SUPPORTING INFORMATION

Origins of Selectivity and General Model for Chiral Phosphoric Acid-Catalyzed Oxetane Desymmetrizations

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Full computational details

Density functional theory calculations were performed with Gaussion 09. Geometry optimizations and vibrational frequencies were computed in the gas-phase at the B3LYP/6-31G(d) level of theory.[1] Normal mode frequency analysis was used to confirm that stationary points were either minima (0 negative frequency) or saddle-points (TS, 1 imaginary frequency) on the potential energy surface. All saddle-points were analyzed with the Intrinsic Reaction Coordinate (IRC) tools to verify that they connected the expected minima. ZPE, enthalpy and free energy corrections were also obtained at this level of theory, using a standard state of 1 atmosphere of pressure and 298 K. Free energy corrections were calculated both with and without Truhlar's quasiharmonic oscillator approximation,[2] the latest being used for the free energies shown throughout the paper. Single-point energy refinements on the optimized structures were then obtained at the CPCM(benzene)/B3LYP-D3(BJ)/6-311+G(d,p) level.[3] Structures were illustrated using CYLview.[4] Other DFT methods were evaluated for the single-point energies and are fully consistent with the trends and magnitudes of the relative activation free energies ($\Delta\Delta G^{\ddagger}$) presented in the main text (see below).

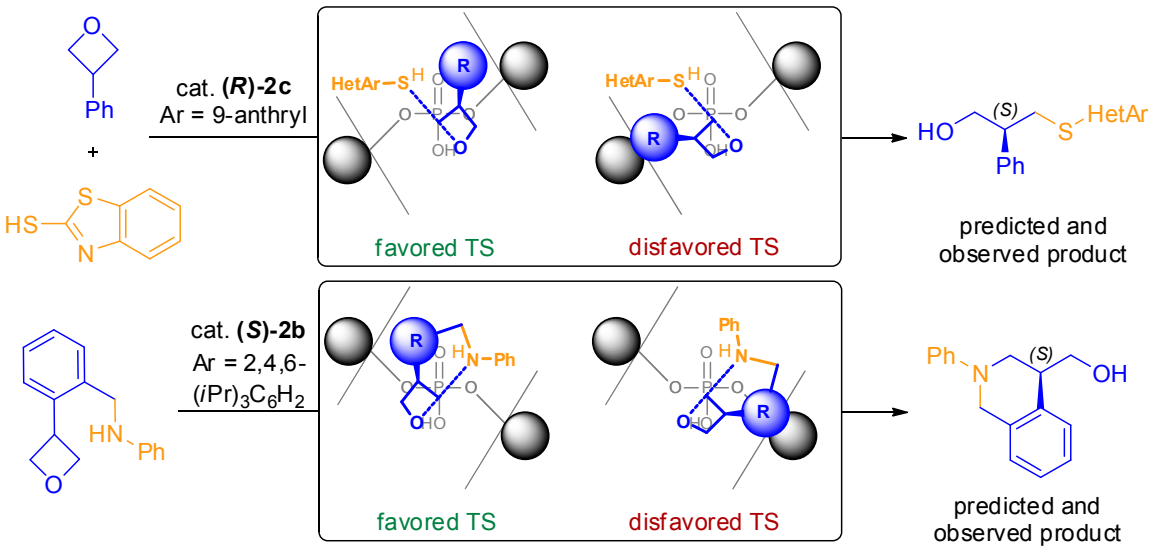
Full list of authors for reference 12 (Gaussian 09):

Gaussian 09, Revision D.01,

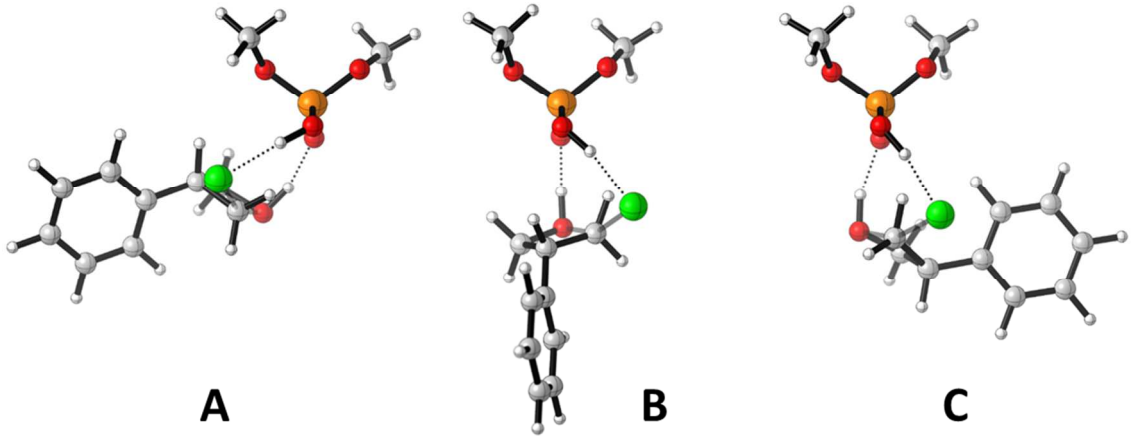
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Additional figures, tables and discussion

"Back-of-the-envelope" model with both enantiomeric TSs:



Transition structures with model catalyst **4** (Goodman projection):



TS conformer	$\Delta G^{\ddagger}$ (kcal/mol)	ΔG_{rel} (kcal/mol)
TS_4_A	19.2	0.0
TS_4_B	19.2	0.0
TS_4_C	22.5	3.3

Conformers of catalyst (*S*)-2a:

Four (4) low-energy conformers were located, which are different orientations of the chair conformation of the *para*-cyclohexyl substituents. Any other conformation (boat, twist-boat) was at least 6.9 kcal/mol higher in energy. Such conformations, when appearing for later stationary points, were systematically higher in energy and are not discussed here.

Catalyst conformer	ΔG_{rel} (kcal/mol)
(*S*)-2a_1	0.0
(*S*)-2a_2	0.3
(*S*)-2a_3	0.3
(*S*)-2a_4	0.4

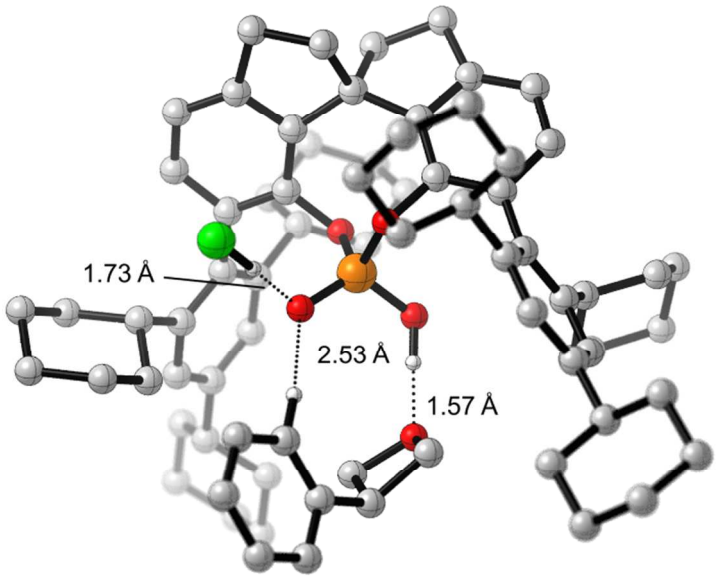
Conformers of the reactant-complex (RC):

15 unique low-energy conformers were located, representing 4 different arrangements of the substrates in the chiral pocket of the catalyst. A lot of high-energy conformers, having non-chair conformations of the cyclohexyl substituents of the catalyst, were also located. As they all were at least 5 kcal/mol higher in energy, we do not discuss them here.

RC conformer	ΔG (kcal/mol)	ΔG_{rel} (kcal/mol)
RC_A1	-4.24	2.69
RC_A2	-3.90	3.03
RC_A3	-4.37	2.56
RC_A4	-4.55	2.38
RC_B1	-3.51	3.42
RC_B2	-3.51	3.42
RC_B3	-3.78	3.15
RC_B4	-3.32	3.60
RC_C1	-4.50	2.42
RC_C3	-5.54	1.39
RC_C4	-5.53	1.40
RC_D1	-6.06	0.86
RC_D2	-6.93	0.00
RC_D3	-6.37	0.56
RC_D4	-6.61	0.32

Arrangements A-C are characterized by the HCl being bonded to the phosphoryl oxygen, while the oxetane oxygen is interacting with the acidic group of the catalyst. Arrangement D, in which the oxetane makes two distinct hydrogen bonds to the catalyst, in addition to the interaction of HCl, is the most favored.

Structure of RC_D2 (called **RC** in the main text):



Conformers of the transition states leading to the (*R*)-product:

10 unique low-energy conformers were located, representing 3 different arrangements (A-C) of the substrates in the chiral pocket of the catalyst. A lot of high-energy conformers, having non-chair conformations of the cyclohexyl substituents of the catalyst, were also located. As they all were at least 5 kcal/mol higher in energy, we do not discuss them here.

TS(*R*) conformer	**ΔG (kcal/mol)**	**ΔG_{rel} (kcal/mol)**
TS(*R*)_A1	11.47	0.00
TS(*R*)_A2	11.70	0.23
TS(*R*)_A3	12.17	0.70
TS(*R*)_A4	12.27	0.80
TS(*R*)_B1	12.10	0.63
TS(*R*)_B2	11.69	0.22
TS(*R*)_B3	12.14	0.67
TS(*R*)_B4	12.07	0.60
TS(*R*)_C3	15.90	4.43
TS(*R*)_C4	15.90	4.43

TS(*R*)_A1 is called **TS(*R*)** in the main text.

Conformers of the transition states leading to the (*S*)-product:

8 unique low-energy conformers were located, representing 2 different arrangements (A-B) of the substrates in the chiral pocket of the catalyst. A lot of high-energy conformers, having non-chair conformations of the cyclohexyl substituents of the catalyst, were also located. As they all were at least 5 kcal/mol higher in energy, we do not discuss them here.

TS(*S*) conformer	**ΔG (kcal/mol)**	**ΔG_{rel} (kcal/mol)**
TS(*S*)_A1	13.34	0.00
TS(*S*)_A2	14.75	1.41
TS(*S*)_A3	13.71	0.36
TS(*S*)_A4	16.10	2.76
TS(*S*)_B1	17.99	4.65
TS(*S*)_B2	17.41	4.07
TS(*S*)_B3	17.87	4.53
TS(*S*)_B4	17.56	4.22

TS(*S*)_A1 is called **TS(*S*)** in the main text.

Comparison of DFT methods for single-point calculations of optimized lowest-energy transition states:

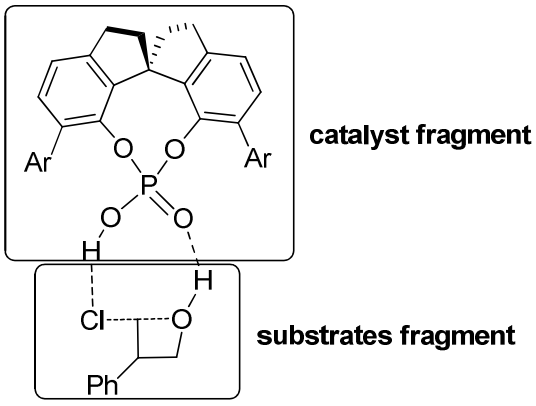
The optimized structures of **TS(*R*)** and **TS(*S*)** were submitted to single-point calculations with a variety of DFT methods, basis sets and solvation models. All of them agree on the sense and relative magnitude of the $\Delta\Delta G^{\ddagger}$ ($\Delta G^{\ddagger}_{(TS\_S)} - \Delta G^{\ddagger}_{(TS\_R)}$) calculated at our preferred B3LYP-D3(BJ)/6-311+G(d,p)/CPCM(benzene)//B3LYP/6-31G(d) level.

	DFT method	Basis set	Solvation model (benzene)	**$\Delta\Delta G^{\ddagger}$ (kcal/mol)**
Experimental				2.06 (94% ee)
Geometry optimizations	B3LYP	6-31G(d)	–	1.1
Single-point refinements	B3LYP-D3(BJ)	6-311+G(d,p)	CPCM	1.9
	B3LYP-D3(BJ)	6-311+G(d,p)	SMD	2.1

	B3LYP-D3(BJ)	6-311+G(d,p)	–	1.6
	B3LYP-D3(BJ)	Def2-TZVP	CPCM	1.7
	B3LYP-D3(BJ)	Def2-TZVPP	CPCM	1.7
	B3LYP	6-311+G(d,p)	CPCM	1.3
	M06-2X	6-311+G(d,p)	CPCM	1.3
	ωB97X-D	6-311+G(d,p)	CPCM	2.0

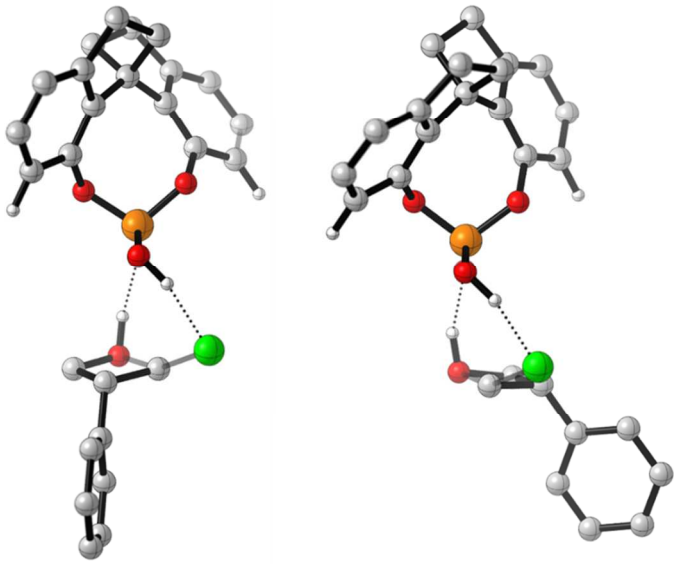
Distortion/interaction analysis:

We performed a distortion/interaction analysis. As such, we computed single-point energies of **TS(*R*)** and **TS(*S*)** in the gas-phase at the B3LYP-D3(BJ)/6-311+G(d,p) level (no solvation model). We then decomposed the overall electronic energy difference ($\Delta\Delta E^{\ddagger} = \Delta E^{\ddagger}_{\mathbf{TS(S)}} - \Delta E^{\ddagger}_{\mathbf{TS(R)}}$) between **TS(*R*)** and **TS(*S*)** in three components: the distortion energy of the catalyst fragment $\Delta\Delta E^{\ddagger}_{cat}$, distortion energy of the substrates fragment $\Delta\Delta E^{\ddagger}_{substrates}$ and interaction energy between these two fragments $\Delta\Delta E^{\ddagger}_{int}$. The breakdown of these fragments is illustrated below. Data for this analysis can be found in the main text of the article.



Truncated versions of the transition states:

Using the optimized geometries of **TS(*R*)** and **TS(*S*)**, we truncated the 6,6'-aryl substituents and replaced them with simple hydrogen atoms. We then calculated single-point energies (without optimization) at the at the B3LYP-D3(BJ)/6-311+G(d,p) level (no solvation model). Structures and relative energies of these TSs are shown below. Distortion of the catalyst backbone is clearly visible in **TS(*S*)**.



Truncated **TS(*R*)**
$\Delta\Delta E^{\ddagger}$ = 0.0

Truncated **TS(*S*)**
$\Delta\Delta E^{\ddagger}$ = 2.0

Cartesian coordinates, energies and vibrational frequencies

Unless specified, coordinates and corrections were obtained at the B3LYP/6-31G(d) level and SCF (electronic) energies were obtained by single-point calculations at the CPCM(benzene)/B3LYP-D3(BJ)/6-311+G(d,p) level.

