasiharmonic free energy correction: +0.152265 hartree
 imaginary frequency: -547.5266

2BCOD^X

C	0.73081	-1.49649	0.43033
C	1.87257	-1.16909	-0.19083
C	2.17299	0.22795	-0.54305
C	1.40593	1.24410	-0.12253
C	0.17018	1.03694	0.70690
C	-0.30076	-0.44652	0.71209
H	0.29770	1.51775	1.68482
C	-1.14318	1.39959	-0.03565
H	-0.86228	-0.67232	1.62617
C	-1.29656	-0.08877	-0.43063
H	0.52517	-2.52791	0.70606
H	2.60918	-1.92975	-0.43279
H	3.06378	0.42788	-1.13191
H	1.68080	2.27091	-0.35825
H	-1.92566	1.70873	0.66636
H	-1.07699	2.13275	-0.84554
H	-0.80402	-0.26840	-1.39339
C	-2.67842	-0.71391	-0.41157
H	-3.31662	-0.28761	-1.19261
H	-2.62633	-1.79561	-0.57350
H	-3.16601	-0.53923	0.55426

SCF energy: -350.126451 hartree
 zero-point correction: +0.185870 hartree
 enthalpy correction: +0.194776 hartree
 free energy correction: +0.153402 hartree
 quasiharmonic free energy correction: +0.153749 hartree

2BCOD^N

C	1.77760	-1.01296	-0.03138
C	2.26167	0.18613	-0.38317
C	1.44789	1.40358	-0.24269
C	0.25665	1.39319	0.37317
C	-0.34735	0.14400	0.94956
C	0.36322	-1.14719	0.44596
H	-0.45167	0.26039	2.03638

C	-1.63756	-0.34762	0.22327
H	0.26888	-1.95155	1.18208
C	-0.74704	-1.27859	-0.63240
H	2.39062	-1.90672	-0.11787
H	3.27371	0.28478	-0.76488
H	1.85361	2.33757	-0.62155
H	-0.29367	2.32337	0.50365
H	-2.22470	-0.94716	0.92909
H	-0.43880	-0.77848	-1.55735
H	-1.11981	-2.27889	-0.86874
C	-2.53498	0.64988	-0.48620
H	-3.33005	0.13142	-1.03166
H	-3.00761	1.34031	0.22071
H	-1.96106	1.24247	-1.20651

SCF energy: -350.125364 hartree

zero-point correction: +0.186106 hartree

enthalpy correction: +0.194922 hartree

free energy correction: +0.153874 hartree

quasiharmonic free energy correction: +0.154059 hartree

3

C	-3.39882	0.59532	0.00042
C	-2.05667	0.67059	0.00024
H	-3.95808	1.52782	0.00064
C	-1.17920	-0.49057	-0.00005
H	-1.60180	1.65713	0.00033
C	0.17358	-0.48081	-0.00032
C	1.01485	0.70324	-0.00046
H	-1.66853	-1.46214	-0.00004
H	0.67432	-1.44505	-0.00047
C	2.36617	0.71415	-0.00035
C	3.24818	-0.44568	-0.00000
H	0.51414	1.66738	-0.00067
H	2.86772	1.68063	-0.00049
C	4.58381	-0.34312	0.00006
H	2.79872	-1.43562	0.00021
H	5.07287	0.62776	-0.00013
H	5.22155	-1.22013	0.00032
C	-4.19979	-0.68055	0.00035
H	-3.98125	-1.29184	0.88267
H	-5.27044	-0.46988	0.00074
H	-3.98181	-1.29139	-0.88243

SCF energy: -350.115452 hartree

zero-point correction: +0.181249 hartree

enthalpy correction: +0.191916 hartree

free energy correction: +0.145364 hartree

quasiharmonic free energy correction: +0.146665 hartree

TS3_{8π}

C	1.77405	0.29876	-0.41939
C	1.44172	-0.91269	0.15260
C	1.09601	1.53259	-0.30662
C	-0.20957	1.87379	0.02801
C	-0.33584	-1.23451	-1.30309
C	-1.38097	-1.23777	-0.41325
C	-1.92259	-0.08863	0.20581
C	-1.43637	1.20647	0.30435
H	-2.17838	1.89924	0.69945
H	-0.33822	2.95407	0.08857
H	-1.81612	-2.19337	-0.12562
H	-2.89106	-0.23748	0.68096
H	2.62552	0.30261	-1.10016
H	1.69643	2.39062	-0.60601
H	2.05308	-1.76474	-0.14364
H	-0.02355	-2.15982	-1.77800
H	-0.07775	-0.31852	-1.81594

C	0.80115	-1.04315	1.50358
H	1.60623	-1.11532	2.24499
H	0.18701	-0.18013	1.75807
H	0.19129	-1.94629	1.58543

SCF energy: -350.085639 hartree
 zero-point correction: +0.182765 hartree
 enthalpy correction: +0.192201 hartree
 free energy correction: +0.150200 hartree
 quasiharmonic free energy correction: +0.150200 hartree
 imaginary frequency: -341.2537

4

C	2.95702	-0.10680	-0.00000
C	1.61746	-0.25851	0.00011
C	0.62911	0.80832	0.00024
H	1.24132	-1.27909	0.00023
C	-0.71555	0.65575	0.00021
C	-1.43208	-0.60768	-0.00007
H	1.00276	1.82835	0.00049
H	-1.31293	1.56314	0.00040
C	-2.77524	-0.75798	-0.00015
C	-3.77118	0.30557	0.00002
H	-0.83643	-1.51625	-0.00025
H	-3.17504	-1.77080	-0.00038
C	-5.08983	0.06902	-0.00007
H	-3.42409	1.33593	0.00025
H	-5.47869	-0.94619	-0.00030
H	-5.81263	0.87736	0.00007
C	3.86609	-1.30569	0.00012
H	3.30465	-2.24265	0.00072
H	4.52032	-1.29478	-0.88005
H	4.52099	-1.29409	0.87978
C	3.67765	1.21339	-0.00033
H	4.32848	1.28469	-0.87977
H	3.01272	2.07654	-0.00106
H	4.32789	1.28559	0.87946

SCF energy: -389.436574 hartree
 zero-point correction: +0.209770 hartree
 enthalpy correction: +0.222539 hartree
 free energy correction: +0.171340 hartree
 quasiharmonic free energy correction: +0.172847 hartree

TS4_{8π}

C	0.87065	1.35780	-0.36008
C	1.35834	0.19324	0.21524
C	-0.42968	1.89675	-0.30134
C	-1.68438	1.36201	-0.01473
C	0.17769	-1.11952	-1.25550
C	-0.66730	-1.79012	-0.40259
C	-1.82923	-1.23465	0.17272
C	-2.25361	0.08568	0.24423
H	-3.28160	0.17592	0.59320
H	-2.44981	2.13691	0.01227
H	-0.41669	-2.80903	-0.11201
H	-2.51078	-1.95106	0.62853
H	1.56419	1.90830	-0.99867
H	-0.47772	2.94065	-0.60854
H	1.01492	-1.64142	-1.71022
H	-0.19080	-0.25021	-1.78234
C	0.84794	-0.27123	1.55269
H	-0.17784	0.03801	1.74508
H	0.91749	-1.35728	1.66193
H	1.48869	0.18366	2.31951
C	2.78497	-0.21484	-0.07418
H	3.09938	0.08957	-1.07572
H	3.46367	0.24436	0.65582
H	2.90455	-1.29910	0.01241

SCF energy: -389.402410 hartree

zero-point correction: +0.210932 hartree

enthalpy correction: +0.221728 hartree

free energy correction: +0.176996 hartree

imaginary frequency: -363.9392

4COT

C	0.56630	1.18683	-0.59848
C	1.28136	0.02022	0.03981
C	-0.68360	1.66913	-0.49543
C	-1.91095	1.22277	0.18488
C	0.33959	-0.89834	0.83765
C	-0.65039	-1.65110	-0.00273
C	-1.90735	-1.25220	-0.24104
C	-2.47905	0.00373	0.24299
H	-3.48462	-0.05341	0.65739
H	-2.50759	2.04777	0.57312
H	-0.32948	-2.60948	-0.40776
H	-2.57661	-1.91613	-0.78583
H	1.24176	1.79979	-1.19963
H	-0.83907	2.62129	-1.00444

H	0.96324	-1.61878	1.38250
H	-0.19010	-0.29331	1.58255
C	2.33501	0.60252	0.99964
H	2.94697	-0.19983	1.42672
H	3.00235	1.29463	0.47518
H	1.85485	1.14731	1.81859
C	2.00150	-0.78185	-1.05577
H	2.73188	-0.15555	-1.57939
H	2.53887	-1.62902	-0.61308
H	1.29303	-1.16553	-1.79504

SCF energy: -389.439209 hartree

zero-point correction: +0.213649 hartree

enthalpy correction: +0.224265 hartree

free energy correction: +0.179701 hartree

quasiharmonic free energy correction: +0.180014 hartree

TS4_{6π}

C	-2.46270	-0.04532	0.38677
C	-1.89737	-1.23935	-0.04297
C	-1.86420	1.20053	0.11431
H	-3.50952	-0.02625	0.67954
C	-0.75521	1.36538	-0.71660
H	-2.49182	2.07496	0.27114
C	0.30188	0.46624	-0.96422
C	-0.51107	-1.37280	-0.19228
H	-2.56011	-2.03158	-0.38723
H	-0.81325	2.23549	-1.37322
C	0.42698	-0.89474	0.90658
H	-0.15967	-2.23052	-0.76494
C	1.32511	0.02881	0.10343
H	0.75399	0.59719	-1.95391
H	0.94573	-1.71818	1.41471
H	-0.14328	-0.33495	1.65411
C	1.90894	1.20621	0.88269
H	2.44339	1.89134	0.21468
H	1.11509	1.76902	1.38299
H	2.61615	0.84928	1.64050
C	2.45481	-0.75314	-0.57089
H	3.15122	-1.13558	0.18289
H	2.07227	-1.60231	-1.14606
H	3.01676	-0.10882	-1.25619

SCF energy: -389.399964 hartree

zero-point correction: +0.211892 hartree

enthalpy correction: +0.221821 hartree

free energy correction: +0.178803 hartree

quasiharmonic free energy correction: +0.178803 hartree

imaginary frequency: -544.5203

4BCOD

C	1.86842	-1.22931	0.09987
C	2.59702	-0.11050	0.21065
C	2.00733	1.20918	-0.06100
C	0.76626	1.34398	-0.55037
C	-0.12614	0.17155	-0.83747
C	0.40922	-1.16246	-0.23626
H	-0.37510	0.15767	-1.90816
C	-1.38134	0.04248	0.09356
H	0.11770	-2.01837	-0.85189
C	-0.58027	-0.97822	0.94650
H	2.31615	-2.20304	0.28373
H	3.64572	-0.15858	0.48909
H	2.61968	2.08968	0.11275
H	0.38054	2.33501	-0.78274
H	-0.08286	-0.48996	1.79120
H	-1.11911	-1.86198	1.30396
C	-2.53769	-0.62502	-0.64636
H	-3.33082	-0.90777	0.05488
H	-2.96699	0.05668	-1.38924
H	-2.21175	-1.53051	-1.16966
C	-1.86038	1.29023	0.82064
H	-2.28551	2.01976	0.12114
H	-2.64044	1.02634	1.54382
H	-1.04184	1.77364	1.36260

SCF energy: -389.440529 hartree

zero-point correction: +0.214009 hartree

enthalpy correction: +0.224174 hartree

free energy correction: +0.180382 hartree

quasiharmonic free energy correction: +0.180731 hartree

5

C	3.99769	0.41346	-0.00012
C	2.71322	0.02615	-0.00114
H	4.21774	1.48195	0.00330
C	1.60248	0.96726	0.00212
H	2.49217	-1.03986	-0.00498
C	0.28444	0.66841	0.00405
C	-0.28442	-0.66841	0.00434
H	1.88343	2.01944	0.00302
H	-0.41073	1.50345	0.00593
C	-1.60246	-0.96725	0.00258
C	-2.71322	-0.02615	-0.00074
H	0.41075	-1.50344	0.00645
H	-1.88342	-2.01943	0.00367
C	-3.99769	-0.41350	-0.00077
H	-2.49217	1.03986	-0.00343
H	-4.21768	-1.48200	0.00168
C	5.17178	-0.51548	-0.00402
H	4.84983	-1.56008	-0.00707
H	5.80246	-0.34760	-0.88400
H	5.80413	-0.35313	0.87577
C	-5.17181	0.51548	-0.00400
H	-5.80336	0.35316	0.87641
H	-4.84988	1.56009	-0.00710
H	-5.80324	0.34771	-0.88339