Oxetane-1a

C	1.23993	-0.78319	-0.00001
C	2.16725	-0.08510	-1.03126
H	1.30926	-1.87471	-0.00003
H	1.67274	0.55169	-1.77370
H	2.86815	-0.76230	-1.53909
O	2.82070	0.68770	0.00001
C	2.16726	-0.08514	1.03125
H	2.86816	-0.76236	1.53906
H	1.67275	0.55162	1.77373
C	-0.20656	-0.35546	0.00000
C	-0.55440	1.00505	0.00000
C	-1.23360	-1.30661	-0.00001
C	-1.89147	1.39850	0.00001
H	0.23144	1.75728	0.00000
C	-2.57427	-0.91542	-0.00000
H	-0.98139	-2.36490	-0.00001
C	-2.90733	0.43896	0.00001
H	-2.14165	2.45628	0.00001
H	-3.35638	-1.67022	-0.00001
H	-3.94961	0.74648	0.00001

There are no imaginary frequencies.

SCF energy: -424.311431 hartree
zero-point correction: +0.169197 hartree
enthalpy correction: +0.178271 hartree
free energy correction: +0.135483 hartree
quasiharmonic free energy correction: +0.136061 hartree

HCl

H	0.00000	0.00000	-1.21785
Cl	0.00000	0.00000	0.07164

There are no imaginary frequencies.

SCF energy: -460.836268 hartree
zero-point correction: +0.006675 hartree
enthalpy correction: +0.009980 hartree
free energy correction: -0.011217 hartree
quasiharmonic free energy correction: -0.011217 hartree

Catalyst (*S*)-2a_1 (lowest-energy catalyst)

C	0.06273	-3.92119	-0.08557
P	0.13173	-0.16099	-0.40048
O	-1.03612	-1.04278	0.29718
O	-0.18325	0.55841	-1.64630
O	0.53826	0.68369	0.90182
O	1.35915	-1.19542	-0.66895
C	1.85884	-2.01247	0.34754
C	1.22684	-3.22333	0.61190
C	3.00689	-1.60110	1.05437
C	1.70554	-4.02171	1.66295
C	3.50747	-2.47529	2.03162
C	2.85700	-3.66655	2.35647
H	4.41065	-2.19447	2.56413
H	3.24278	-4.29803	3.15286
C	-1.68914	-1.96117	-0.54461
C	-1.09215	-3.19881	-0.77923
C	-2.91873	-1.60479	-1.12831
C	-1.64507	-4.04093	-1.75720
C	-3.48897	-2.52407	-2.02411
C	-2.84521	-3.71115	-2.37652
H	-4.44641	-2.27796	-2.47220
H	-3.28495	-4.36887	-3.12224
C	0.79592	-5.20994	1.88295
H	1.23867	-6.13241	1.48172
H	0.59460	-5.39344	2.94441
C	-0.46881	-4.80442	1.09683
H	-1.11759	-4.19023	1.73215
H	-1.05737	-5.65773	0.74697
C	-0.75662	-5.24502	-1.98731
H	-1.19753	-6.15840	-1.56417
H	-0.59125	-5.44210	-3.05268
C	0.54248	-4.85104	-1.24868
H	1.19169	-4.27436	-1.91756
H	1.11464	-5.71100	-0.88661
C	3.65524	-0.26848	0.80504
C	3.64139	0.73581	1.81503
C	4.29970	-0.00585	-0.43266
C	4.24457	1.97240	1.54011

C	4.89112	1.24465	-0.63984	H	6.27741	-1.88991	-0.73363
C	4.86998	2.25482	0.32519	C	5.43623	-2.16329	-4.11332
H	4.23614	2.74175	2.30791	H	3.59525	-1.32422	-4.91490
H	5.38785	1.43248	-1.58757	H	3.35198	-2.54357	-3.67010
C	-3.63568	-0.32560	-0.80325	H	5.49325	-3.51847	-2.42866
C	-3.81766	0.67041	-1.79507	H	7.07696	-2.90192	-2.88786
C	-4.20015	-0.14446	0.48562	H	6.04443	-1.33804	-4.51322
C	-4.56587	1.80969	-1.47246	H	5.49543	-2.97747	-4.84726
C	-4.92899	1.01921	0.75050	C	-4.08425	-1.18562	1.59465
C	-5.13030	2.01055	-0.21303	C	-3.34759	-0.64417	2.84271
H	-4.71320	2.57244	-2.23295	C	-5.45985	-1.76914	1.99689
H	-5.36121	1.14700	1.73960	H	-3.49275	-2.02743	1.21994
C	3.05318	0.51470	3.21098	C	-3.20962	-1.72339	3.92750
C	4.17982	0.31469	4.25699	H	-3.90363	0.21008	3.25505
C	2.10724	1.64199	3.69271	H	-2.36132	-0.26768	2.55066
H	2.45743	-0.40394	3.18960	C	-5.32165	-2.84608	3.08465
C	3.61966	0.01563	5.65592	H	-6.10873	-0.96259	2.36666
H	4.85242	-0.49132	3.93943	H	-5.95726	-2.18467	1.11116
H	4.79367	1.22637	4.29465	C	-4.57212	-2.31580	4.31642
C	1.53418	1.33412	5.08589	H	-2.70915	-1.30606	4.81115
H	1.28561	1.77750	2.98175	H	-2.55812	-2.52835	3.55396
H	2.65003	2.59628	3.73819	H	-6.31353	-3.21836	3.37279
C	2.64571	1.10765	6.12004	H	-4.77430	-3.70703	2.67222
H	4.44419	-0.09130	6.37282	H	-5.17899	-1.53510	4.79938
H	3.09674	-0.95198	5.63490	H	-4.44507	-3.11504	5.05844
H	0.87728	2.15326	5.40497	C	-3.25311	0.54990	-3.20798
H	0.90348	0.43524	5.02501	C	-4.36789	0.26781	-4.24609
H	2.21423	0.84477	7.09437	C	-2.43590	1.78803	-3.64630
H	3.19989	2.04688	6.26641	H	-2.56030	-0.29775	-3.22682
C	5.50724	3.61167	0.07832	C	-3.79737	0.08851	-5.66151
C	4.83112	4.37870	-1.08223	H	-5.08103	1.10529	-4.24134
C	7.03222	3.51594	-0.16037	H	-4.94215	-0.62188	-3.95730
H	5.36086	4.21065	0.98997	C	-1.85454	1.59961	-5.05609
C	5.46261	5.76332	-1.29297	H	-3.07785	2.68059	-3.64600
H	3.75616	4.47456	-0.88473	H	-1.63227	1.95908	-2.92582
H	4.92525	3.79168	-2.00705	C	-2.95051	1.29594	-6.08858
C	7.66282	4.90101	-0.37262	H	-4.61353	-0.07844	-6.37720
H	7.50667	3.00543	0.68725	H	-3.17238	-0.81668	-5.68397
H	7.22152	2.89094	-1.04494	H	-1.12979	0.77292	-5.03633
C	6.97924	5.66605	-1.51574	H	-1.29354	2.49628	-5.35090
H	5.26614	6.38830	-0.40905	H	-3.60376	2.17579	-6.19110
H	4.98360	6.26719	-2.14209	H	-2.50877	1.11905	-7.07828
H	7.57386	5.48380	0.55635	H	1.43838	1.05587	0.82662
H	8.73710	4.79646	-0.57177	C	-5.94172	3.26058	0.08304
H	7.41438	6.66862	-1.61587	C	-7.41990	2.94064	0.40568
H	7.17271	5.14553	-2.46555	C	-5.32317	4.12095	1.20921
C	4.42806	-1.05713	-1.52984	H	-5.93742	3.87518	-0.83023
C	3.85671	-0.59035	-2.88905	C	-8.23787	4.21410	0.66892
C	5.89538	-1.52409	-1.69547	H	-7.46351	2.29118	1.29194
H	3.85450	-1.94009	-1.23132	H	-7.86035	2.36734	-0.41981
C	3.98387	-1.68908	-3.95559	C	-6.14200	5.39438	1.47048
H	4.39992	0.30155	-3.23253	H	-5.27208	3.52678	2.13310
H	2.80895	-0.29599	-2.76732	H	-4.28865	4.37722	0.94894
C	6.02361	-2.61647	-2.76855	C	-7.61121	5.07014	1.77976
H	6.52299	-0.66473	-1.97201	H	-9.27116	3.94936	0.92853

H	-8.29227	4.80665	-0.25667
H	-5.69545	5.96456	2.29541
H	-6.09474	6.04312	0.58297
H	-8.18526	5.99552	1.91779
H	-7.66736	4.52214	2.73240

There are no imaginary frequencies.

SCF energy: -3170.492433 hartree
zero-point correction: +1.360242 hartree
enthalpy correction: +1.424071 hartree
free energy correction: +1.257674 hartree
quasiharmonic free energy correction: +1.279320 hartree

Catalyst (*S*)-2a_2

C	-0.07988	-3.84724	-0.90549
P	-0.12818	-0.32442	0.43908
O	1.00162	-0.96375	-0.53260
O	0.25027	0.02119	1.81946
O	-0.59266	0.84742	-0.55354
O	-1.34536	-1.40547	0.46477
C	-1.88813	-1.91115	-0.71882
C	-1.27118	-2.99506	-1.33450
C	-3.06375	-1.32964	-1.23605
C	-1.79593	-3.47462	-2.54564
C	-3.60330	-1.89658	-2.40048
C	-2.97057	-2.94611	-3.06897
H	-4.52514	-1.48512	-2.79943
H	-3.38943	-3.33290	-3.99461
C	1.69465	-2.06939	-0.00825
C	1.10799	-3.33055	-0.09433
C	2.95210	-1.87163	0.59117
C	1.70530	-4.40210	0.58836
C	3.56336	-2.99450	1.17261
C	2.93486	-4.24006	1.21718
H	4.54245	-2.86969	1.62420
H	3.40929	-5.07137	1.73286
C	-0.90319	-4.55215	-3.11988
H	-1.33431	-5.55167	-2.96700
H	-0.74757	-4.43820	-4.19862
C	0.39538	-4.36904	-2.30677
H	1.01872	-3.59916	-2.77631
H	0.99505	-5.28095	-2.23050
C	0.82480	-5.63241	0.52017
H	1.24173	-6.38952	-0.15850
H	0.71016	-6.11641	1.49678
C	-0.50730	-5.06359	-0.01956
H	-1.12001	-4.69691	0.81206
H	-1.10021	-5.79727	-0.57475
C	-3.70033	-0.13892	-0.57701
C	-3.71649	1.12816	-1.22981
C	-4.29124	-0.27209	0.70472
C	-4.27788	2.22364	-0.55855
C	-4.84108	0.85917	1.31885
C	-4.83581	2.11867	0.71900
H	-4.28834	3.18792	-1.05819
H	-5.29407	0.75482	2.30163
C	3.65491	-0.54422	0.59056
C	3.89219	0.14703	1.80510
C	4.14759	-0.01095	-0.62838
C	4.62379	1.34099	1.76616
C	4.86228	1.19079	-0.60405
C	5.11770	1.88500	0.58087
H	4.81393	1.87024	2.69664
H	5.23951	1.59069	-1.54173
C	-3.21424	1.33318	-2.66133
C	-4.40619	1.42646	-3.64899
C	-2.29773	2.56560	-2.85523
H	-2.62159	0.45687	-2.94461
C	-3.93725	1.54905	-5.10644
H	-5.06150	0.55438	-3.53489
H	-5.01652	2.30211	-3.38397
C	-1.81506	2.67890	-4.31047
H	-1.43194	2.50452	-2.18766
H	-2.83924	3.48473	-2.59222
C	-2.99034	2.74221	-5.29650
H	-4.80578	1.64047	-5.77162
H	-3.41772	0.62374	-5.39624
H	-1.17670	3.56465	-4.42087
H	-1.18524	1.80962	-4.54920
H	-2.62138	2.77544	-6.32962
H	-3.54885	3.67611	-5.13345
C	-5.43715	3.31964	1.42903
C	-6.68987	3.86568	0.70346
C	-4.41069	4.45388	1.65337
H	-5.76398	2.97908	2.42312
C	-7.30848	5.05571	1.45264
H	-7.42729	3.06144	0.58679
H	-6.41025	4.18085	-0.31240
C	-5.03153	5.64365	2.40116
H	-3.54616	4.06485	2.20556
H	-4.02998	4.79694	0.68058
C	-6.28175	6.17429	1.68330
H	-7.69187	4.71047	2.42438
H	-8.17317	5.43954	0.89621
H	-5.30562	5.32736	3.41860
H	-4.28814	6.44297	2.51456
H	-6.73283	6.99240	2.25918
H	-5.98772	6.60051	0.71241
C	-4.42619	-1.61950	1.40489
C	-3.86298	-1.63811	2.84420
C	-5.90014	-2.09594	1.39717
H	-3.85830	-2.36192	0.83532
C	-4.01191	-3.02907	3.48108
H	-4.39835	-0.90534	3.46462
H	-2.81065	-1.33396	2.83061
C	-6.05047	-3.48202	2.04136
H	-6.51995	-1.36947	1.94236

H	-6.27697	-2.11340	0.36645
C	-5.47054	-3.51131	3.46311
H	-3.62894	-3.01106	4.50938
H	-3.38626	-3.74692	2.92950
H	-5.52702	-4.22552	1.42192
H	-7.10787	-3.77693	2.05377
H	-6.07405	-2.85926	4.11235
H	-5.54359	-4.52276	3.88338
C	3.96786	-0.70985	-1.97300
C	3.17056	0.14710	-2.98435
C	5.31879	-1.14809	-2.58760
H	3.39125	-1.62700	-1.81475
C	2.97621	-0.58920	-4.31890
H	3.70604	1.08905	-3.17038
H	2.20142	0.41512	-2.54998
C	5.12262	-1.88053	-3.92445
H	5.95357	-0.26517	-2.74735
H	5.85553	-1.79006	-1.87747
C	4.31651	-1.03497	-4.92180
H	2.43465	0.05245	-5.02631
H	2.34137	-1.47347	-4.15447
H	6.09743	-2.14909	-4.35230
H	4.59159	-2.82701	-3.74245
H	4.90188	-0.14450	-5.19611
H	4.15081	-1.59671	-5.85052
C	3.40079	-0.35768	3.15907
C	4.56369	-0.89783	4.02771
C	2.60749	0.70589	3.95476
H	2.70798	-1.18711	2.98252
C	4.06139	-1.46178	5.36595
H	5.27752	-0.08325	4.21974
H	5.12203	-1.66887	3.48141
C	2.09506	0.13529	5.28617
H	3.24895	1.57386	4.16485
H	1.76914	1.05490	3.34682
C	3.23836	-0.42536	6.14455
H	4.91088	-1.80760	5.97014
H	3.43674	-2.34627	5.17074
H	1.36877	-0.66300	5.07544
H	1.55046	0.91162	5.83965
H	3.89766	0.40083	6.45160
H	2.84440	-0.86927	7.06846
H	-1.48255	1.18246	-0.32890
C	5.90729	3.18366	0.58987
C	7.35298	2.99786	0.07364
C	5.19855	4.31162	-0.19536
H	5.97856	3.51492	1.63709
C	8.14965	4.31136	0.10796
H	7.32240	2.62078	-0.95870
H	7.85908	2.22760	0.66916
C	5.99775	5.62374	-0.15971
H	5.06554	3.99608	-1.24020
H	4.19139	4.46535	0.21167
C	7.43363	5.42671	-0.66796
H	9.15681	4.14973	-0.29782
H	8.28264	4.62693	1.15358
H	5.48480	6.39142	-0.75357
H	6.02930	5.99981	0.87389
H	7.99686	6.36586	-0.59266
H	7.40565	5.16358	-1.73604

There are no imaginary frequencies.