SCF energy: -389.439807 hartree

zero-point correction: +0.209704 hartree

enthalpy correction: +0.222530 hartree

free energy correction: +0.171226 hartree

quasiharmonic free energy correction: +0.172620 hartree

TS5_{8π}

C	0.07169	1.74025	-0.28505
C	0.72470	0.93757	0.63225
C	-1.28376	1.61602	-0.63430
C	-2.22266	0.63708	-0.31290
C	0.72475	-0.93754	-0.63228
C	0.07171	-1.74028	0.28496
C	-1.28372	-1.61606	0.63425
C	-2.22264	-0.63711	0.31295
H	-3.23409	-0.93785	0.58494
H	-3.23413	0.93781	-0.58482
H	0.65536	-2.48796	0.82293
H	-1.67881	-2.42530	1.24545
H	0.65532	2.48792	-0.82305
H	-1.67888	2.42525	-1.24549

H	0.10344	0.41714	1.35218
H	0.10354	-0.41711	-1.35224
C	2.14541	1.19352	1.04632
H	2.17007	1.84583	1.92697
H	2.65905	0.26584	1.31640
H	2.71193	1.68388	0.24894
C	2.14550	-1.19347	-1.04625
H	2.17022	-1.84566	-1.92699
H	2.65918	-0.26576	-1.31615
H	2.71191	-1.68394	-0.24887

SCF energy: -389.409667 hartree
 zero-point correction: +0.211088 hartree
 enthalpy correction: +0.222098 hartree
 free energy correction: +0.176426 hartree
 quasiharmonic free energy correction: +0.176426 hartree
 imaginary frequency: -367.2916

5COT

C	0.10244	1.58887	-0.61043
C	1.18759	0.55312	-0.44926
C	-1.13909	1.70110	-0.10794
C	-2.02248	0.81008	0.66220
C	0.71293	-0.75506	0.20618
C	-0.30958	-1.44424	-0.65677
C	-1.63815	-1.36286	-0.50894
C	-2.30258	-0.49082	0.45925
H	-3.12592	-0.92190	1.02668
H	-2.63754	1.33212	1.39445
H	0.08866	-2.10785	-1.42617
H	-2.27786	-1.99562	-1.12216
H	0.44764	2.46468	-1.16209
H	-1.61501	2.66430	-0.29748
H	1.55655	0.30363	-1.45658
H	0.24294	-0.49071	1.16262
C	2.35035	1.20673	0.31687
H	3.25291	0.59141	0.28326
H	2.59611	2.18270	-0.11236
H	2.07223	1.36248	1.36538
C	1.87459	-1.71917	0.47592
H	2.45103	-1.89666	-0.44077
H	2.55668	-1.33166	1.23644
H	1.49538	-2.68343	0.82626

SCF energy: -389.437363 hartree
 zero-point correction: +0.213824 hartree
 enthalpy correction: +0.224492 hartree
 free energy correction: +0.179643 hartree
 quasiharmonic free energy correction: +0.179913 hartree

TS5_{6π}

C	-2.19796	0.54972	-0.59286
C	-1.55780	1.36322	0.33378
C	-1.91573	-0.82682	-0.69468
H	-3.12061	0.89117	-1.05554
C	-1.10664	-1.52612	0.20209
H	-2.62106	-1.41646	-1.27600
C	-0.02201	-1.05618	0.97332
C	-0.25738	1.07098	0.76352
H	-2.12940	2.15480	0.81510
H	-1.48516	-2.51673	0.46150
C	0.83624	0.73021	-0.24175
H	0.10560	1.58079	1.65896
C	1.30224	-0.56856	0.37993
H	0.10230	-1.60680	1.91098
H	1.96043	-0.32193	1.22548
H	0.36246	0.51811	-1.20789
C	2.00348	-1.57330	-0.52609
H	2.22035	-2.50516	0.00642
H	1.36622	-1.81398	-1.38359
H	2.95095	-1.16773	-0.89762
C	1.88542	1.82131	-0.41288
H	2.67477	1.49828	-1.10016
H	1.44159	2.73777	-0.81339
H	2.35233	2.06103	0.54947

SCF energy: -389.402745 hartree

zero-point correction: +0.211993 hartree

enthalpy correction: +0.222142 hartree

free energy correction: +0.178349 hartree

quasiharmonic free energy correction: +0.178508 hartree

imaginary frequency: -541.7911

5BCOD

C	-1.50199	0.77171	-1.00775
C	-2.39723	0.13553	-0.24004
C	-2.00813	-1.00510	0.60495
C	-0.77675	-1.53123	0.55268
C	0.29091	-0.99991	-0.35983
C	-0.05853	0.36692	-1.01486
H	0.59726	-1.79131	-1.05817
C	1.49292	-0.32259	0.36025
H	0.34001	0.42892	-2.03238
C	0.92169	1.07461	-0.01686
H	-1.80821	1.61098	-1.62820

H	-3.43702	0.44981	-0.23158
H	-2.75425	-1.42854	1.27138
H	-0.52042	-2.39036	1.17054
H	1.52205	-0.50119	1.44351
H	1.65427	1.72511	-0.51080
C	0.27612	1.81758	1.14359
H	1.04049	2.10043	1.87538
H	-0.22846	2.72851	0.80762
H	-0.46463	1.19094	1.64978
C	2.84285	-0.63688	-0.26582
H	3.62862	-0.00146	0.15559
H	3.12382	-1.68236	-0.10226
H	2.81541	-0.46320	-1.34825

SCF energy: -389.442397 hartree

zero-point correction: +0.214079 hartree

enthalpy correction: +0.224429 hartree

free energy correction: +0.179999 hartree

quasiharmonic free energy correction: +0.180376 hartree

6

C	3.96253	-0.69426	0.00021
C	2.61821	-0.69808	0.00009
H	4.47171	-1.65502	0.00036
C	1.80310	0.50756	-0.00009
H	2.11166	-1.65915	0.00014
C	0.45127	0.56852	-0.00025
C	-0.45127	-0.56852	-0.00036
H	2.34275	1.45212	-0.00009
H	0.00195	1.55773	-0.00034
C	-1.80310	-0.50757	-0.00025
C	-2.61822	0.69808	0.00005
H	-0.00195	-1.55773	-0.00054
H	-2.34275	-1.45212	-0.00035
C	-3.96253	0.69426	0.00019
H	-2.11166	1.65915	0.00021
H	-4.47171	1.65502	0.00050
C	-4.82973	-0.53758	0.00010
H	-4.64431	-1.15924	0.88282
H	-5.88784	-0.27080	-0.00035
H	-4.64363	-1.15959	-0.88222
C	4.82973	0.53758	0.00019
H	4.64372	1.15961	0.88252
H	5.88784	0.27080	0.00056
H	4.64423	1.15921	-0.88252

SCF energy: -389.431643 hartree

zero-point correction: +0.209414 hartree

enthalpy correction: +0.220939 hartree

free energy correction: +0.171747 hartree

quasiharmonic free energy correction: +0.173721 hartree

TS6_{8π}

C	-1.68127	-0.49075	0.43393
C	-1.04348	-1.27116	-0.50933
C	-1.61090	0.90902	0.60894
C	-0.65921	1.86077	0.26225
C	1.04238	-1.27203	0.50931
C	1.68084	-0.49215	-0.43394
C	1.61170	0.90768	-0.60893
C	0.66081	1.86023	-0.26222
H	0.99626	2.87304	-0.48185
H	-0.99379	2.87386	0.48192
H	2.29310	-1.01404	-1.16904
H	2.43765	1.31830	-1.18923
H	-2.29397	-1.01211	1.16902
H	-2.43651	1.32034	1.18925

H	-1.20848	-2.34501	-0.42127
H	1.20647	-2.34601	0.42122
C	-0.75520	-0.80025	-1.90787
H	-0.47726	0.25283	-1.94575
H	0.03202	-1.39056	-2.38259
H	-1.67101	-0.92676	-2.49819
C	0.75450	-0.80093	1.90786
H	0.47722	0.25232	1.94579
H	-0.03305	-1.39075	2.38264
H	1.67028	-0.92802	2.49811

SCF energy: -389.396697 hartree

zero-point correction: +0.211133 hartree

enthalpy correction: +0.221906 hartree

free energy correction: +0.177192 hartree

quasiharmonic free energy correction: +0.177192 hartree

imaginary frequency: -365.7996

7

C	-4.06414	0.42552	-0.00051
C	-2.73335	0.61522	-0.00043
H	-4.70178	1.30629	-0.00089
C	-1.75857	-0.46559	0.00023
H	-2.36441	1.63713	-0.00084
C	-0.41180	-0.33657	0.00055
C	0.32526	0.91473	0.00044
H	-2.16130	-1.47615	0.00054
H	0.17134	-1.25355	0.00104
C	1.67145	1.03726	0.00025
C	2.64967	-0.04076	-0.00005
H	-0.25441	1.83342	0.00061
H	2.08812	2.04350	0.00034
C	3.97353	0.17705	-0.00009
H	2.29228	-1.06905	-0.00034
H	4.32989	1.20809	0.00010
C	-4.75178	-0.91501	0.00002
H	-4.48287	-1.50374	0.88386
H	-5.83674	-0.79791	-0.00202
H	-4.47978	-1.50611	-0.88126
C	5.01747	-0.89596	-0.00037
H	4.56327	-1.89019	-0.00065
H	5.66496	-0.81331	-0.88023
H	5.66493	-0.81380	0.87953

SCF energy: -389.435763 hartree

zero-point correction: +0.209665 hartree

enthalpy correction: +0.221799 hartree

free energy correction: +0.171745 hartree

quasiharmonic free energy correction: +0.173309 hartree

TS7_{8π}

C	-0.88645	1.42316	0.17216
C	-1.28703	0.38019	-0.63436
C	0.43203	1.90617	0.29568
C	1.64746	1.37010	-0.11217
C	-0.48522	-1.36411	0.63003
C	0.39001	-1.77805	-0.35723
C	1.59764	-1.16987	-0.75739
C	2.10300	0.11885	-0.60667
H	3.12553	0.19641	-0.97526
H	2.46570	2.08424	-0.02862
H	0.08272	-2.63352	-0.95931
H	2.23599	-1.81192	-1.36276
H	-1.64209	1.90780	0.79175
H	0.51733	2.87422	0.78722

H	-0.61619	0.09761	-1.43738
H	-1.41910	-1.92212	0.70435
C	-2.73961	0.03522	-0.82393
H	-3.17706	0.65129	-1.61842
H	-2.87024	-1.01069	-1.11452
H	-3.31024	0.21336	0.09267
C	-0.04047	-0.73224	1.91702
H	0.88181	-0.16349	1.80540
H	-0.80833	-0.07960	2.34085
H	0.14599	-1.54005	2.63525

SCF energy: -389.403100 hartree
 zero-point correction: +0.210942 hartree
 enthalpy correction: +0.221949 hartree
 free energy correction: +0.176377 hartree
 quasiharmonic free energy correction: +0.176377 hartree
 imaginary frequency: -366.1720

7COT

C	-0.70745	1.39496	-0.53807
C	-1.40311	0.05625	-0.57700
C	0.47661	1.85184	-0.08958
C	1.66608	1.23781	0.51368
C	-0.62669	-1.15371	-0.01683
C	0.60059	-1.43478	-0.85172
C	1.83907	-0.94680	-0.70736
C	2.27516	0.06777	0.25023
H	3.23200	-0.11186	0.73835
H	2.17780	1.89686	1.21426
H	0.44786	-2.14807	-1.66127
H	2.61873	-1.34404	-1.35685
H	-1.36157	2.18196	-0.91843
H	0.58101	2.93521	-0.15417
H	-1.58960	-0.15921	-1.63938
H	-1.28818	-2.01465	-0.18296
C	-2.77769	0.20327	0.09683
H	-3.37978	0.96434	-0.40844
H	-3.32888	-0.74230	0.06344
H	-2.66989	0.50320	1.14352
C	-0.40498	-1.07241	1.50208
H	-1.33708	-1.30522	2.02490
H	0.34971	-1.79795	1.81796
H	-0.07774	-0.08335	1.82552

SCF energy: -389.431714 hartree
 zero-point correction: +0.214088 hartree
 enthalpy correction: +0.224944 hartree
 free energy correction: +0.179240 hartree
 quasiharmonic free energy correction: +0.180123 hartree

TS7_{6π}^X

C	2.22767	0.51974	-0.63955
C	1.34870	1.50466	-0.18362
C	2.28498	-0.78481	-0.11298
H	3.11920	0.86315	-1.15951
C	1.35749	-1.24625	0.81544
H	3.22781	-1.31324	-0.23106
C	0.04692	-0.75626	0.82694
C	0.06231	1.35279	0.36914
H	1.80025	2.49390	-0.08584
H	1.70529	-1.89993	1.61358
C	-1.15053	0.80930	-0.39832
H	-0.20042	2.14896	1.07388
C	-0.74751	-0.65491	-0.47326
H	-0.55546	-0.96798	1.71259
H	-0.04068	-0.77829	-1.30008
H	-1.24293	1.29165	-1.38173
C	-1.84968	-1.70033	-0.60337
H	-1.41942	-2.70582	-0.63533
H	-2.42793	-1.54821	-1.52121
H	-2.54280	-1.65856	0.24338
C	-2.43538	1.06615	0.38511
H	-3.30491	0.65859	-0.13859
H	-2.59406	2.14146	0.51425
H	-2.39376	0.61381	1.38244