SCF energy: -3170.492569 hartree
zero-point correction: +1.360732 hartree
enthalpy correction: +1.424265 hartree
free energy correction: +1.260668 hartree
quasiharmonic free energy correction: +1.279904 hartree

Catalyst (*S*)-2a_3

C	0.12505	-4.01096	-0.09774
P	0.09906	-0.24182	-0.34200
O	-0.96327	-1.15918	0.46777
O	-0.37442	0.52380	-1.50747
O	0.66612	0.55742	0.92858
O	1.28176	-1.25602	-0.81048
C	1.93606	-2.07956	0.10787
C	1.36449	-3.30256	0.44167
C	3.16780	-1.65817	0.64831
C	1.99566	-4.10438	1.40612
C	3.81222	-2.53479	1.53479
C	3.22865	-3.73830	1.93473
H	4.77714	-2.24624	1.93951
H	3.73074	-4.37088	2.66248
C	-1.69931	-2.07254	-0.30892
C	-1.12131	-3.30046	-0.62825
C	-2.99144	-1.72102	-0.74286
C	-1.78199	-4.14033	-1.53968
C	-3.65647	-2.63757	-1.57316
C	-3.05055	-3.81720	-2.00778
H	-4.66167	-2.39574	-1.90360
H	-3.57091	-4.47396	-2.70057
C	1.13858	-5.30615	1.73734
H	1.53201	-6.21987	1.27016
H	1.08767	-5.50085	2.81459
C	-0.22772	-4.91021	1.13757
H	-0.78817	-4.30810	1.86221
H	-0.84967	-5.76834	0.86583
C	-0.91773	-5.33343	-1.88783
H	-1.28869	-6.25231	-1.41271
H	-0.89055	-5.52737	-2.96615
C	0.46064	-4.92420	-1.32334
H	1.00557	-4.33052	-2.06640
H	1.08972	-5.77712	-1.04994
C	3.74787	-0.31055	0.32286
C	3.86540	0.68586	1.33662
C	4.17965	-0.01757	-0.99570
C	4.36563	1.94761	0.98631

C	4.68065	1.25913	-1.27751	H	6.16557	-1.80048	-1.66040
C	4.77147	2.26301	-0.31362	C	4.76441	-2.09651	-4.84830
H	4.44938	2.70513	1.75989	H	2.77958	-1.33440	-5.31093
H	5.01057	1.48070	-2.28947	H	2.80515	-2.57011	-4.05838
C	-3.67320	-0.44938	-0.32425	H	5.17372	-3.45564	-3.21570
C	-3.95569	0.56601	-1.27469	H	6.62403	-2.76333	-3.93399
C	-4.09736	-0.29222	1.01796	H	5.25736	-1.24304	-5.33773
C	-4.65272	1.70437	-0.85524	H	4.73173	-2.90444	-5.59076
C	-4.78049	0.87485	1.37998	C	-3.88784	-1.36450	2.08208
C	-5.07027	1.88708	0.46549	C	-3.03064	-0.87297	3.27178
H	-4.86927	2.47775	-1.58682	C	-5.23110	-1.94172	2.59079
H	-5.10743	0.99567	2.41045	H	-3.34637	-2.20102	1.62753
C	3.53104	0.42641	2.80798	C	-2.81788	-1.98451	4.31129
C	4.82723	0.25541	3.64155	H	-3.52772	-0.02020	3.75592
C	2.64228	1.50995	3.46627	H	-2.06715	-0.50671	2.90037
H	2.97482	-0.51440	2.87343	C	-5.01516	-3.05107	3.63134
C	4.52553	-0.08571	5.10877	H	-5.83077	-1.13646	3.03836
H	5.46332	-0.51936	3.19607	H	-5.81229	-2.32473	1.74222
H	5.40651	1.18895	3.59259	C	-4.15124	-2.56599	4.80486
C	2.32826	1.16135	4.93037	H	-2.23346	-1.59967	5.15730
H	1.70634	1.62344	2.90926	H	-2.21749	-2.79010	3.86111
H	3.15071	2.48368	3.43807	H	-5.98366	-3.41740	3.99644
C	3.60755	0.96174	5.75467	H	-4.52066	-3.90752	3.14878
H	5.46318	-0.17285	5.67294	H	-4.69939	-1.78944	5.35932
H	4.03934	-1.07145	5.15577	H	-3.97261	-3.38655	5.51213
H	1.70814	1.95050	5.37418	C	-3.54835	0.46311	-2.74256
H	1.72776	0.24046	4.95976	C	-4.76304	0.17390	-3.65874
H	3.35792	0.66768	6.78221	C	-2.79725	1.71385	-3.25740
H	4.14551	1.91906	5.82580	H	-2.85232	-0.37645	-2.84335
C	5.28674	3.64560	-0.67669	C	-4.34148	0.00682	-5.12713
C	6.54187	4.05194	0.12912	H	-5.48093	1.00322	-3.57553
C	4.18858	4.72705	-0.54178	H	-5.29411	-0.72356	-3.31674
H	5.58010	3.61465	-1.73691	C	-2.36217	1.53725	-4.72007
C	7.05414	5.44233	-0.27814	H	-3.44799	2.59745	-3.18818
H	7.32790	3.29863	-0.00808	H	-1.92644	1.89451	-2.62308
H	6.30029	4.05734	1.20177	C	-3.55555	1.22483	-5.63467
C	4.70315	6.11702	-0.94584	H	-5.22631	-0.16556	-5.75449
H	3.32070	4.44811	-1.15228	H	-3.71368	-0.89202	-5.21933
H	3.83891	4.75697	0.50052	H	-1.63024	0.71880	-4.77906
C	5.95673	6.50940	-0.15027	H	-1.84493	2.44135	-5.06742
H	7.40514	5.40758	-1.32029	H	-4.22544	2.09761	-5.66435
H	7.92430	5.71409	0.33319	H	-3.21763	1.05598	-6.66577
H	4.94161	6.11556	-2.01984	H	1.52049	0.98809	0.73206
H	3.91169	6.86410	-0.80492	C	-5.81050	3.14044	0.90226
H	6.33255	7.48392	-0.48718	C	-4.94001	4.41162	0.76717
H	5.68927	6.62707	0.91055	C	-7.15297	3.32845	0.15872
C	4.16990	-1.05258	-2.11548	H	-6.04754	3.02426	1.97099
C	3.35624	-0.60138	-3.35104	C	-5.68628	5.67014	1.23620
C	5.60648	-1.44814	-2.53676	H	-4.64286	4.53489	-0.28404
H	3.69720	-1.96472	-1.73742	H	-4.01140	4.28221	1.33691
C	3.34238	-1.68761	-4.43749	C	-7.89716	4.58775	0.62950
H	3.79922	0.31334	-3.77066	H	-6.96128	3.40455	-0.92112
H	2.33439	-0.34920	-3.04986	H	-7.77919	2.43850	0.30006
C	5.59552	-2.52796	-3.63062	C	-7.02247	5.84351	0.49895
H	6.13668	-0.55911	-2.90746	H	-5.05412	6.55610	1.09335

H	-5.87783	5.59548	2.31723
H	-8.82690	4.70930	0.05867
H	-8.19269	4.46130	1.68189
H	-7.55774	6.72224	0.88137
H	-6.82477	6.03671	-0.56605

There are no imaginary frequencies.

SCF energy: -3170.492757 hartree
zero-point correction: +1.360961 hartree
enthalpy correction: +1.424371 hartree
free energy correction: +1.261511 hartree
quasiharmonic free energy correction: +1.280157 hartree

Catalyst (*S*)-2a_4

C	0.10812	-3.83961	-1.00830
P	0.09024	-0.13174	-0.30159
O	-1.02190	-1.20678	0.18296
O	-0.30537	0.89949	-1.27551
O	0.56264	0.32627	1.16192
O	1.31042	-1.01358	-0.91933
C	1.89532	-2.05239	-0.19267
C	1.30376	-3.31065	-0.22127
C	3.08279	-1.80147	0.52431
C	1.86487	-4.34058	0.55061
C	3.66311	-2.88439	1.20277
C	3.05517	-4.14053	1.24099
H	4.59601	-2.72423	1.73418
H	3.50459	-4.94516	1.81757
C	-1.70141	-1.88393	-0.84597
C	-1.09874	-2.99857	-1.42686
C	-2.96294	-1.41752	-1.26086
C	-1.69233	-3.57123	-2.56330
C	-3.56581	-2.08321	-2.34036
C	-2.92638	-3.12166	-3.01906
H	-4.54767	-1.75299	-2.66475
H	-3.39536	-3.57399	-3.88943
C	0.98913	-5.57338	0.50442
H	1.41694	-6.34404	-0.15216
H	0.86191	-6.03490	1.49017
C	-0.33137	-5.01597	-0.06869
H	-0.94342	-4.60758	0.74400
H	-0.93068	-5.76695	-0.59202
C	-0.80324	-4.65142	-3.14171
H	-1.20495	-5.65431	-2.94030
H	-0.69979	-4.56788	-4.22958
C	0.53138	-4.42040	-2.39868
H	1.12760	-3.66887	-2.92893
H	1.14016	-5.32528	-2.30578
C	3.68453	-0.42611	0.59275
C	3.72773	0.27982	1.82915
C	4.21756	0.18027	-0.57539
C	4.26872	1.57459	1.84515
C	4.74854	1.47134	-0.49041
C	4.77691	2.19577	0.70374
H	4.30323	2.11583	2.78694
H	5.15492	1.92414	-1.39041
C	-3.67756	-0.29024	-0.57241
C	-3.90256	0.94084	-1.24137
C	-4.18877	-0.48183	0.73435
C	-4.62730	1.94143	-0.58441
C	-4.89846	0.55974	1.34323
C	-5.13008	1.78006	0.70894
H	-4.79711	2.88127	-1.10199
H	-5.29257	0.41184	2.34630
C	3.26681	-0.32405	3.15823
C	4.48407	-0.73421	4.02666
C	2.33622	0.59376	3.98862
H	2.69668	-1.23372	2.94253
C	4.05247	-1.41061	5.33662
H	5.14667	-1.39824	3.45832
H	5.07593	0.16428	4.25445
C	1.89421	-0.08745	5.29403
H	1.45246	0.86813	3.40312
H	2.85516	1.52948	4.23860
C	3.09664	-0.52091	6.14375
H	4.93718	-1.66358	5.93539
H	3.55157	-2.36161	5.10200
H	1.24850	0.59175	5.86506
H	1.28196	-0.96829	5.05195
H	2.75812	-1.04562	7.04631
H	3.63887	0.37319	6.48646
C	5.34206	3.60444	0.77191
C	4.53896	4.60317	-0.09409
C	6.84240	3.65904	0.40136
H	5.25502	3.94009	1.81660
C	5.10359	6.02869	0.00759
H	3.48412	4.58729	0.20732
H	4.56597	4.27517	-1.14306
C	7.40379	5.08574	0.50378
H	7.40740	2.97775	1.05000
H	6.97566	3.29203	-0.62645
C	6.59622	6.07355	-0.35113
H	4.96737	6.39871	1.03473
H	4.53354	6.70332	-0.64375
H	7.37690	5.41059	1.55464
H	8.45934	5.09438	0.20310
H	6.98706	7.09164	-0.22808
H	6.72041	5.81729	-1.41396
C	4.29383	-0.54356	-1.91573
C	3.59877	0.22469	-3.06396
C	5.75866	-0.87028	-2.29750
H	3.77924	-1.50480	-1.81973
C	3.67642	-0.55570	-4.38512
H	4.08265	1.20236	-3.20160
H	2.55528	0.42235	-2.79745
C	5.83810	-1.64235	-3.62376
H	6.33144	0.06435	-2.38443

H	6.23010	-1.44849	-1.49237
C	5.12669	-0.89391	-4.76080
H	3.19919	0.02114	-5.18757
H	3.09920	-1.48768	-4.28801
H	5.37047	-2.62983	-3.49367
H	6.88776	-1.82814	-3.88632
H	5.67044	0.03855	-4.97530
H	5.15453	-1.48910	-5.68280
C	-4.05012	-1.79789	1.49371
C	-3.32025	-1.63963	2.84771
C	-5.42195	-2.48509	1.69773
H	-3.44818	-2.48612	0.89112
C	-3.18412	-2.98580	3.57684
H	-3.87755	-0.94146	3.48838
H	-2.33361	-1.19375	2.67888
C	-5.28149	-3.82901	2.42881
H	-6.07981	-1.82272	2.27812
H	-5.90877	-2.63021	0.72487
C	-4.54619	-3.66984	3.76771
H	-2.69180	-2.83867	4.54703
H	-2.52673	-3.64817	2.99281
H	-6.27164	-4.27587	2.58793
H	-4.72220	-4.53026	1.79130
H	-5.16245	-3.06237	4.44753
H	-4.41894	-4.64705	4.25173
C	-3.40313	1.21633	-2.65726
C	-4.55855	1.19668	-3.68865
C	-2.62111	2.54517	-2.78366
H	-2.70351	0.41985	-2.93165
C	-4.04414	1.40363	-5.12193
H	-5.27704	1.99076	-3.43718
H	-5.11324	0.25200	-3.62206
C	-2.09182	2.74215	-4.21233
H	-3.27685	3.39129	-2.53213
H	-1.79370	2.54421	-2.07032
C	-3.22264	2.69516	-5.25032
H	-4.88696	1.41484	-5.82602
H	-3.41444	0.54607	-5.40227
H	-1.35701	1.95430	-4.43245
H	-1.55315	3.69637	-4.28254
H	-3.88696	3.55977	-5.09993
H	-2.81705	2.78736	-6.26663
H	1.43740	0.76032	1.14010
C	-5.89124	2.88854	1.41685
C	-5.00000	4.12186	1.69457
C	-7.17277	3.31487	0.66521
H	-6.20750	2.49256	2.39422
C	-5.76387	5.22388	2.44461
H	-4.62955	4.52024	0.73923
H	-4.11463	3.81373	2.26451
C	-7.93637	4.41568	1.41802
H	-6.90152	3.68233	-0.33488
H	-7.81679	2.44009	0.50978
C	-7.04331	5.63329	1.70029
H	-5.11386	6.09577	2.59381
H	-6.03126	4.85980	3.44803
H	-8.82221	4.71727	0.84404
H	-8.30684	4.01077	2.37178
H	-7.59654	6.38561	2.27732
H	-6.77011	6.10959	0.74675

There are no imaginary frequencies.

SCF energy: -3170.492523 hartree
zero-point correction: +1.360857 hartree
enthalpy correction: +1.424368 hartree
free energy correction: +1.260809 hartree
quasiharmonic free energy correction: +1.280067 hartree

Catalyst 4

O	0.84784	-0.85928	-0.49367
O	-1.43822	0.09688	-0.55035
P	-0.00172	0.36450	0.10648
O	0.04896	0.54975	1.57491
O	0.51998	1.62634	-0.75708
H	0.43322	2.43949	-0.23265
C	2.18998	-1.06977	-0.01659
H	2.50563	-2.03886	-0.40601
H	2.85253	-0.28662	-0.39892
H	2.21255	-1.07746	1.07670
C	-2.25609	-0.95837	-0.01038
H	-3.23660	-0.85407	-0.47712
H	-1.82768	-1.93327	-0.26286
H	-2.34567	-0.85734	1.07511

There are no imaginary frequencies.

SCF energy: -722.925992 hartree
zero-point correction: +0.106293 hartree
enthalpy correction: +0.116491 hartree
free energy correction: +0.071674 hartree
quasiharmonic free energy correction: +0.072419 hartree

TS_4_A

O	-2.05387	-0.74460	-1.23558
O	-4.26034	-0.10499	-0.03183
P	-2.66512	0.00534	0.05304
O	-2.39495	-0.89121	1.31843
O	-2.17470	1.42256	0.04546
H	-0.81342	2.30953	0.39914
C	-2.17873	-2.17958	-1.36962
H	-1.87068	-2.41289	-2.38988

H	-1.52027	-2.67870	-0.65422
H	-3.21506	-2.49394	-1.21563
C	-4.99662	0.87266	-0.79100
H	-4.79280	0.76182	-1.86111
H	-6.05092	0.67270	-0.59573
H	-4.73661	1.88321	-0.46740
C	0.83945	2.07768	-0.69740
C	1.17956	0.64420	-0.24624
O	0.16298	2.51339	0.53820
H	1.70285	2.72689	-0.84276
H	0.15781	2.15519	-1.54603
C	0.62942	0.87065	1.16713
H	1.31532	1.09660	1.97595
H	-0.36460	0.60445	1.46426
Cl	0.46468	-1.68062	1.69449
H	-1.43846	-1.23266	1.45854
H	0.56152	-0.09207	-0.75995
C	2.63758	0.24470	-0.33431
C	2.99710	-0.96464	-0.93853
C	3.65063	1.07185	0.17092
C	4.33726	-1.33740	-1.04440
H	2.21898	-1.62534	-1.30951
C	4.99106	0.70007	0.07067
H	3.39812	2.01394	0.65460
C	5.33825	-0.50563	-0.54156
H	4.59755	-2.28224	-1.51361
H	5.76295	1.35168	0.47130
H	6.38223	-0.79627	-0.62118

1 imaginary frequency: -388.81 cm^{-1}.