SCF energy: -389.398900 hartree

zero-point correction: +0.212338 hartree

enthalpy correction: +0.222320 hartree

free energy correction: +0.178991 hartree

quasiharmonic free energy correction: +0.179065 hartree

imaginary frequency: -543.5068

TS7_{6π}^N

C	1.45126	1.16445	0.81473
C	0.44593	1.71120	0.01648
C	2.16300	-0.00329	0.48802
H	1.92783	1.83266	1.52859
C	1.83084	-0.78321	-0.61323
H	3.14722	-0.11440	0.93691
C	0.52500	-0.86813	-1.11073
C	-0.41746	1.07039	-0.89426
H	0.47280	2.80106	-0.04209
H	2.64713	-1.21901	-1.18823
C	-1.51276	0.05423	-0.55263

H	-0.71939	1.73669	-1.70901
C	-0.69986	-1.20126	-0.24669
H	0.42740	-1.22505	-2.13694
H	-1.17590	-2.09583	-0.66949
H	-2.05157	-0.12758	-1.49061
C	-2.51443	0.54943	0.48579
H	-2.98717	1.47762	0.14837
H	-3.30314	-0.19131	0.65695
H	-2.01642	0.75581	1.43794
C	-0.46103	-1.50253	1.23035
H	-1.40957	-1.79418	1.69250
H	0.24166	-2.33265	1.34287
H	-0.06382	-0.65141	1.78528

SCF energy: -389.393169 hartree

zero-point correction: +0.212512 hartree

enthalpy correction: +0.222488 hartree

free energy correction: +0.179109 hartree

quasiharmonic free energy correction: +0.179437 hartree

imaginary frequency: -549.8864

7BCOD^x

C	1.74866	-0.93944	-0.42709
C	2.31341	-0.00697	0.35223
C	1.63237	1.26687	0.63545
C	0.48000	1.59845	0.03651
C	-0.18242	0.71552	-0.98412
C	0.38532	-0.73164	-1.01580
H	-0.19153	1.24530	-1.94607
C	-1.56522	0.12091	-0.58341
H	0.34735	-1.13903	-2.03119
C	-0.86629	-1.22321	-0.21101
H	2.26628	-1.87443	-0.62917
H	3.29400	-0.17377	0.78894
H	2.09711	1.95185	1.33918
H	0.01586	2.56079	0.24546
H	-2.15782	-0.02600	-1.49376
H	-1.34877	-2.10767	-0.64194
C	-2.41210	0.83484	0.45643
H	-2.74713	1.80862	0.08347
H	-3.30285	0.24780	0.70323
H	-1.85194	1.00646	1.38098
C	-0.64313	-1.45683	1.27769
H	-1.60151	-1.59360	1.78959
H	-0.04273	-2.35682	1.44056
H	-0.11991	-0.62048	1.74947

SCF energy: -389.437219 hartree

zero-point correction: +0.214520 hartree

enthalpy correction: +0.224695 hartree
 free energy correction: +0.180845 hartree
 quasiharmonic free energy correction: +0.181124 hartree

7BCOD^N

C	1.38983	1.29725	0.62023
C	2.44816	0.72859	0.02568
C	2.37927	-0.64444	-0.49833
C	1.32060	-1.43564	-0.27171
C	0.11357	-0.97490	0.49299
C	0.08282	0.56834	0.69612
H	-0.01527	-1.59094	1.39411
C	-1.17313	-0.85092	-0.37400
H	-0.46491	0.83616	1.60679
C	-0.86028	0.66609	-0.53682
H	1.45612	2.30482	1.02357
H	3.38691	1.26717	-0.06623
H	3.23241	-1.02513	-1.05284
H	1.31943	-2.46351	-0.63088
H	-1.15369	-1.41963	-1.31171
H	-0.24125	0.80496	-1.43075
C	-2.44434	-1.17050	0.40066
H	-3.33863	-0.87556	-0.15781
H	-2.50940	-2.24458	0.60159
H	-2.46533	-0.65201	1.36613
C	-1.98641	1.68373	-0.52028
H	-1.58427	2.70209	-0.53093
H	-2.63658	1.57215	-1.39469
H	-2.60608	1.57843	0.37635

SCF energy: -389.440569 hartree
 zero-point correction: +0.214105 hartree
 enthalpy correction: +0.224452 hartree
 free energy correction: +0.179920 hartree
 quasiharmonic free energy correction: +0.180488 hartree

8

C	-3.57981	0.01612	0.00009
C	-2.25160	0.24645	0.00060
C	-1.20050	-0.75886	0.00053
H	-1.93659	1.28758	0.00117
C	0.13218	-0.52330	0.00023
C	0.77307	0.78004	-0.00038
H	0.78392	-1.39276	0.00041
C	2.10600	1.00533	-0.00049
C	3.16325	0.00456	0.00006
H	2.44486	2.04033	-0.00105
C	4.46720	0.32032	-0.00023
H	4.74585	1.37506	-0.00090
C	5.58826	-0.67211	0.00024
H	6.22832	-0.54149	0.87977
H	5.20897	-1.69731	0.00134
H	6.22758	-0.54313	-0.88008
C	-4.55859	1.15893	0.00032
H	-4.05364	2.12754	0.00092
H	-5.21121	1.10965	-0.87982
H	-5.21170	1.10884	0.88005
C	-4.22088	-1.34461	-0.00084
H	-4.86568	-1.45486	-0.88077
H	-3.50542	-2.16641	-0.00109
H	-4.86629	-1.45583	0.87852
H	-1.51108	-1.79981	0.00088
H	0.12668	1.65315	-0.00085
H	2.88396	-1.04768	0.00075

SCF energy: -428.756728 hartree

zero-point correction: +0.237973 hartree

enthalpy correction: +0.252283 hartree

free energy correction: +0.197243 hartree

quasiharmonic free energy correction: +0.199322 hartree

TS8_{8π}

C	-0.92884	-0.88026	0.35743
C	1.14133	-1.59941	-0.89751
C	2.21227	-0.77360	-0.53164
C	-0.55692	1.12143	-0.65236
C	0.21022	1.74367	0.32088
C	1.56251	1.48561	0.57996
C	2.39616	0.46182	0.12627
H	3.16613	-1.19412	-0.84874
H	2.05489	2.20968	1.22712
H	-0.84422	-2.14707	-1.33710
H	-0.01270	0.62921	-1.44970