SCF energy: -1608.090532 hartree
zero-point correction: +0.288819 hartree
enthalpy correction: +0.310105 hartree
free energy correction: +0.236506 hartree
quasiharmonic free energy correction: +0.242005 hartree

TS_4_B

O	3.68910	-0.31059	-0.94583
O	3.41905	-0.13336	1.61702
P	2.63595	0.00358	0.22757
O	1.66994	-1.23628	0.21660
O	2.05156	1.37982	0.12666
H	0.65920	2.26876	-0.02852
C	4.54698	0.73854	-1.43487
H	5.08922	0.31522	-2.28128
H	3.95366	1.59731	-1.75784
H	5.25497	1.04958	-0.65971
C	4.01191	-1.39028	2.00211
H	4.51390	-1.20797	2.95330
H	3.23774	-2.15184	2.12269
H	4.74049	-1.71707	1.25390
C	-0.99987	1.85046	1.01559
C	-1.34074	0.49800	0.35935
O	-0.32202	2.45655	-0.14787
H	-1.86006	2.47477	1.25600
H	-0.31534	1.80503	1.86439
C	-0.73374	0.91401	-0.98628
H	-1.38753	1.22532	-1.79334
H	0.27308	0.67667	-1.26568
Cl	-0.45577	-1.55845	-1.83342
H	1.02524	-1.39136	-0.57351
H	-0.75341	-0.31577	0.78382
C	-2.80547	0.11457	0.33483
C	-3.19529	-1.17731	0.70417
C	-3.79314	1.03193	-0.05087
C	-4.54153	-1.54330	0.69841
H	-2.43621	-1.90471	0.97644
C	-5.13939	0.66756	-0.06118
H	-3.51656	2.04061	-0.35314
C	-5.51760	-0.62177	0.31767
H	-4.82547	-2.55217	0.98492
H	-5.89151	1.39062	-0.36533
H	-6.56619	-0.90669	0.31117

1 imaginary frequency: -387.37 cm^{-1}.

SCF energy: -1608.090084 hartree
zero-point correction: +0.288580 hartree
enthalpy correction: +0.309895 hartree
free energy correction: +0.236062 hartree
quasiharmonic free energy correction: +0.241609 hartree

TS_4_C

O	-2.39084	1.76248	0.06878
O	-3.89868	-0.28203	-0.39107
P	-2.38708	0.16219	-0.10448
O	-2.09639	-0.37713	1.33812
O	-1.51730	-0.27946	-1.24785
H	-0.60633	-1.64700	-1.66696
C	-2.49477	2.59862	-1.09879
H	-2.39248	3.62601	-0.74669
H	-3.47006	2.46814	-1.57933
H	-1.69988	2.36351	-1.81145
C	-4.91529	-0.12440	0.61979
H	-4.99501	0.92295	0.92728
H	-5.85006	-0.44735	0.15941
H	-4.68415	-0.74783	1.48644
C	1.41937	-1.71660	-1.98184
C	2.02955	-1.56530	-0.57160
O	0.13859	-2.31451	-1.55724
H	1.23763	-0.76449	-2.48341
H	1.92245	-2.41132	-2.65597
C	0.67338	-1.82855	0.08892
H	-0.01763	-1.01993	0.16475
H	0.47389	-2.71705	0.66973

Cl	0.62235	-0.74445	2.48589
H	-1.15374	-0.38172	1.76360
H	2.70710	-2.39597	-0.35713
C	2.73583	-0.25680	-0.29237
C	4.07366	-0.26450	0.11329
C	2.09165	0.97395	-0.47912
C	4.75936	0.93135	0.33198
H	4.58186	-1.21344	0.26828
C	2.77405	2.16849	-0.25997
H	1.04643	1.00168	-0.77839
C	4.11094	2.15129	0.14443
H	5.79734	0.90694	0.65236
H	2.25889	3.11533	-0.39712
H	4.64056	3.08413	0.31752

1 imaginary frequency: -362.80 cm^{-1}.

SCF energy: -1608.084714 hartree
zero-point correction: +0.288307 hartree
enthalpy correction: +0.309681 hartree
free energy correction: +0.235069 hartree
quasiharmonic free energy correction: +0.241384 hartree

RC_A1

C	-0.10215	-4.60735	-0.03736
O	1.12117	-1.81176	-0.49379
O	-1.25312	-1.79508	0.52062
C	-1.85691	-2.64237	-0.42295
C	-1.25910	-3.86807	-0.70534
C	-3.06802	-2.24701	-1.02482
C	-1.80430	-4.66794	-1.72312
C	-3.62486	-3.12211	-1.97102
C	-2.98915	-4.30436	-2.35144
H	-4.57176	-2.85152	-2.42655
H	-3.42334	-4.93257	-3.12528
C	1.73622	-2.72967	0.37155
C	1.09330	-3.93610	0.63243
C	2.99114	-2.41747	0.92807
C	1.62784	-4.79261	1.60742
C	3.53941	-3.35261	1.82175
C	2.85403	-4.50891	2.19802
H	4.51675	-3.14650	2.24652
H	3.28308	-5.17937	2.93853
C	-0.93207	-5.87766	-1.97632
H	-1.38671	-6.79133	-1.56844
H	-0.76753	-6.05911	-3.04457
C	0.36707	-5.51252	-1.22773
H	1.01956	-4.92322	-1.88268
H	0.93538	-6.38388	-0.88875
C	0.69486	-5.95790	1.85909
H	1.09244	-6.89016	1.43418
H	0.53856	-6.14295	2.92796
C	-0.59844	-5.51478	1.13838
H	-1.21361	-4.91065	1.81531
H	-1.21040	-6.35220	0.78942
C	-3.78049	-0.97719	-0.65559
C	-3.92763	0.07691	-1.59662
C	-4.36828	-0.85789	0.62815
C	-4.62899	1.22676	-1.21507
C	-5.05019	0.32039	0.95371
C	-5.18976	1.37873	0.05639
H	-4.74629	2.02798	-1.93931
H	-5.49927	0.41263	1.93951
C	3.74836	-1.16877	0.57822
C	4.03003	-0.19561	1.57082
C	4.24661	-0.98930	-0.73891
C	4.79179	0.92600	1.21645
C	4.99732	0.15381	-1.03249
C	5.28564	1.12715	-0.07267
H	5.01591	1.66969	1.97757
H	5.38197	0.27650	-2.04150
C	-3.40521	-0.01308	-3.03016
C	-4.55861	-0.29069	-4.02892
C	-2.62535	1.23634	-3.50204
H	-2.70806	-0.85606	-3.08761
C	-4.04473	-0.46514	-5.46616
H	-5.12399	-1.17876	-3.72198
H	-5.26858	0.54862	-3.99129
C	-2.09025	1.05596	-4.93177
H	-1.79913	1.44659	-2.81737
H	-3.28212	2.11736	-3.48409
C	-3.22096	0.74658	-5.92396
H	-4.88869	-0.63208	-6.14841
H	-3.41904	-1.36856	-5.51661
H	-1.54744	1.95798	-5.24314
H	-1.35988	0.23385	-4.94243
H	-2.81307	0.57323	-6.92831
H	-3.88162	1.62314	-6.00184
C	-5.94651	2.63533	0.45379
C	-7.23300	2.83939	-0.38105
C	-5.06552	3.90419	0.39741
H	-6.25937	2.50809	1.50114
C	-8.00453	4.09412	0.05598
H	-7.87000	1.94987	-0.29719
H	-6.96441	2.92960	-1.44358
C	-5.83850	5.15924	0.83099
H	-4.18188	3.76388	1.03268
H	-4.69632	4.04263	-0.62941
C	-7.12020	5.34850	0.00536
H	-8.37207	3.95255	1.08329
H	-8.89224	4.22725	-0.57580
H	-6.10398	5.06929	1.89478
H	-5.19476	6.04415	0.74572
H	-7.67826	6.22309	0.36365
H	-6.84912	5.55748	-1.04046
C	-4.36763	-1.99639	1.64437

C	-3.81667	-1.59141	3.02945
C	-5.78167	-2.61227	1.78863
H	-3.72089	-2.79637	1.27003
C	-3.82229	-2.77903	4.00470
H	-4.42754	-0.78232	3.45308
H	-2.80409	-1.18924	2.92211
C	-5.79050	-3.79384	2.77097
H	-6.47947	-1.83914	2.14106
H	-6.14622	-2.93340	0.80433
C	-5.22257	-3.39533	4.14102
H	-3.44916	-2.45762	4.98545
H	-3.12254	-3.54840	3.64336
H	-5.18648	-4.61380	2.35424
H	-6.81115	-4.18404	2.87871
H	-5.89468	-2.66120	4.61024
H	-5.19534	-4.26548	4.80999
C	4.05565	-2.02113	-1.84651
C	3.32134	-1.45090	-3.08271
C	5.39917	-2.66335	-2.27060
H	3.43587	-2.83608	-1.45993
C	3.12222	-2.52482	-4.16353
H	3.90364	-0.62045	-3.50716
H	2.35490	-1.03649	-2.77599
C	5.19859	-3.73421	-3.35408
H	6.07489	-1.88417	-2.65099
H	5.89252	-3.09872	-1.39217
C	4.45264	-3.17335	-4.57404
H	2.62479	-2.08765	-5.03903
H	2.44425	-3.30170	-3.77841
H	6.16940	-4.14784	-3.65702
H	4.62225	-4.57093	-2.93176
H	5.08401	-2.41924	-5.06764
H	4.27977	-3.96671	-5.31295
C	3.56705	-0.32078	3.02022
C	4.75003	-0.62817	3.97219
C	2.80502	0.92556	3.52766
H	2.86607	-1.15944	3.08599
C	4.28495	-0.80346	5.42602
H	5.47601	0.19615	3.91765
H	5.28456	-1.52605	3.63657
C	2.32845	0.74231	4.97670
H	3.45774	1.80883	3.47918
H	1.95302	1.11774	2.86981
C	3.49645	0.41839	5.91927
H	5.15060	-0.98846	6.07583
H	3.64687	-1.69706	5.49437
H	1.59164	-0.07264	5.01415
H	1.80256	1.64456	5.31225
H	4.17190	1.28584	5.97064
H	3.12976	0.24768	6.93981
P	-0.02288	-0.83281	0.10336
O	0.38303	-0.01492	1.28272
O	-0.43678	-0.05345	-1.19779
H	-0.55515	0.75268	2.48780
H	-0.30614	0.95373	-1.12167
Cl	-1.21303	1.48947	3.37741
O	-0.10211	2.51261	-1.01008
C	-0.96534	3.24158	-0.07847
C	1.09954	2.99995	-0.32721
C	0.25571	3.87599	0.63466
H	-1.55644	2.55702	0.53548
H	-1.62115	3.92950	-0.61919
H	1.64656	2.17970	0.14460
H	1.74552	3.53932	-1.02643
H	0.33535	3.55336	1.67489
C	0.42010	5.37221	0.53842
C	0.63088	6.13582	1.69288
C	0.36629	6.03182	-0.69944
C	0.78521	7.52147	1.61729
H	0.67277	5.63940	2.65954
C	0.52016	7.41506	-0.77854
H	0.20258	5.45797	-1.60945
C	0.73077	8.16535	0.38105
H	0.94747	8.09590	2.52552
H	0.47564	7.90820	-1.74612
H	0.85064	9.24365	0.31967
C	6.13036	2.34762	-0.39847
C	7.58519	1.96904	-0.76321
C	5.51481	3.22833	-1.51009
H	6.17709	2.96435	0.51197
C	8.44475	3.20861	-1.05453
H	7.57593	1.31567	-1.64758
H	8.02617	1.38086	0.05131
C	6.37472	4.46849	-1.79916
H	5.41354	2.63508	-2.43023
H	4.49901	3.52832	-1.22145
C	7.82034	4.08600	-2.14969
H	9.45863	2.90237	-1.34288
H	8.54919	3.80059	-0.13291
H	5.92674	5.05352	-2.61269
H	6.37803	5.12026	-0.91281
H	8.42537	4.98820	-2.30654
H	7.82787	3.53485	-3.10203

There are no imaginary frequencies.

SCF energy: -4055.692172 hartree
zero-point correction: +1.540571 hartree
enthalpy correction: +1.616439 hartree
free energy correction: +1.421273 hartree
quasiharmonic free energy correction: +1.449446 hartree

RC_A2

C	-0.17191	-4.59314	-0.04578
O	-1.29642	-1.75366	0.41390
O	1.12513	-1.82305	-0.47795
C	1.63634	-2.70997	0.48291
C	0.97859	-3.91878	0.69895

C	2.81980	-2.37320	1.17031	H	1.11592	1.74636	5.41046
C	1.43599	-4.76501	1.72259	H	0.86603	0.05276	5.00169
C	3.29147	-3.29511	2.11835	H	2.14579	0.20728	7.12312
C	2.59600	-4.46448	2.42559	H	3.34589	1.24539	6.35922
H	4.21894	-3.07160	2.63494	C	5.98642	2.44675	0.14013
H	2.96353	-5.13020	3.20257	C	5.52716	3.23706	-1.10636
C	-1.91099	-2.63108	-0.49305	C	7.49416	2.11501	0.03773
C	-1.30639	-3.85737	-0.75234	H	5.86140	3.11057	1.00960
C	-3.12842	-2.25732	-1.09290	C	6.37914	4.49512	-1.33428
C	-1.83223	-4.67152	-1.76752	H	4.46845	3.50698	-1.00362
C	-3.67616	-3.15289	-2.02655	H	5.59369	2.58995	-1.99206
C	-3.02143	-4.32762	-2.40019	C	8.34474	3.37351	-0.19314
H	-4.62608	-2.89926	-2.48598	H	7.81820	1.59553	0.94836
H	-3.44560	-4.96528	-3.17185	H	7.65127	1.41175	-0.79286
C	0.50612	-5.94518	1.89684	C	7.87397	4.15534	-1.42833
H	0.94471	-6.86482	1.48473	H	6.22010	5.19721	-0.50201
H	0.28129	-6.14906	2.94994	H	6.04687	5.01152	-2.24388
C	-0.73731	-5.50647	1.09626	H	8.27742	4.02314	0.69246
H	-1.39605	-4.90584	1.73441	H	9.40213	3.09724	-0.29578
H	-1.32405	-6.34450	0.70813	H	8.46660	5.07135	-1.54821
C	-0.93495	-5.86705	-2.00686	H	8.05021	3.54838	-2.32896
H	-1.38630	-6.79229	-1.62253	C	4.31322	-2.06826	-1.38969
H	-0.73874	-6.03355	-3.07220	C	3.86586	-1.58995	-2.78866
C	0.34175	-5.49269	-1.21974	C	5.71075	-2.73096	-1.47074
H	1.01064	-4.89935	-1.85392	H	3.61642	-2.85717	-1.08921
H	0.90330	-6.36201	-0.86413	C	3.88871	-2.73976	-3.80783
C	3.59397	-1.11408	0.89956	H	4.53222	-0.79055	-3.14143
C	3.70199	-0.10174	1.88845	H	2.86401	-1.15272	-2.72834
C	4.28484	-0.96979	-0.33083	C	5.73956	-3.87383	-2.49773
C	4.47447	1.03260	1.60566	H	6.45708	-1.97243	-1.74765
C	5.03686	0.18791	-0.55633	H	6.00014	-3.10323	-0.47953
C	5.14450	1.20674	0.39346	C	5.27164	-3.40367	-3.88288
H	4.56687	1.80728	2.36282	H	3.58916	-2.36794	-4.79591
H	5.56595	0.28830	-1.50002	H	3.14033	-3.49406	-3.51981
C	-3.84465	-0.98232	-0.75182	H	5.08314	-4.68613	-2.15113
C	-4.04859	0.01492	-1.73985	H	6.75087	-4.29701	-2.55892
C	-4.37808	-0.79587	0.55054	H	5.99725	-2.67907	-4.28201
C	-4.76880	1.16618	-1.39510	H	5.25484	-4.24711	-4.58550
C	-5.08216	0.37853	0.83558	C	-4.26980	-1.84671	1.65155
C	-5.29184	1.37636	-0.11927	C	-3.53744	-1.32430	2.91016
H	-4.93258	1.92877	-2.15259	C	-5.65284	-2.42342	2.03977
H	-5.49105	0.50795	1.83419	H	-3.68385	-2.68955	1.27169
C	3.05945	-0.21996	3.26979	C	-3.41234	-2.41791	3.98198
C	4.10745	-0.59961	4.34813	H	-4.09196	-0.47327	3.33139
C	2.30779	1.04939	3.73485	H	-2.54675	-0.95063	2.63069
H	2.31854	-1.02582	3.23170	C	-5.52900	-3.51407	3.11560
C	3.45842	-0.81780	5.72348	H	-6.29652	-1.61519	2.41515
H	4.65843	-1.49818	4.04689	H	-6.14895	-2.82454	1.14671
H	4.85370	0.20567	4.41561	C	-4.78083	-3.00503	4.35709
C	1.63679	0.83107	5.10035	H	-2.91327	-2.01463	4.87273
H	1.55905	1.34129	2.99335	H	-2.76409	-3.22205	3.60162
H	3.01028	1.89045	3.82196	H	-6.52555	-3.88088	3.39432
C	2.65383	0.41055	6.17140	H	-4.98737	-4.37483	2.69537
H	4.22794	-1.06152	6.46780	H	-5.38410	-2.22623	4.84763
H	2.78921	-1.68928	5.66893	H	-4.66302	-3.81469	5.08914