C	-1.90896	1.66749	-1.02365
H	-1.79066	2.49473	-1.73344
H	-2.53946	0.91614	-1.50508
H	-2.43812	2.05495	-0.14719
C	-2.43406	-1.01325	0.38888
H	-2.85432	-1.18344	-0.60560
H	-2.71584	-1.86012	1.02711
H	-2.90257	-0.12082	0.81563
C	-0.32279	-0.71194	1.72737
H	0.76267	-0.64119	1.70876
H	-0.72624	0.16313	2.24580
H	-0.59057	-1.60189	2.31162
H	-0.27580	2.49127	0.94927
H	3.44769	0.65384	0.33559
H	1.43907	-2.39613	-1.57770

SCF energy: -428.718225 hartree

zero-point correction: +0.239384 hartree

enthalpy correction: +0.251565 hartree

free energy correction: +0.203865 hartree

quasiharmonic free energy correction: +0.203865 hartree

imaginary frequency: -385.5723

8COT

C	0.38177	1.75649	0.32024
C	-0.93959	1.04762	0.15430
C	1.68573	1.41874	0.33267
C	2.44257	0.16834	0.23269
C	-0.96690	-0.49706	0.31145
C	-0.30535	-1.17307	-0.87334
C	0.99061	-1.39966	-1.13142
C	2.17353	-1.00422	-0.37176
H	-1.00366	-1.55393	-1.61953
H	-1.57597	1.44340	0.96333
C	-2.43602	-0.96499	0.33655
H	-2.48070	-2.03669	0.55616
H	-2.99764	-0.43677	1.11451
H	-2.93969	-0.80372	-0.62042
C	-0.35891	-0.90197	1.66448
H	-0.38104	-1.99085	1.77310
H	0.66891	-0.56872	1.79128
H	-0.95856	-0.46666	2.47218
C	-1.56300	1.52480	-1.17102
H	-2.61125	1.22732	-1.25518
H	-1.52295	2.61574	-1.24264
H	-1.00729	1.11505	-2.01975
H	2.34846	2.26638	0.50411
H	2.97676	-1.73976	-0.36644
H	0.21690	2.82698	0.45655

H	3.43065	0.24179	0.68476
H	1.21043	-1.98967	-2.02117

SCF energy: -428.744161 hartree
 zero-point correction: +0.242425 hartree
 enthalpy correction: +0.254424 hartree
 free energy correction: +0.206781 hartree
 quasiharmonic free energy correction: +0.207435 hartree

TS8_{6π}^X

C	2.52697	0.46362	0.35691
C	1.80056	1.29449	-0.48909
C	2.20204	-0.89611	0.52383
C	1.23673	-1.56458	-0.23203
H	2.96019	-1.51202	1.00244
C	0.06471	-1.05192	-0.82225
C	0.43964	1.07065	-0.72699
H	2.33932	2.04526	-1.06475
C	-0.51264	0.81193	0.43431
C	-1.13851	-0.49609	-0.03647
H	-0.23809	-1.60231	-1.72019
H	0.09676	0.59558	1.31965
C	-2.30195	-0.27332	-1.00636
H	-2.61801	-1.22921	-1.43818
H	-3.16301	0.16100	-0.48861
H	-2.02617	0.39126	-1.83178
C	-1.58820	-1.42520	1.09107
H	-1.91508	-2.39358	0.69532
H	-0.76802	-1.60387	1.79312
H	-2.42896	-0.98280	1.63895
C	-1.43903	1.98180	0.74728
H	-2.15754	1.71418	1.53027
H	-0.86187	2.84263	1.09779
H	-2.00317	2.29325	-0.13801
H	-0.00798	1.59220	-1.57518
H	1.52902	-2.57062	-0.53886
H	3.52064	0.76742	0.67680

SCF energy: -428.714683 hartree
 zero-point correction: +0.240071 hartree
 enthalpy correction: +0.251473 hartree
 free energy correction: +0.205430 hartree
 quasiharmonic free energy correction: +0.205501 hartree
 imaginary frequency: -535.8827

TS8_{6π}^N

C	-2.17799	0.60557	0.56354
C	-1.45300	1.43514	-0.29340
C	-2.21176	-0.79443	0.45118
C	-1.42152	-1.48052	-0.46468
H	-3.07416	-1.29655	0.88330
C	-0.17922	-1.00950	-0.90481
C	-0.28312	1.15781	-1.02590
H	-1.98087	2.34876	-0.57385
C	1.10823	0.85761	-0.46165
C	0.97644	-0.58714	0.02421
H	0.18083	-1.43557	-1.84376
C	0.69563	-0.72049	1.52264
H	-0.11981	-0.08564	1.86918
H	0.44387	-1.75614	1.77004
H	1.59773	-0.44610	2.07981
C	2.22059	-1.42431	-0.29324
H	2.45506	-1.39568	-1.36265
H	3.08842	-1.03928	0.25486
H	2.07277	-2.47055	-0.00298
C	1.62359	1.91219	0.51287
H	2.63294	1.66512	0.86119
H	1.66365	2.89302	0.02804
H	0.96381	1.99550	1.38159
H	1.78123	0.83960	-1.32941
H	-0.22851	1.74758	-1.94640
H	-2.99743	1.06338	1.11312
H	-1.86669	-2.33901	-0.96665

SCF energy: -428.707865 hartree

zero-point correction: +0.240351 hartree

enthalpy correction: +0.251664 hartree

free energy correction: +0.205650 hartree

quasiharmonic free energy correction: +0.206087 hartree

imaginary frequency: -543.1955

8BCOD^x

C	-1.75928	1.35558	-0.29799
C	-2.67850	0.50940	0.18693
C	-2.39033	-0.92645	0.32583
C	-1.25735	-1.47114	-0.14132
C	-0.18732	-0.66456	-0.81818
C	-0.38346	0.87020	-0.63940
C	1.16409	-0.54394	-0.03463
H	0.02478	1.42409	-1.49266
C	0.65801	0.82576	0.51201
H	-1.98702	2.41213	-0.41856
H	-3.66388	0.86629	0.47235
H	-3.14291	-1.55749	0.79078
H	-1.10259	-2.54611	-0.06563

C	1.62216	1.98477	0.68854
H	2.13521	2.22406	-0.24891
H	2.38477	1.75578	1.44158
H	1.08997	2.88347	1.01729
H	-0.06045	-1.02284	-1.84994
C	2.33396	-0.40619	-1.00585
H	2.53333	-1.36830	-1.49094
H	3.24590	-0.09608	-0.48301
H	2.13113	0.32733	-1.79381
C	1.47744	-1.59366	1.02193
H	2.36841	-1.30076	1.58996
H	1.67933	-2.57076	0.56712
H	0.64775	-1.71000	1.72621
H	0.11972	0.64051	1.45102