C	-3.54606	-0.11510	-3.17574
C	-4.71153	-0.37383	-4.16372
C	-2.72610	1.10602	-3.65270
H	-2.87369	-0.97781	-3.22780
C	-4.21076	-0.55924	-5.60419
H	-5.40768	0.47678	-4.12527
H	-5.28949	-1.25231	-3.84958
C	-2.21557	0.91515	-5.08945
H	-3.34742	2.01212	-3.61636
H	-1.88590	1.26457	-2.97060
C	-3.36659	0.63644	-6.06722
H	-5.06279	-0.71099	-6.28011
H	-3.60217	-1.47414	-5.65861
H	-1.50562	0.07607	-5.11187
H	-1.65074	1.80140	-5.40383
H	-4.00971	1.52719	-6.13319
H	-2.97627	0.45825	-7.07770
P	-0.08960	-0.81600	-0.11792
O	-0.39832	0.02107	-1.31303
O	0.27807	-0.06184	1.21178
H	0.59577	0.79117	-2.45944
H	0.30369	0.94970	1.10837
Cl	1.30278	1.52930	-3.31038
O	0.31264	2.52421	0.98812
C	1.35766	3.18935	0.20714
C	-0.73210	3.17288	0.19132
C	0.31196	4.06491	-0.52873
H	1.88908	2.47791	-0.43117
H	2.05841	3.71050	0.86456
H	-1.23890	2.44566	-0.44847
H	-1.44968	3.68617	0.83767
H	0.32680	3.91990	-1.61090
C	0.29839	5.53577	-0.19168
C	0.30876	6.49604	-1.21025
C	0.27746	5.97399	1.14191
C	0.29865	7.85968	-0.90938
H	0.32604	6.17173	-2.24825
C	0.26729	7.33448	1.44531
H	0.26975	5.24385	1.94879
C	0.27783	8.28299	0.41949
H	0.30735	8.58934	-1.71482
H	0.25126	7.65510	2.48375
H	0.27001	9.34357	0.65604
C	-6.07496	2.63875	0.19979
C	-7.55005	2.34201	0.55773
C	-5.41630	3.48635	1.31287
H	-6.08315	3.25571	-0.71188
C	-8.34042	3.62831	0.84135
H	-7.58288	1.69242	1.44430
H	-8.01884	1.77675	-0.25752
C	-6.20704	4.77281	1.59537
H	-5.35243	2.88927	2.23399
H	-4.38380	3.72750	1.02820
C	-7.67378	4.47188	1.93831
H	-9.37138	3.38006	1.12490
H	-8.40679	4.22312	-0.08197
H	-5.73200	5.33362	2.41066
H	-6.16935	5.42232	0.70809
H	-8.22856	5.40657	2.09084
H	-7.71684	3.92363	2.89146

There are no imaginary frequencies.

SCF energy: -4055.691450 hartree
zero-point correction: +1.540358 hartree
enthalpy correction: +1.616295 hartree
free energy correction: +1.420433 hartree
quasiharmonic free energy correction: +1.449270 hartree

RC_A3

C	0.13340	-4.62977	-0.12061
O	-1.09602	-1.88139	0.54906
O	1.21696	-1.77665	-0.59521
C	1.88009	-2.65931	0.27290
C	1.31437	-3.90706	0.52360
C	3.11596	-2.27551	0.83032
C	1.92311	-4.74794	1.46989
C	3.73041	-3.18482	1.70592
C	3.13153	-4.39471	2.05805
H	4.69519	-2.92116	2.12680
H	3.61295	-5.05275	2.77721
C	-1.74978	-2.76405	-0.32487
C	-1.10710	-3.94420	-0.68572
C	-3.03928	-2.44357	-0.79021
C	-1.68475	-4.75660	-1.67388
C	-3.62503	-3.33872	-1.70084
C	-2.94644	-4.46144	-2.17814
H	-4.62802	-3.12684	-2.05754
H	-3.40841	-5.09815	-2.92858
C	1.08581	-5.98636	1.70060
H	1.53394	-6.86688	1.21902
H	0.98110	-6.22968	2.76408
C	-0.25664	-5.60620	1.04202
H	-0.88189	-5.06515	1.76184
H	-0.82867	-6.46849	0.68662
C	-0.75126	-5.89152	-2.03835
H	-1.11056	-6.85076	-1.64025
H	-0.65407	-6.01923	-3.12250
C	0.57491	-5.46346	-1.37005
H	1.13919	-4.81219	-2.04760
H	1.21989	-6.30632	-1.10327
C	3.80164	-0.98594	0.47835
C	3.99156	0.03070	1.45215
C	4.32936	-0.81522	-0.82554
C	4.67437	1.19622	1.08415
C	4.99637	0.37579	-1.13525
C	5.17776	1.39813	-0.20441
H	4.82450	1.96896	1.83302

H	5.40092	0.50659	-2.13596
C	-3.79035	-1.22980	-0.32396
C	-4.14984	-0.20586	-1.23989
C	-4.19909	-1.13058	1.03010
C	-4.89787	0.88330	-0.77651
C	-4.93432	-0.01062	1.43584
C	-5.29795	1.00892	0.55627
H	-5.17969	1.65654	-1.48572
H	-5.25107	0.06187	2.47386
C	3.53318	-0.11549	2.90278
C	4.72848	-0.41700	3.84308
C	2.76414	1.11037	3.44938
H	2.84645	-0.96708	2.95924
C	4.27568	-0.64345	5.29373
H	5.28510	-1.29063	3.48315
H	5.43163	0.42793	3.80482
C	2.28950	0.87723	4.89244
H	1.90861	1.33784	2.80795
H	3.41380	1.99682	3.43413
C	3.46208	0.54486	5.82623
H	5.14857	-0.82564	5.93443
H	3.65955	-1.55366	5.33948
H	1.75343	1.76350	5.25626
H	1.56620	0.04896	4.90478
H	3.09761	0.33368	6.83999
H	4.11878	1.42415	5.90683
C	5.91538	2.67062	-0.58695
C	7.21839	2.86712	0.22311
C	5.02368	3.92901	-0.47971
H	6.20512	2.57237	-1.64403
C	7.96770	4.14003	-0.19987
H	7.86192	1.98655	0.10285
H	6.97375	2.92891	1.29337
C	5.77459	5.20220	-0.89906
H	4.12726	3.79532	-1.09837
H	4.67652	4.03794	0.55834
C	7.07278	5.38387	-0.09808
H	8.31308	4.02756	-1.23842
H	8.86828	4.26647	0.41483
H	6.01685	5.14113	-1.97041
H	5.12450	6.07810	-0.77725
H	7.61418	6.27257	-0.44706
H	6.82369	5.56436	0.95844
C	4.28131	-1.91116	-1.88653
C	3.64613	-1.45359	-3.21839
C	5.69003	-2.50388	-2.13772
H	3.66467	-2.73335	-1.50982
C	3.60673	-2.59789	-4.24342
H	4.22287	-0.61892	-3.64037
H	2.63752	-1.06953	-3.03422
C	5.65251	-3.64206	-3.16951
H	6.35975	-1.70895	-2.49592
H	6.11334	-2.86243	-1.19060
C	5.00256	-3.19109	-4.48578
H	3.17482	-2.23907	-5.18632
H	2.93612	-3.39018	-3.87637
H	5.08132	-4.48633	-2.75496
H	6.66866	-4.01534	-3.35308
H	5.63983	-2.42972	-4.96026
H	4.94499	-4.03173	-5.18963
C	-3.93390	-2.22344	2.06107
C	-3.13033	-1.72386	3.28429
C	-5.24794	-2.90044	2.52263
H	-3.33464	-3.00896	1.58986
C	-2.86572	-2.85875	4.28587
H	-3.68825	-0.92354	3.79144
H	-2.18492	-1.28560	2.94660
C	-4.98159	-4.03233	3.52650
H	-5.90366	-2.14994	2.98643
H	-5.78911	-3.28664	1.64939
C	-4.16751	-3.54079	4.73250
H	-2.32102	-2.47020	5.15614
H	-2.20744	-3.60662	3.81799
H	-5.93201	-4.46906	3.86017
H	-4.42908	-4.83945	3.02229
H	-4.77180	-2.82284	5.30726
H	-3.94842	-4.37605	5.41045
C	-3.78240	-0.24610	-2.72167
C	-5.01966	-0.52443	-3.61105
C	-3.07216	1.03787	-3.21066
H	-3.07561	-1.06761	-2.87869
C	-4.64498	-0.61963	-5.09826
H	-5.75202	0.28386	-3.46992
H	-5.51982	-1.44644	-3.28832
C	-2.68606	0.93598	-4.69423
H	-3.73308	1.90632	-3.07643
H	-2.18255	1.21211	-2.59891
C	-3.90618	0.63870	-5.57721
H	-5.54686	-0.78764	-5.70173
H	-3.99931	-1.49739	-5.25043
H	-1.94107	0.13725	-4.81856
H	-2.19599	1.86298	-5.01619
H	-4.59616	1.49567	-5.54325
H	-3.60199	0.52493	-6.62584
P	-0.00451	-0.85670	-0.06832
O	-0.48773	0.00282	-1.18761
O	0.46659	-0.12531	1.24111
H	0.36268	0.81305	-2.42838
H	0.34440	0.88506	1.20182
Cl	0.96015	1.58051	-3.33457
O	0.16539	2.44938	1.14105
C	1.00656	3.18925	0.19784
C	-1.05034	2.98622	0.52316
C	-0.22356	3.91285	-0.40579
H	1.52440	2.51288	-0.48746
H	1.72652	3.81525	0.73146
H	-1.61300	2.19875	0.01504
H	-1.67461	3.48412	1.27079
H	-0.36083	3.68518	-1.46492
C	-0.33247	5.39898	-0.16925

C	-0.57353	6.27012	-1.23831
C	-0.19299	5.94138	1.11791
C	-0.67394	7.64739	-1.03130
H	-0.68117	5.86522	-2.24188
C	-0.29276	7.31585	1.32795
H	-0.00363	5.28192	1.96265
C	-0.53402	8.17452	0.25255
H	-0.86081	8.30680	-1.87480
H	-0.18179	7.71735	2.33187
H	-0.61151	9.24607	0.41574
C	-6.13345	2.18403	1.03666
C	-5.46520	3.55310	0.77818
C	-7.55839	2.16411	0.43325
H	-6.24442	2.07980	2.12686
C	-6.32450	4.71706	1.29671
H	-5.29956	3.68023	-0.30108
H	-4.47366	3.57320	1.24899
C	-8.41649	3.32860	0.95055
H	-7.48473	2.22286	-0.66234
H	-8.03912	1.20423	0.66004
C	-7.74009	4.68434	0.70097
H	-5.83605	5.67318	1.06899
H	-6.39283	4.65558	2.39317
H	-9.40677	3.30343	0.47769
H	-8.58426	3.20203	2.03062
H	-8.34796	5.49679	1.11939
H	-7.68017	4.86468	-0.38277

There are no imaginary frequencies.

SCF energy: -4055.692100 hartree
zero-point correction: +1.540293 hartree
enthalpy correction: +1.616162 hartree
free energy correction: +1.420967 hartree
quasiharmonic free energy correction: +1.449172 hartree

RC_A4

C	0.03891	-4.61805	-0.29466
O	-1.19539	-1.89118	0.45829
O	1.16528	-1.75157	-0.57817
C	1.77985	-2.68217	0.27533
C	1.19914	-3.93891	0.43165
C	2.98626	-2.33481	0.91562
C	1.76391	-4.83450	1.35519
C	3.56152	-3.29702	1.76065
C	2.94747	-4.52362	2.01304
H	4.50581	-3.06053	2.23989
H	3.39558	-5.22517	2.71231
C	-1.82368	-2.72830	-0.47674
C	-1.17618	-3.89571	-0.86907
C	-3.09390	-2.37600	-0.97125
C	-1.72463	-4.65794	-1.91239
C	-3.65494	-3.22685	-1.93814
C	-2.96789	-4.33221	-2.44279
H	-4.64328	-2.99064	-2.31910
H	-3.40865	-4.93119	-3.23583
C	0.91142	-6.07693	1.48588
H	1.37063	-6.93305	0.97186
H	0.76653	-6.37796	2.52964
C	-0.40256	-5.64813	0.80144
H	-1.04713	-5.13656	1.52578
H	-0.97079	-6.48447	0.38344
C	-0.78469	-5.78016	-2.29926
H	-1.16108	-6.75499	-1.95918
H	-0.65181	-5.85678	-3.38443
C	0.52017	-5.39231	-1.56714
H	1.10972	-4.71236	-2.19294
H	1.15210	-6.25094	-1.32025
C	3.68397	-1.02302	0.69354
C	3.81100	-0.08104	1.74691
C	4.29214	-0.76008	-0.56078
C	4.51836	1.10413	1.50497
C	4.98185	0.44333	-0.74262
C	5.10697	1.39426	0.27309
H	4.62652	1.82483	2.31167
H	5.45009	0.63318	-1.70451
C	-3.84601	-1.16877	-0.48935
C	-4.15792	-0.11050	-1.38426
C	-4.29749	-1.10361	0.85302
C	-4.89676	0.97958	-0.90986
C	-5.02766	0.01614	1.26930
C	-5.33846	1.07154	0.41244
H	-5.13443	1.78369	-1.60062
H	-5.37628	0.06291	2.29851
C	3.25980	-0.32358	3.15137
C	4.38919	-0.70197	4.14408
C	2.46564	0.86900	3.73484
H	2.56597	-1.16984	3.10512
C	3.83546	-1.03542	5.53827
H	4.96861	-1.54922	3.75856
H	5.09292	0.14000	4.21779
C	1.88838	0.53210	5.11891
H	1.66074	1.15946	3.05467
H	3.12415	1.74367	3.83495
C	2.98977	0.11486	6.10378
H	4.66019	-1.27444	6.22258
H	3.21479	-1.94111	5.46880
H	1.33431	1.39444	5.51204
H	1.16003	-0.28543	5.01588
H	2.55292	-0.17239	7.06907
H	3.64293	0.97834	6.30091
C	5.88463	2.68446	0.06963
C	5.30190	3.56641	-1.05841
C	7.38926	2.42441	-0.17913
H	5.80821	3.26202	1.00377
C	6.09117	4.87408	-1.22767
H	4.24650	3.78358	-0.85022
H	5.31927	3.00677	-2.00405

C	8.17708	3.73240	-0.34976
H	7.80181	1.83440	0.64899
H	7.50335	1.81076	-1.08426
C	7.58501	4.60717	-1.46462
H	5.97330	5.48799	-0.32214
H	5.67168	5.45910	-2.05608
H	8.15852	4.29181	0.59757
H	9.23163	3.50998	-0.55816
H	8.13443	5.55446	-1.53854
H	7.71150	4.09558	-2.43038
C	4.30361	-1.77917	-1.69695
C	3.75262	-1.22501	-3.02949
C	5.72181	-2.36638	-1.90410
H	3.66068	-2.61961	-1.41647
C	3.77028	-2.29501	-4.13220
H	4.35779	-0.36810	-3.35655
H	2.73626	-0.84621	-2.88082
C	5.74193	-3.42974	-3.01310
H	6.41631	-1.55457	-2.16426
H	6.08513	-2.79404	-0.96072
C	5.17494	-2.88312	-4.33164
H	3.39802	-1.86739	-5.07181
H	3.07454	-3.10455	-3.86254
H	5.14247	-4.29555	-2.69376
H	6.76558	-3.79848	-3.16043
H	5.84384	-2.09726	-4.71358
H	5.15509	-3.67277	-5.09413
C	-4.06960	-2.22397	1.86308
C	-3.27666	-1.75781	3.10676
C	-5.39785	-2.89193	2.29532
H	-3.47510	-3.00841	1.38395
C	-3.03663	-2.91428	4.08909
H	-3.83469	-0.96264	3.62179
H	-2.32268	-1.32211	2.79164
C	-5.15733	-4.04575	3.28149
H	-6.05045	-2.14250	2.76519
H	-5.93280	-3.25557	1.40862
C	-4.35175	-3.58838	4.50673
H	-2.49814	-2.54871	4.97311
H	-2.38122	-3.66053	3.61468
H	-6.11712	-4.47682	3.59509
H	-4.60868	-4.84997	2.76850
H	-4.95385	-2.87415	5.08834
H	-4.15199	-4.43987	5.17031
C	-3.74645	-0.11335	-2.85502
C	-4.95942	-0.36102	-3.78672
C	-3.01589	1.17734	-3.29234
H	-3.03994	-0.93491	-3.01297
C	-4.54017	-0.42749	-5.26336
H	-5.68782	0.45165	-3.64987
H	-5.47863	-1.28432	-3.49998
C	-2.58584	1.10740	-4.76579
H	-3.67577	2.04650	-3.15859
H	-2.14429	1.33326	-2.65043
C	-3.78020	0.83588	-5.69213
H	-5.42401	-0.57637	-5.89775
H	-3.89540	-1.30611	-5.41449
H	-1.84086	0.30799	-4.88612
H	-2.08236	2.03923	-5.05110
H	-4.46638	1.69599	-5.66101
H	-3.44421	0.74297	-6.73311
P	-0.07667	-0.84764	-0.06959
O	-0.50557	0.05831	-1.17414
O	0.33311	-0.17398	1.29038
H	0.37592	0.92775	-2.34635
H	0.28269	0.84249	1.26907
Cl	0.99936	1.73670	-3.19768
O	0.19277	2.41614	1.26068
C	1.13769	3.16672	0.43104
C	-0.94427	3.04203	0.57978
C	-0.00668	4.00446	-0.19418
H	1.65961	2.50887	-0.26937
H	1.85510	3.70641	1.05474
H	-1.47525	2.31401	-0.03919
H	-1.62290	3.50207	1.30344
H	-0.07086	3.88563	-1.27773
C	-0.06572	5.46493	0.18085
C	-0.17051	6.44691	-0.81140
C	-0.01364	5.87218	1.52335
C	-0.22282	7.80151	-0.47619
H	-0.20982	6.14673	-1.85600
C	-0.06603	7.22359	1.86110
H	0.06942	5.12521	2.31038
C	-0.17112	8.19386	0.86132
H	-0.30366	8.54834	-1.26163
H	-0.02457	7.52017	2.90597
H	-0.21179	9.24734	1.12474
C	-6.12894	2.27039	0.91011
C	-5.30110	3.57611	0.86970
C	-7.46431	2.45999	0.15388
H	-6.38023	2.08080	1.96489
C	-6.09705	4.77798	1.40111
H	-4.99053	3.77420	-0.16633
H	-4.37907	3.44255	1.45048
C	-8.25893	3.66170	0.68835
H	-7.25735	2.61086	-0.91524
H	-8.06109	1.54219	0.22745
C	-7.42590	4.95148	0.65065
H	-5.49318	5.69129	1.32457
H	-6.30358	4.62965	2.47162
H	-9.18297	3.78727	0.10943
H	-8.56651	3.46009	1.72540
H	-7.99687	5.78686	1.07580
H	-7.21696	5.21608	-0.39668

There are no imaginary frequencies.

SCF energy: -4055.691953 hartree
zero-point correction: +1.539926 hartree
enthalpy correction: +1.615897 hartree

free energy correction: +1.420197 hartree
quasiharmonic free energy correction: +1.448735 hartree

RC_B1

C	-0.04044	-4.51081	-0.12832
O	-1.15535	-1.68538	0.43993
O	1.21525	-1.72875	-0.58859
C	1.76112	-2.60769	0.35730
C	1.13188	-3.83133	0.57946
C	2.95652	-2.25272	1.01258
C	1.64495	-4.68312	1.57141
C	3.47593	-3.17413	1.93628
C	2.81879	-4.36523	2.24374
H	4.41343	-2.93532	2.42779
H	3.22636	-5.03508	2.99683
C	-1.83569	-2.57144	-0.41389
C	-1.23033	-3.77891	-0.74185
C	-3.10278	-2.20810	-0.90896
C	-1.80876	-4.57603	-1.74162
C	-3.69802	-3.08939	-1.82626
C	-3.04494	-4.23753	-2.28087
H	-4.68415	-2.84666	-2.20971
H	-3.50753	-4.85924	-3.04326
C	0.75611	-5.89318	1.75031
H	1.20362	-6.78714	1.29347
H	0.58041	-6.13349	2.80507
C	-0.52988	-5.46843	1.01353
H	-1.17572	-4.90233	1.69507
H	-1.11152	-6.31117	0.62831
C	-0.90049	-5.74034	-2.07763
H	-1.30581	-6.68957	-1.70039
H	-0.76761	-5.86231	-3.15839
C	0.41664	-5.36141	-1.35960
H	1.02940	-4.73312	-2.01576
H	1.01687	-6.22900	-1.06807
C	3.71230	-0.98340	0.73032
C	3.79583	0.04253	1.70885
C	4.42858	-0.85416	-0.48463
C	4.59122	1.16290	1.44360
C	5.20157	0.29467	-0.69568
C	5.30386	1.31372	0.25074
H	4.66168	1.94043	2.19860
H	5.76052	0.38925	-1.62350
C	-3.80936	-0.96305	-0.45451
C	-4.21405	-0.84114	0.90226
C	-4.11532	0.07756	-1.36852
C	-4.88045	0.31710	1.31376
C	-4.78867	1.21283	-0.89495
C	-5.17270	1.36434	0.43692
H	-5.18892	0.39747	2.35276
H	-5.02833	2.00955	-1.59488
C	3.08187	-0.04355	3.05700
C	4.05076	-0.43921	4.20018
C	2.34540	1.25610	3.45889
H	2.32078	-0.82875	2.98555
C	3.31389	-0.61049	5.53799
H	4.58307	-1.36305	3.94708
H	4.82077	0.34016	4.29938
C	1.58201	1.07912	4.78052
H	1.66250	1.56568	2.66307
H	3.07030	2.07293	3.58376
C	2.52008	0.64781	5.91748
H	4.03046	-0.86206	6.33103
H	2.62398	-1.46365	5.45875
H	1.07065	2.01400	5.04507
H	0.79624	0.32171	4.64476
H	1.95106	0.47516	6.84030
H	3.22368	1.46616	6.13292
C	6.18963	2.52331	-0.00099
C	7.37793	2.58436	0.98721
C	5.40823	3.85715	0.01801
H	6.61472	2.41280	-1.01019
C	8.29028	3.79067	0.71692
H	7.95075	1.65042	0.92875
H	6.98946	2.64581	2.01397
C	6.32352	5.06212	-0.25247
H	4.59979	3.81858	-0.72395
H	4.92656	3.98153	0.99851
C	7.50193	5.10859	0.73118
H	8.77075	3.66828	-0.26526
H	9.10008	3.82209	1.45722
H	6.71246	4.99693	-1.27955
H	5.74395	5.99273	-0.19865
H	8.16332	5.95136	0.49255
H	7.11822	5.28967	1.74647
C	4.46288	-1.95549	-1.53941
C	4.12007	-1.46062	-2.96208
C	5.82889	-2.68562	-1.53854
H	3.71008	-2.70688	-1.28075
C	4.14994	-2.61121	-3.97975
H	4.84150	-0.69276	-3.27571
H	3.13228	-0.98742	-2.96226
C	5.86381	-3.82954	-2.56392
H	6.62534	-1.96305	-1.76849
H	6.04028	-3.07046	-0.53246
C	5.50219	-3.33905	-3.97360
H	3.92552	-2.22600	-4.98209
H	3.34896	-3.32548	-3.73923
H	5.14919	-4.60837	-2.25825
H	6.85544	-4.30115	-2.56488
H	6.28485	-2.65097	-4.32755
H	5.48715	-4.18175	-4.67714
C	-3.78640	0.01550	-2.85923
C	-5.07119	-0.19087	-3.70140
C	-3.01824	1.25949	-3.36790
H	-3.13525	-0.84629	-3.03757
C	-4.76896	-0.27702	-5.20478
H	-5.76054	0.64589	-3.51587

H	-5.59686	-1.09505	-3.36822
C	-2.72610	1.17806	-4.87528
H	-3.60576	2.16740	-3.17117
H	-2.08244	1.34948	-2.80569
C	-4.00600	0.96175	-5.69448
H	-5.70380	-0.39972	-5.76758
H	-4.16387	-1.17419	-5.40096
H	-2.21694	2.09443	-5.20312
H	-2.02783	0.35230	-5.06397
H	-4.65576	1.84563	-5.60158
H	-3.76347	0.86284	-6.76044
C	-4.00678	-1.94558	1.93490
C	-3.17111	-1.48403	3.15195
C	-5.35240	-2.54841	2.40791
H	-3.45436	-2.76429	1.46320
C	-2.95986	-2.62621	4.15761
H	-3.68589	-0.65534	3.65891
H	-2.20725	-1.09391	2.80798
C	-5.13994	-3.68777	3.41688
H	-5.96443	-1.76169	2.87170
H	-5.91925	-2.91004	1.54049
C	-4.29362	-3.23444	4.61576
H	-2.38964	-2.26255	5.02233
H	-2.34549	-3.41083	3.69012
H	-4.63369	-4.52520	2.91370
H	-6.11013	-4.07203	3.75807
H	-4.85467	-2.48125	5.18921
H	-4.11658	-4.07663	5.29736
P	-0.02294	-0.74962	-0.24021
O	-0.40940	-0.03288	-1.49215
O	0.36832	0.14552	0.99119
H	0.00567	-0.70591	-3.04406
H	0.41542	1.13449	0.75781
Cl	0.31330	-1.21661	-4.22860
O	0.39702	2.66572	0.36549
C	1.00554	3.03569	-0.91527
C	-0.89393	3.20425	-0.06768
C	-0.25463	3.83742	-1.32985
H	1.19579	2.14833	-1.52435
H	1.92466	3.60572	-0.75699
H	-1.29625	3.89583	0.67778
H	-1.60584	2.39969	-0.27356
H	-0.70306	3.48454	-2.26129
C	-0.12958	5.34134	-1.34423
C	0.43143	6.03127	-0.25795
C	-0.57479	6.07924	-2.44722
C	0.54227	7.42061	-0.27720
H	0.78416	5.47507	0.60816
C	-0.46486	7.47113	-2.46931
H	-1.01115	5.55882	-3.29683
C	0.09394	8.14596	-1.38406
H	0.97948	7.93817	0.57265
H	-0.81596	8.02583	-3.33543
H	0.18071	9.22901	-1.39901
C	-5.89390	2.61874	0.90240
C	-7.33138	2.32560	1.39222
C	-5.10464	3.38442	1.98901
H	-5.97985	3.28819	0.03295
C	-8.05679	3.60582	1.83524
H	-7.28875	1.62098	2.23520
H	-7.89452	1.82201	0.59649
C	-5.83117	4.66389	2.43203
H	-4.96045	2.72966	2.86011
H	-4.10125	3.62501	1.61407
C	-7.26106	4.36516	2.90701
H	-9.05945	3.35913	2.20752
H	-8.20109	4.25947	0.96204
H	-5.26153	5.16274	3.22675
H	-5.87011	5.36853	1.58792
H	-7.77563	5.29696	3.17462
H	-7.21801	3.75773	3.82343

There are no imaginary frequencies.