SCF energy: -428.755665 hartree

zero-point correction: +0.242052 hartree

enthalpy correction: +0.253738 hartree

free energy correction: +0.206780 hartree

quasiharmonic free energy correction: +0.207186 hartree

8BCOD^N

C	1.36952	-1.50487	-0.27682
C	2.36742	-0.82467	0.30451
C	2.34827	0.64519	0.38110
C	1.39591	1.36998	-0.22267
C	0.30547	0.74258	-1.04551
C	0.18052	-0.79423	-0.84969
C	-1.14627	0.89152	-0.50348
H	-0.13554	-1.27938	-1.78042
C	-1.08217	-0.56634	0.05736
H	1.40023	-2.59112	-0.32526
H	3.21654	-1.35036	0.73197
H	3.14190	1.14054	0.93354
H	1.42492	2.45704	-0.17139
H	-1.83723	0.90432	-1.35622
C	-1.48573	2.04088	0.43028
C	-0.78899	-0.63504	1.55423
C	-2.28724	-1.43585	-0.27740
H	-2.50976	-1.40780	-1.34954
H	-3.17674	-1.08901	0.26241
H	-2.11004	-2.47985	0.00631
H	0.09096	-0.05017	1.83334
H	-0.61072	-1.67145	1.85945
H	-1.64703	-0.25826	2.12243
H	-0.80103	2.08120	1.28323
H	-2.50549	1.93995	0.81712
H	-1.42266	3.00014	-0.09446

H	0.42144	1.07935	-2.08407
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SCF energy: -428.753433 hartree

zero-point correction: +0.242285 hartree

enthalpy correction: +0.253879 hartree

free energy correction: +0.207253 hartree

quasiharmonic free energy correction: +0.207560 hartree

9

C	3.53574	0.19062	0.00016
C	2.18965	0.26422	0.00080
C	1.26394	-0.85743	0.00084
H	1.75531	1.26145	0.00145
C	-0.08753	-0.78180	0.00031
C	-0.87546	0.43799	-0.00075
H	-0.63065	-1.72257	0.00065
C	-2.22633	0.51605	-0.00097
C	-3.15300	-0.60706	-0.00024
H	-2.66077	1.51191	-0.00181
C	-4.49510	-0.52127	0.00027
C	4.37399	1.44015	0.00033
H	3.75915	2.34301	0.00079
H	5.02841	1.46677	0.88008
H	5.02791	1.46734	-0.87978
C	4.33178	-1.08558	-0.00090
H	4.98679	-1.11964	0.87772
H	3.71777	-1.98568	0.00009
H	4.98412	-1.11982	-0.88150
H	1.69536	-1.85442	0.00144
H	-0.33100	1.37819	-0.00150
H	-2.72306	-1.60508	-0.00012
H	-5.05320	-1.45612	0.00074
C	-5.33223	0.72263	0.00029
H	-5.98456	0.74324	0.88014
H	-4.73876	1.63765	-0.00030
H	-5.98550	0.74265	-0.87888

SCF energy: -428.754109 hartree

zero-point correction: +0.238111 hartree

enthalpy correction: +0.252473 hartree

free energy correction: +0.196930 hartree

quasiharmonic free energy correction: +0.199359 hartree

TS9_{8π}

C	0.59178	-1.71394	-0.43420
C	-0.29563	-1.45992	0.59545
C	1.79336	-1.04340	-0.74130
C	2.25799	0.23494	-0.44881
C	-1.35731	0.36550	-0.33278
C	-0.82049	1.29616	0.54423
C	0.47815	1.84165	0.58794
C	1.71908	1.41621	0.12017
H	3.28804	0.38398	-0.77026
H	0.53732	2.76480	1.16417
H	0.32004	-2.50708	-1.13055
C	-2.79915	-0.04688	-0.12967
H	-3.46983	0.68161	-0.60324
H	-2.99989	-1.01786	-0.59230
H	-3.05768	-0.10866	0.93136
H	-1.19124	-2.08155	0.60452
C	0.13881	-0.99283	1.95716
H	0.96613	-0.28512	1.91272
H	-0.68545	-0.53805	2.51293
H	0.47808	-1.87078	2.52048
H	2.48937	2.17338	0.26082
H	2.46193	-1.60762	-1.39083
H	-1.48294	1.64787	1.33735
C	-0.90745	0.32836	-1.77096
H	0.14514	0.57952	-1.89203
H	-1.09619	-0.64551	-2.23089
H	-1.49765	1.07589	-2.31765

SCF energy: -428.712893 hartree

zero-point correction: +0.239246 hartree

enthalpy correction: +0.251415 hartree

free energy correction: +0.203907 hartree

quasiharmonic free energy correction: +0.203907 hartree

imaginary frequency: - 374.7772

10

C	4.03310	-0.08651	0.00049
C	2.69513	-0.25113	0.00039
C	1.69467	0.80458	-0.00084
H	2.32929	-1.27553	0.00150
C	0.35162	0.63515	-0.00151
C	-0.35161	-0.63512	-0.00165
H	-0.25494	1.53643	-0.00220
C	-1.69467	-0.80456	-0.00101
C	-2.69513	0.25114	0.00035
H	-2.05639	-1.82890	-0.00147
C	-4.03310	0.08650	0.00051
C	-4.95462	1.27601	0.00206
H	-5.60917	1.25746	0.88198
H	-4.40259	2.21862	0.00324
H	-5.60922	1.25970	-0.87787
C	4.95460	-1.27603	0.00211
H	4.40256	-2.21863	0.00328
H	5.60929	-1.25974	-0.87775
H	5.60906	-1.25748	0.88211
C	4.74021	1.24110	-0.00085
H	5.39092	1.31880	-0.87993
H	4.06568	2.09682	-0.00300
H	5.38900	1.32165	0.87940
H	2.05640	1.82892	-0.00109
H	0.25495	-1.53640	-0.00253
H	-2.32931	1.27554	0.00141
C	-4.74019	-1.24112	-0.00072
H	-5.39079	-1.31898	-0.87987
H	-4.06564	-2.09682	-0.00262
H	-5.38909	-1.32151	0.87947