SCF energy: -4055.690336 hartree
zero-point correction: +1.539900 hartree
enthalpy correction: +1.616009 hartree
free energy correction: +1.418400 hartree
quasiharmonic free energy correction: +1.448782 hartree

RC_B2

C	0.00623	-4.47356	-0.51521
O	-1.16995	-1.72847	0.29359
O	1.23917	-1.64215	-0.62891
C	1.75269	-2.60779	0.24842
C	1.14077	-3.85894	0.30580
C	2.90055	-2.30219	1.00585
C	1.62790	-4.80543	1.22300
C	3.39910	-3.31039	1.84646
C	2.76095	-4.54260	1.98311
H	4.30117	-3.10607	2.41389
H	3.14826	-5.28466	2.67683
C	-1.80848	-2.53433	-0.66512
C	-1.17546	-3.69693	-1.08946
C	-3.06291	-2.13668	-1.16545
C	-1.71143	-4.39977	-2.17965
C	-3.61953	-2.93574	-2.17762
C	-2.93782	-4.02787	-2.71916
H	-4.59606	-2.66715	-2.56775
H	-3.36943	-4.57925	-3.55068
C	0.75653	-6.04086	1.23164
H	1.23514	-6.87070	0.69279
H	0.54898	-6.40191	2.24537
C	-0.50925	-5.55192	0.50138
H	-1.18260	-5.06581	1.21717
H	-1.06878	-6.35405	0.01117
C	-0.77321	-5.51065	-2.60331
H	-1.17072	-6.49934	-2.33534

H	-0.60785	-5.52065	-3.68641
C	0.51597	-5.18528	-1.81162
H	1.13428	-4.48297	-2.38182
H	1.12439	-6.06844	-1.59285
C	3.62221	-0.98541	0.92667
C	3.61376	-0.09359	2.02950
C	4.39522	-0.67758	-0.22134
C	4.37779	1.07775	1.95093
C	5.13563	0.50972	-0.24230
C	5.14599	1.40291	0.83210
H	4.38357	1.76057	2.79704
H	5.73909	0.73025	-1.11846
C	-3.79285	-0.93505	-0.63710
C	-4.23012	-0.91011	0.71482
C	-4.08954	0.16402	-1.48474
C	-4.92648	0.20730	1.18540
C	-4.79178	1.25482	-0.95268
C	-5.21496	1.30746	0.37477
H	-5.25973	0.21327	2.21981
H	-5.02315	2.09550	-1.60198
C	2.84313	-0.37783	3.31731
C	3.78177	-0.86249	4.45176
C	2.01767	0.82291	3.83667
H	2.12957	-1.18384	3.11317
C	2.99662	-1.24201	5.71709
H	4.38105	-1.71601	4.11450
H	4.49667	-0.06023	4.68677
C	1.20609	0.43832	5.08376
H	1.35429	1.19303	3.05045
H	2.68851	1.65283	4.09946
C	2.11335	-0.08546	6.20713
H	3.68950	-1.55431	6.50957
H	2.36267	-2.11326	5.49526
H	0.62795	1.30280	5.43558
H	0.47434	-0.33644	4.81213
H	1.51199	-0.40401	7.06863
H	2.75635	0.73437	6.56110
C	5.98265	2.67154	0.81164
C	5.59365	3.63321	-0.33423
C	7.49962	2.37173	0.76240
H	5.79087	3.20220	1.75688
C	6.43295	4.91995	-0.31173
H	4.52502	3.87550	-0.26471
H	5.73372	3.12492	-1.29883
C	8.33912	3.65814	0.78394
H	7.77253	1.72271	1.60395
H	7.72553	1.80499	-0.15231
C	7.93800	4.61538	-0.34815
H	6.20129	5.48620	0.60283
H	6.15350	5.56448	-1.15504
H	8.20014	4.16437	1.75099
H	9.40618	3.41042	0.71411
H	8.51597	5.54619	-0.28319
H	8.19102	4.15743	-1.31611
C	4.52380	-1.63793	-1.39989
C	4.27187	-0.97623	-2.77277
C	5.90138	-2.34582	-1.38915
H	3.76921	-2.42344	-1.29094
C	4.39799	-1.99339	-3.91744
H	4.99751	-0.16715	-2.93757
H	3.27627	-0.51924	-2.78727
C	6.03238	-3.35600	-2.53945
H	6.69575	-1.58964	-1.47151
H	6.04993	-2.84756	-0.42424
C	5.76097	-2.70094	-3.90171
H	4.23756	-1.49101	-4.87942
H	3.59655	-2.74061	-3.82449
H	5.31320	-4.17380	-2.38283
H	7.03080	-3.81278	-2.52543
H	6.55313	-1.96650	-4.11274
H	5.81146	-3.45143	-4.70141
C	-3.71938	0.21280	-2.96650
C	-4.97887	0.05150	-3.85582
C	-2.95612	1.49824	-3.36735
H	-3.05132	-0.62556	-3.18817
C	-4.63461	0.06743	-5.35237
H	-5.68025	0.86955	-3.63526
H	-5.50610	-0.87608	-3.59806
C	-2.62067	1.52074	-4.86805
H	-3.56162	2.38360	-3.12732
H	-2.03767	1.56284	-2.77348
C	-3.87403	1.34356	-5.73726
H	-5.55207	-0.02683	-5.94829
H	-4.01405	-0.80882	-5.59052
H	-2.11510	2.46280	-5.11965
H	-1.90565	0.71763	-5.08974
H	-4.53761	2.21213	-5.60617
H	-3.59936	1.31789	-6.79971
C	-4.01316	-2.06871	1.68459
C	-3.19748	-1.65242	2.93139
C	-5.34672	-2.72734	2.11468
H	-3.43921	-2.84842	1.17433
C	-2.96101	-2.84124	3.87481
H	-3.73903	-0.86735	3.47827
H	-2.24291	-1.21795	2.61739
C	-5.11115	-3.91347	3.06394
H	-5.98104	-1.98216	2.61548
H	-5.89922	-3.05638	1.22526
C	-4.28139	-3.50575	4.29066
H	-2.40468	-2.51065	4.76166
H	-2.32412	-3.58283	3.36896
H	-4.58286	-4.71086	2.51992
H	-6.07348	-4.33825	3.37827
H	-4.86341	-2.79902	4.90114
H	-4.08774	-4.37981	4.92610
P	-0.02951	-0.71623	-0.24707
O	-0.37572	0.10877	-1.44311
O	0.29127	0.06630	1.07802
H	0.11700	-0.41827	-3.02536
H	0.34649	1.07258	0.93555

Cl	0.48809	-0.81736	-4.23470
O	0.33352	2.62728	0.66960
C	1.05821	3.10105	-0.51154
C	-0.92063	3.17508	0.14707
C	-0.17407	3.90608	-0.99763
H	1.33709	2.26518	-1.15853
H	1.94009	3.67757	-0.22016
H	-1.40947	3.80591	0.89488
H	-1.58976	2.37588	-0.18368
H	-0.51710	3.61005	-1.99154
C	-0.08352	5.40922	-0.89843
C	0.32722	6.03193	0.29083
C	-0.40712	6.21392	-1.99704
C	0.41063	7.42066	0.37617
H	0.58349	5.42332	1.15558
C	-0.32426	7.60546	-1.91459
H	-0.72628	5.74650	-2.92585
C	0.08476	8.21301	-0.72754
H	0.73050	7.88528	1.30520
H	-0.57950	8.21268	-2.77904
H	0.14998	9.29564	-0.66115
C	-5.96807	2.51537	0.90823
C	-7.40609	2.16194	1.35427
C	-5.20751	3.22109	2.05476
H	-6.05438	3.23909	0.08342
C	-8.16235	3.39018	1.88426
H	-7.36187	1.39561	2.14151
H	-7.94932	1.71071	0.51447
C	-5.96790	4.44687	2.58433
H	-5.05109	2.50850	2.87706
H	-4.20819	3.51290	1.70616
C	-7.39393	4.08021	3.02063
H	-9.16328	3.09503	2.22465
H	-8.31233	4.10639	1.06254
H	-5.41664	4.89703	3.42001
H	-6.01662	5.21258	1.79567
H	-7.93220	4.97598	3.35592
H	-7.34361	3.40265	3.88602

There are no imaginary frequencies.

SCF energy: -4055.690500 hartree
zero-point correction: +1.540009 hartree
enthalpy correction: +1.616081 hartree
free energy correction: +1.418679 hartree
quasiharmonic free energy correction: +1.448945 hartree

RC_B3

C	0.09655	-4.52157	-0.41007
O	-1.07374	-1.79685	0.46829
O	1.23187	-1.66502	-0.69326
C	1.85992	-2.60024	0.14036
C	1.28715	-3.86228	0.28658
C	3.07725	-2.25625	0.76021
C	1.88657	-4.77643	1.16871
C	3.68024	-3.23205	1.56974
C	3.08477	-4.47151	1.80311
H	4.63467	-2.99867	2.03027
H	3.55802	-5.18783	2.47008
C	-1.77549	-2.63354	-0.41823
C	-1.15161	-3.78416	-0.88622
C	-3.08184	-2.27824	-0.80480
C	-1.76398	-4.51411	-1.91661
C	-3.70240	-3.09904	-1.76068
C	-3.04110	-4.17798	-2.35175
H	-4.71711	-2.86095	-2.06408
H	-3.52834	-4.74881	-3.13819
C	1.05208	-6.03178	1.28636
H	1.49939	-6.86163	0.72130
H	0.95101	-6.37450	2.32238
C	-0.29064	-5.59182	0.66951
H	-0.90887	-5.11071	1.43660
H	-0.86953	-6.41856	0.24724
C	-0.84114	-5.61007	-2.40696
H	-1.19187	-6.60295	-2.09253
H	-0.77091	-5.63256	-3.50017
C	0.50453	-5.24554	-1.73598
H	1.05546	-4.54119	-2.36923
H	1.14854	-6.11246	-1.55786
C	3.77091	-0.93870	0.54771
C	3.86137	0.01192	1.59918
C	4.42345	-0.68747	-0.68348
C	4.59863	1.18239	1.38702
C	5.14031	0.50610	-0.83848
C	5.24856	1.45315	0.17922
H	4.67572	1.90159	2.19719
H	5.65067	0.69357	-1.78038
C	-3.80393	-1.10694	-0.20296
C	-4.12959	-1.11794	1.17816
C	-4.20912	-0.00780	-1.00657
C	-4.82295	-0.03039	1.72180
C	-4.90534	1.04759	-0.40410
C	-5.21869	1.06622	0.95686
H	-5.07421	-0.04329	2.77988
H	-5.21840	1.88240	-1.02454
C	3.22156	-0.21160	2.96858
C	4.26048	-0.67153	4.02270
C	2.47001	1.02298	3.52059
H	2.47953	-1.01162	2.86699
C	3.59984	-0.98555	5.37436
H	4.80694	-1.55043	3.66252
H	5.01000	0.12320	4.15236
C	1.78015	0.70269	4.85554
H	1.73880	1.38062	2.79059
H	3.17694	1.84853	3.68526
C	2.78733	0.20563	5.90286
H	4.36397	-1.27964	6.10599
H	2.93421	-1.85291	5.25272

H	1.25456	1.59183	5.22774
H	1.01240	-0.06691	4.68934
H	2.27144	-0.06765	6.83256
H	3.47553	1.02595	6.15691
C	6.07267	2.71566	-0.01757
C	7.27714	2.77996	0.95034
C	5.22766	4.00593	0.09053
H	6.48115	2.68262	-1.03902
C	8.12298	4.04430	0.73452
H	7.89354	1.88077	0.82652
H	6.90943	2.76281	1.98634
C	6.07673	5.26920	-0.12311
H	4.40993	3.96987	-0.64117
H	4.75725	4.04830	1.08345
C	7.27097	5.31760	0.84088
H	8.58818	4.00338	-0.26172
H	8.94575	4.07362	1.46046
H	6.44751	5.28439	-1.15883
H	5.45288	6.16444	-0.00405
H	7.88486	6.20524	0.64124
H	6.89975	5.41945	1.87171
C	4.44815	-1.70003	-1.82417
C	3.94864	-1.12274	-3.16748
C	5.85905	-2.31591	-1.99345
H	3.77671	-2.52663	-1.56967
C	3.98152	-2.18051	-4.28113
H	4.57920	-0.27265	-3.46521
H	2.93065	-0.73658	-3.04853
C	5.89314	-3.36731	-3.11327
H	6.57832	-1.51612	-2.22218
H	6.18292	-2.76088	-1.04368
C	5.37989	-2.79433	-4.44250
H	3.64564	-1.73530	-5.22576
H	3.25977	-2.97583	-4.04327
H	5.26632	-4.22391	-2.82309
H	6.91352	-3.75530	-3.23148
H	6.07752	-2.01898	-4.79403
H	5.36824	-3.57514	-5.21418
C	-3.95587	0.07391	-2.51138
C	-5.27157	-0.10946	-3.30970
C	-3.26159	1.38967	-2.94011
H	-3.28216	-0.74086	-2.79567
C	-5.04090	-0.04810	-4.82694
H	-5.98099	0.67851	-3.01713
H	-5.74680	-1.06063	-3.03722
C	-3.03905	1.45423	-4.45990
H	-3.87382	2.25084	-2.63690
H	-2.30413	1.47023	-2.41416
C	-4.34848	1.25934	-5.23689
H	-5.99772	-0.15716	-5.35455
H	-4.41505	-0.89914	-5.13250
H	-2.58082	2.41655	-4.72586
H	-2.32121	0.67775	-4.75435
H	-5.02442	2.10440	-5.03467
H	-4.15492	1.26515	-6.31731
C	-3.81427	-2.29196	2.10085
C	-2.94638	-1.88892	3.31580
C	-5.10264	-3.00785	2.57538
H	-3.24244	-3.03548	1.53701
C	-2.62754	-3.09960	4.20674
H	-3.47762	-1.13654	3.91588
H	-2.02193	-1.41814	2.96446
C	-4.78226	-4.21537	3.47032
H	-5.73216	-2.29968	3.13277
H	-5.68986	-3.32521	1.70421
C	-3.90496	-3.81771	4.66662
H	-2.03564	-2.78069	5.07452
H	-1.99730	-3.80561	3.64460
H	-4.25708	-4.97713	2.87475
H	-5.71328	-4.68164	3.81832
H	-4.47710	-3.14771	5.32587
H	-3.65265	-4.70290	5.26497
P	-0.01719	-0.76651	-0.19591
O	-0.49802	0.03145	-1.36362
O	0.41279	0.04413	1.08048
H	-0.17866	-0.53060	-2.98101
H	0.44401	1.04725	0.91290
Cl	0.05775	-0.95319	-4.21591
O	0.39783	2.59939	0.62368
C	0.97735	3.05254	-0.64314
C	-0.91106	3.13608	0.24473
C	-0.31419	3.82844	-1.00709
H	1.19633	2.20418	-1.29650
H	1.87626	3.64847	-0.46577
H	-1.30232	3.79279	1.02661
H	-1.61757	2.33013	0.02750
H	-0.76910	3.48872	-1.94021
C	-0.23594	5.33520	-0.97992
C	0.32187	6.01141	0.11656
C	-0.72152	6.08985	-2.05419
C	0.39036	7.40349	0.13542
H	0.70586	5.44252	0.96093
C	-0.65416	7.48449	-2.03818
H	-1.15582	5.58030	-2.91137
C	-0.09806	8.14547	-0.94305
H	0.82573	7.91014	0.99277
H	-1.03628	8.05227	-2.88243
H	-0.04438	9.23067	-0.92842
C	-5.96587	2.22873	1.58962
C	-5.15601	3.54551	1.53444
C	-7.37066	2.43741	0.97867
H	-6.10956	1.98390	2.65312
C	-5.90543	4.70934	2.20103
H	-4.95202	3.79929	0.48411
H	-4.17990	3.39453	2.01363
C	-8.11807	3.60164	1.64728
H	-7.27148	2.64169	-0.09701
H	-7.95005	1.50974	1.06549
C	-7.30260	4.90221	1.59341
H	-5.31956	5.63323	2.11181

H	-6.00475	4.50609	3.27776
H	-9.09538	3.74421	1.16840
H	-8.32084	3.34550	2.69794
H	-7.83596	5.70815	2.11367
H	-7.20000	5.22116	0.54530

There are no imaginary frequencies.