SCF energy: -468.073642 hartree

zero-point correction: +0.266207 hartree

enthalpy correction: +0.282032 hartree

free energy correction: +0.223201 hartree

quasiharmonic free energy correction: +0.225947 hartree

TS10_{8π}

C	0.04295	-1.58323	-0.70521
C	-0.77925	-1.10389	0.31696
C	1.42749	-1.46945	-0.87796
C	2.39757	-0.60064	-0.36689
C	-0.77925	1.10389	-0.31696
C	0.04295	1.58323	0.70521
C	1.42749	1.46944	0.87796
C	2.39757	0.60064	0.36689

H	3.40704	-0.90564	-0.63947
H	1.83052	2.17122	1.60763
H	-0.46433	-2.12648	-1.50485
C	-2.24023	1.49239	-0.23295
H	-2.36238	2.52124	-0.59521
H	-2.86706	0.85484	-0.86180
H	-2.61844	1.45097	0.79269
C	-2.24023	-1.49239	0.23295
H	-2.61844	-1.45096	-0.79269
H	-2.36238	-2.52123	0.59521
H	-2.86706	-0.85484	0.86180
C	-0.26369	-1.05852	1.73472
H	0.79321	-0.80593	1.79543
H	-0.83303	-0.35518	2.34996
H	-0.39462	-2.06058	2.16446
H	3.40704	0.90564	0.63947
H	1.83052	-2.17122	-1.60763
H	-0.46433	2.12648	1.50485
C	-0.26369	1.05852	-1.73472
H	0.79321	0.80593	-1.79543
H	-0.83303	0.35518	-2.34996
H	-0.39462	2.06058	-2.16446

SCF energy: -468.026119 hartree

zero-point correction: +0.267689 hartree

enthalpy correction: +0.281047 hartree

free energy correction: +0.231342 hartree

quasiharmonic free energy correction: +0.231342 hartree

imaginary frequency: -387.0718

10COT

C	0.03602	1.67529	-0.23216
C	-1.05952	0.62438	-0.16042
C	1.36038	1.75863	-0.00220
C	2.42088	0.81761	0.37148
C	-0.57276	-0.81399	0.22653
C	0.40298	-1.32834	-0.82147
C	1.73779	-1.23458	-0.87939
C	2.61414	-0.45755	-0.00831
H	-0.06420	-1.91840	-1.61058
C	-1.73943	-1.82690	0.21727
H	-1.36002	-2.80445	0.53389
H	-2.53333	-1.54216	0.91230
H	-2.17560	-1.95149	-0.77768
C	-0.00306	-0.83476	1.66031
H	0.61408	-1.72638	1.80574
H	0.60302	0.03901	1.89694
H	-0.82666	-0.87563	2.37998

C	-1.74995	0.61665	-1.54072
H	-2.67700	0.03653	-1.51543
H	-2.01261	1.63789	-1.83534
H	-1.09329	0.20685	-2.31297
H	1.74783	2.77464	-0.08400
H	3.54985	-0.93066	0.28528
H	-0.40684	2.64025	-0.48980
H	3.21283	1.27233	0.96538
H	2.24275	-1.79889	-1.66333
C	-2.07997	1.16825	0.86378
H	-2.41557	2.16461	0.55763
H	-2.96686	0.53081	0.92187
H	-1.64337	1.25684	1.86188

SCF energy: -468.049580 hartree

zero-point correction: +0.270301 hartree

enthalpy correction: +0.283644 hartree

free energy correction: +0.233244 hartree

quasiharmonic free energy correction: +0.234298 hartree

TS10_{6π}

C	-2.34506	-0.85572	0.41149
C	-1.34834	-1.63679	-0.18010
C	-2.58136	0.48673	0.08058
C	-1.75654	1.18791	-0.79562
H	-3.57683	0.87213	0.28805
C	-0.39703	0.90892	-0.95867
C	-0.12467	-1.24730	-0.75059
H	-1.66722	-2.65650	-0.40507
C	1.10672	-0.63139	-0.05634
C	0.62692	0.81899	0.18895
H	0.04808	1.27954	-1.88443
C	1.69783	1.90367	-0.00187
H	1.25444	2.89071	0.16900
H	2.51407	1.77304	0.71828
H	2.12635	1.89975	-1.00720
C	0.04225	1.03911	1.58943
H	-0.44776	2.01580	1.64007
H	-0.68618	0.28633	1.88658
H	0.85735	1.02853	2.32057
C	2.26456	-0.69350	-1.06281
H	3.17409	-0.24946	-0.64789
H	2.48230	-1.73897	-1.30560
H	2.02309	-0.17912	-1.99864
H	0.18079	-1.92838	-1.55330
H	-2.23805	1.87463	-1.49125
H	-3.16715	-1.38643	0.88654
C	1.51970	-1.42663	1.18585

H	1.78906	-2.44974	0.90088
H	2.39391	-0.96887	1.66525
H	0.70987	-1.48699	1.91635

SCF energy: -468.016559 hartree
 zero-point correction: +0.268653 hartree
 enthalpy correction: +0.281082 hartree
 free energy correction: +0.233099 hartree
 quasiharmonic free energy correction: +0.233502 hartree
 imaginary frequency: -534.9868

10BCOD

C	-1.74245	1.25259	-0.61108
C	-2.71142	0.49312	-0.08124
C	-2.48185	-0.92445	0.24156
C	-1.33700	-1.54374	-0.07904
C	-0.22859	-0.85247	-0.82114
C	-0.37749	0.69268	-0.87714
C	1.13318	-0.66739	-0.07488
H	0.00817	1.08823	-1.82388
C	0.73039	0.83113	0.22517
H	-1.92953	2.29906	-0.84183
H	-3.69209	0.91403	0.12171
H	-3.27552	-1.47179	0.74248
H	-1.20724	-2.60023	0.14908
C	0.15889	1.03177	1.62946
C	1.78542	1.90251	-0.03160
H	2.19979	1.84821	-1.04187
H	2.61440	1.81424	0.68126
H	1.34539	2.89824	0.09559
H	-0.64715	0.33173	1.86002
H	-0.24489	2.04463	1.72866
H	0.94852	0.90874	2.37920
C	2.28705	-0.78828	-1.07103
H	2.41245	-1.83648	-1.36430
H	3.23070	-0.44401	-0.63361
H	2.10502	-0.21079	-1.98336
H	-0.10744	-1.34724	-1.79585
C	1.41084	-1.56577	1.12463
H	1.56520	-2.60039	0.79702
H	2.32239	-1.24297	1.64151
H	0.58996	-1.56338	1.84619

SCF energy: -468.064656 hartree
 zero-point correction: +0.270345 hartree
 enthalpy correction: +0.283197 hartree
 free energy correction: +0.234258 hartree
 quasiharmonic free energy correction: +0.234570 hartree