SCF energy: -4055.691093 hartree
zero-point correction: +1.540205 hartree
enthalpy correction: +1.616157 hartree
free energy correction: +1.419769 hartree
quasiharmonic free energy correction: +1.449102 hartree

RC_B4

C	0.13540	-4.42936	-0.82808
O	-1.10338	-1.82826	0.29704
O	1.25218	-1.55307	-0.72752
C	1.84611	-2.57356	0.02916
C	1.28335	-3.84848	-0.00259
C	3.02185	-2.29553	0.75408
C	1.84843	-4.85599	0.79714
C	3.59478	-3.35598	1.47460
C	3.00712	-4.61938	1.52646
H	4.51799	-3.16987	2.01380
H	3.45431	-5.40596	2.12910
C	-1.75811	-2.56706	-0.70422
C	-1.10071	-3.65280	-1.27142
C	-3.05336	-2.18443	-1.10031
C	-1.66168	-4.27047	-2.39948
C	-3.62719	-2.90582	-2.16049
C	-2.92851	-3.90521	-2.84135
H	-4.63483	-2.65009	-2.47225
H	-3.37940	-4.39313	-3.70183
C	1.02614	-6.12262	0.72384
H	1.51049	-6.87530	0.08584
H	0.88076	-6.58771	1.70545
C	-0.29044	-5.62115	0.09960
H	-0.94867	-5.23584	0.88723
H	-0.84004	-6.39565	-0.44339
C	-0.70280	-5.29354	-2.97188
H	-1.04929	-6.31964	-2.78632
H	-0.58886	-5.19132	-4.05689
C	0.60946	-4.99253	-2.20884
H	1.17470	-4.21439	-2.73403
H	1.25933	-5.86689	-2.10299
C	3.70747	-0.95673	0.75505
C	3.73385	-0.16115	1.92902
C	4.42433	-0.53800	-0.39448
C	4.47788	1.02580	1.91882
C	5.14383	0.66106	-0.34590
C	5.19050	1.45904	0.80001
H	4.51023	1.63417	2.81921
H	5.70103	0.96866	-1.22650
C	-3.81534	-1.08735	-0.41415
C	-4.19116	-1.23268	0.94659
C	-4.21562	0.07428	-1.12768
C	-4.94102	-0.21985	1.55604
C	-4.96731	1.05040	-0.46191
C	-5.34055	0.93137	0.87865
H	-5.23202	-0.33664	2.59741
H	-5.27746	1.93188	-1.01596
C	3.01326	-0.56005	3.21554
C	3.99066	-1.12249	4.27851
C	2.19672	0.58891	3.85396
H	2.30013	-1.35511	2.97092
C	3.24703	-1.60473	5.53461
H	4.58214	-1.94351	3.85733
H	4.70822	-0.33498	4.55205
C	1.42358	0.10096	5.08872
H	1.51072	1.02029	3.12033
H	2.87244	1.39849	4.16404
C	2.36826	-0.49975	6.13965
H	3.96641	-1.96961	6.27959
H	2.61419	-2.46335	5.26540
H	0.85067	0.93018	5.52401
H	0.68944	-0.65667	4.77807
H	1.79631	-0.89261	6.99038
H	3.01417	0.29664	6.53921
C	6.00327	2.74261	0.84667
C	5.52262	3.79205	-0.18173
C	7.51851	2.48249	0.67562
H	5.86264	3.18226	1.84602
C	6.34252	5.08918	-0.10481
H	4.45796	4.00520	-0.01866
H	5.60238	3.37107	-1.19418
C	8.33712	3.78052	0.75088
H	7.85670	1.77186	1.44022
H	7.69347	1.99863	-0.29606
C	7.84554	4.81900	-0.26808
H	6.16636	5.57130	0.86851
H	5.99653	5.79692	-0.86906
H	8.25569	4.20189	1.76412
H	9.40079	3.56211	0.59047
H	8.41330	5.75267	-0.16545
H	8.03758	4.44632	-1.28533
C	4.51263	-1.38726	-1.65895
C	4.15475	-0.61403	-2.94773
C	5.90936	-2.04262	-1.79439
H	3.79167	-2.20673	-1.57702
C	4.24161	-1.51744	-4.18726
H	4.84204	0.23371	-3.07871
H	3.14613	-0.19571	-2.86094
C	5.99893	-2.93936	-3.03904
H	6.67431	-1.25471	-1.85399
H	6.13280	-2.62349	-0.89015
C	5.62408	-2.17344	-4.31653
H	4.00686	-0.93589	-5.08735

H	3.47067	-2.29852	-4.11734
H	5.31583	-3.79311	-2.91670
H	7.00956	-3.35968	-3.12648
H	6.37870	-1.39454	-4.50401
H	5.64893	-2.84588	-5.18402
C	-3.89925	0.30642	-2.60483
C	-5.17447	0.16676	-3.47461
C	-3.22576	1.67327	-2.87626
H	-3.18919	-0.45903	-2.93410
C	-4.88279	0.37497	-4.96793
H	-5.91652	0.90787	-3.14326
H	-5.63572	-0.81580	-3.31205
C	-2.94355	1.88692	-4.37279
H	-3.87226	2.48692	-2.51823
H	-2.29297	1.72541	-2.30391
C	-4.21348	1.73232	-5.22199
H	-5.81312	0.29199	-5.54528
H	-4.22009	-0.42732	-5.32380
H	-2.50313	2.88124	-4.52775
H	-2.19082	1.16054	-4.70599
H	-4.92262	2.53616	-4.97121
H	-3.97495	1.84675	-6.28729
C	-3.85182	-2.46231	1.78429
C	-3.01005	-2.10946	3.03358
C	-5.11501	-3.25667	2.19653
H	-3.24806	-3.14364	1.17707
C	-2.64906	-3.36333	3.84396
H	-3.57804	-1.42209	3.67658
H	-2.10297	-1.57899	2.72594
C	-4.75316	-4.50828	3.01258
H	-5.77614	-2.61287	2.79376
H	-5.68274	-3.53783	1.30028
C	-3.90087	-4.15887	4.24188
H	-2.07646	-3.08080	4.73702
H	-1.98746	-4.00471	3.24199
H	-4.19347	-5.20663	2.37236
H	-5.66755	-5.03318	3.31864
H	-4.50349	-3.55733	4.93898
H	-3.61956	-5.07254	4.78166
P	-0.03122	-0.72309	-0.19859
O	-0.46791	0.19637	-1.29159
O	0.32288	-0.05524	1.17999
H	-0.00376	-0.08307	-2.93751
H	0.38271	0.95865	1.11788
Cl	0.34789	-0.27193	-4.20283
O	0.37569	2.53277	0.98512
C	1.00871	3.09310	-0.21087
C	-0.91172	3.12370	0.61436
C	-0.27435	3.88130	-0.57830
H	1.27963	2.30450	-0.91719
H	1.88579	3.68738	0.05905
H	-1.30211	3.74143	1.42811
H	-1.63490	2.35179	0.33656
H	-0.69328	3.58035	-1.54101
C	-0.20965	5.38561	-0.48246
C	0.29893	6.01802	0.66295
C	-0.65781	6.18279	-1.54229
C	0.35608	7.40846	0.74372
H	0.65387	5.41718	1.49794
C	-0.60164	7.57580	-1.46455
H	-1.05350	5.70771	-2.43710
C	-0.09457	8.19285	-0.32101
H	0.75330	7.88050	1.63851
H	-0.95400	8.17676	-2.29869
H	-0.04963	9.27673	-0.25829
C	-6.15430	2.00544	1.58133
C	-5.40317	3.35496	1.66363
C	-7.54793	2.20682	0.94269
H	-6.31910	1.66491	2.61500
C	-6.22351	4.42354	2.40245
H	-5.18119	3.70739	0.64597
H	-4.43505	3.20560	2.15910
C	-8.36691	3.27567	1.68267
H	-7.42459	2.50777	-0.10760
H	-8.08757	1.25157	0.92971
C	-7.60982	4.60939	1.76816
H	-5.67752	5.37571	2.41249
H	-6.34474	4.12277	3.45387
H	-9.33473	3.41792	1.18479
H	-8.58958	2.92065	2.70005
H	-8.19394	5.34315	2.33831
H	-7.49155	5.02321	0.75550

There are no imaginary frequencies.

SCF energy: -4055.690424 hartree
zero-point correction: +1.540226 hartree
enthalpy correction: +1.616241 hartree
free energy correction: +1.419116 hartree
quasiharmonic free energy correction: +1.449159 hartree

RC_C1

C	-0.30259	-4.60560	-0.08802
O	-1.35787	-1.76091	0.50041
O	1.01970	-1.84870	-0.50260
C	1.59904	-2.79868	0.35257
C	0.91371	-3.98562	0.59417
C	2.86120	-2.53755	0.91905
C	1.41433	-4.87335	1.55923
C	3.37325	-3.50332	1.80150
C	2.64709	-4.64062	2.15847
H	4.35502	-3.33631	2.23338
H	3.04934	-5.33583	2.89116
C	-1.98683	-2.57592	-0.45484
C	-1.43106	-3.81820	-0.74994
C	-3.18216	-2.13171	-1.05380
C	-2.00164	-4.58674	-1.77801
C	-3.76734	-2.97588	-2.01085

C	-3.17217	-4.17509	-2.40376
H	-4.70371	-2.66786	-2.46442
H	-3.62641	-4.77914	-3.18529
C	0.44016	-6.00835	1.79260
H	0.27440	-6.20243	2.85843
H	0.80555	-6.94813	1.35557
C	-0.83444	-5.50964	1.07492
H	-1.42888	-4.89223	1.75837
H	-1.47538	-6.32020	0.71465
C	-1.17149	-5.82314	-2.04358
H	-1.65833	-6.72498	-1.64681
H	-1.01098	-5.99802	-3.11353
C	0.13789	-5.51201	-1.28841
H	0.81176	-4.93785	-1.93512
H	0.67501	-6.40663	-0.95930
C	3.66369	-1.31146	0.59076
C	4.17719	-1.13244	-0.72046
C	3.97388	-0.36300	1.59878
C	4.97317	-0.01478	-0.99228
C	4.77965	0.73433	1.26553
C	5.29129	0.93363	-0.01694
H	5.36947	0.10792	-1.99676
H	5.02464	1.45906	2.03845
C	-3.85023	-0.84245	-0.66903
C	-4.44484	-0.72239	0.61126
C	-3.94658	0.23269	-1.59221
C	-5.08840	0.47379	0.94959
C	-4.60534	1.40259	-1.19650
C	-5.17746	1.55229	0.07018
H	-5.54484	0.56531	1.93217
H	-4.67994	2.22173	-1.90591
C	3.95384	-2.13989	-1.84476
C	3.25832	-1.52067	-3.07954
C	5.27399	-2.83287	-2.26261
H	3.29537	-2.93276	-1.47692
C	3.03021	-2.56677	-4.18187
H	2.30535	-1.07364	-2.77633
H	3.87774	-0.70691	-3.48269
C	5.04278	-3.87554	-3.36738
H	5.73543	-3.30396	-1.38528
H	5.98782	-2.07724	-2.62000
C	4.33887	-3.26164	-4.58655
H	2.56300	-2.09430	-5.05567
H	2.31619	-3.32206	-3.81971
H	5.99911	-4.32539	-3.66469
H	4.42500	-4.69364	-2.96785
H	4.14439	-4.03312	-5.34302
H	5.00804	-2.52523	-5.05639
C	6.18231	2.12643	-0.32293
C	5.60067	3.04277	-1.42369
C	7.62285	1.69887	-0.69051
H	6.24946	2.72860	0.59584
C	6.50700	4.25217	-1.70223
H	4.59807	3.37957	-1.12973
H	5.47481	2.46371	-2.34972
C	8.52767	2.90890	-0.97039
H	8.04134	1.08734	0.11869
H	7.59078	1.05466	-1.58102
C	7.93649	3.81795	-2.05782
H	6.08071	4.86127	-2.50973
H	6.53596	4.89515	-0.81000
H	8.65280	3.48868	-0.04364
H	9.52980	2.56803	-1.26087
H	8.57528	4.69777	-2.20770
H	7.92242	3.27487	-3.01466
C	3.49384	-0.48953	3.04244
C	4.65815	-0.83927	4.00274
C	2.76230	0.77293	3.55539
H	2.76879	-1.30844	3.09293
C	4.17350	-1.01668	5.45004
H	5.40697	-0.03473	3.96410
H	5.17080	-1.74823	3.66274
C	2.26442	0.58652	4.99688
H	3.44118	1.63711	3.52462
H	1.92338	0.99730	2.89124
C	3.41238	0.22061	5.94845
H	5.02710	-1.23156	6.10657
H	3.51124	-1.89359	5.50238
H	1.50606	-0.20916	5.01638
H	1.75925	1.49885	5.33709
H	4.11014	1.06895	6.01744
H	3.02975	0.04826	6.96286
C	-3.41438	0.14491	-3.02220
C	-4.56627	-0.08347	-4.03513
C	-2.59076	1.37414	-3.47135
H	-2.74406	-0.71942	-3.08371
C	-4.04412	-0.25661	-5.46963
H	-5.25003	0.77719	-3.99380
H	-5.16211	-0.95696	-3.74481
C	-2.04798	1.19479	-4.89829
H	-3.21857	2.27589	-3.44779
H	-1.76429	1.54731	-2.77664
C	-3.17824	0.93388	-5.90466
H	-4.88626	-0.38869	-6.16172
H	-3.44653	-1.17859	-5.52530
H	-1.47379	2.08292	-5.19294
H	-1.34381	0.35013	-4.91244
H	-3.81009	1.83187	-5.97761
H	-2.76636	0.76014	-6.90733
C	-4.48376	-1.87183	1.61402
C	-3.89643	-1.50419	2.99503
C	-5.91977	-2.42962	1.77380
H	-3.87695	-2.69491	1.22288
C	-3.93633	-2.70056	3.95842
H	-4.46710	-0.67443	3.43460
H	-2.86978	-1.14302	2.87584
C	-5.96209	-3.62084	2.74349
H	-6.58009	-1.63315	2.14572
H	-6.31251	-2.72449	0.79212
C	-5.35806	-3.26177	4.10917

H	-3.53666	-2.40501	4.93688
H	-3.27339	-3.49357	3.57919
H	-5.39848	-4.46000	2.30860
H	-6.99607	-3.97048	2.86278
H	-5.99301	-2.50703	4.59708
H	-5.35592	-4.14026	4.76773
P	-0.09272	-0.83820	0.10294
O	0.33891	-0.05309	1.29544
O	-0.47805	-0.02638	-1.18711
H	-0.60003	0.79627	2.44612
H	-0.25127	0.96418	-1.12249
Cl	-1.24549	1.58780	3.29703
O	0.09366	2.50126	-1.02311
C	1.28978	2.88954	-0.26996
C	-0.75251	3.34015	-0.17262
C	0.47441	3.87159	0.61077
H	2.03073	3.34307	-0.93458
H	1.71945	2.03412	0.25706
H	-1.29469	4.07489	-0.77446
H	-1.45299	2.73743	0.41188
H	0.45194	3.57212	1.66066
C	0.79428	5.34110	0.49373
C	1.02193	6.10823	1.64271
C	0.87220	5.97166	-0.75797
C	1.31999	7.46908	1.54850
H	0.96306	5.63408	2.61968
C	1.16934	7.33019	-0.85553
H	0.69879	5.39534	-1.66471
C	1.39479	8.08421	0.29880
H	1.49285	8.04676	2.45272
H	1.22514	7.80110	-1.83354
H	1.62654	9.14317	0.22293
C	-5.87781	2.83498	0.48715
C	-4.89410	4.02124	0.62338
C	-7.04599	3.21345	-0.45102
H	-6.30847	2.66032	1.48475
C	-5.60555	5.30477	1.07983
H	-4.40994	4.19858	-0.34852
H	-4.09617	3.75535	1.32806
C	-7.75689	4.49546	0.01008
H	-6.66101	3.36293	-1.46988
H	-7.75762	2.38011	-0.50746
C	-6.77324	5.66697	0.15064
H	-4.88768	6.13345	1.13196
H	-5.98829	5.16025	2.10106
H	-8.55956	4.75298	-0.69299
H	-8.24052	4.31126	0.98102
H	-7.29347	6.55883	0.52306
H	-6.37785	5.92770	-0.84268

There are no imaginary frequencies.

SCF energy: -4055.692380 hartree
zero-point correction: +1.540330 hartree
enthalpy correction: +1.616267 hartree
free energy correction: +1.420574 hartree
quasiharmonic free energy correction: +1.449236 hartree

RC_C3

C	1.01501	-4.54494	0.25207
O	1.63709	-1.61722	-0.52809
O	-0.62070	-1.96014	0.67439
C	-1.13539	-3.01268	-0.09617
C	-0.32517	-4.11816	-0.34270
C	-2.45757	-2.93578	-0.57379
C	-0.78334	-5.11101	-1.22317
C	-2.91085	-4.00540	-1.36394
C	-2.07862	-5.06506	-1.72588
H	-3.93463	-3.98068	-1.72315
H	-2.44555	-5.84380	-2.38986
C	2.44838	-2.30319	0.39052
C	2.08713	-3.59133	0.77594
C	3.62052	-1.68138	0.86418
C	2.84278	-4.23491	1.76986
C	4.39602	-2.40329	1.78554
C	4.00142	-3.65151	2.26820
H	5.31822	-1.95690	2.14321
H	4.59889	-4.15864	3.02179
C	0.30573	-6.12646	-1.49376
H	0.40375	-6.35780	-2.56053
H	0.10437	-7.07844	-0.98293
C	1.55967	-5.43137	-0.91846
H	2.00410	-4.77777	-1.67806
H	2.33235	-6.13275	-0.58912
C	2.20520	-5.55115	2.15672
H	2.76395	-6.40358	1.74563
H	2.16738	-5.69486	3.24255
C	0.80303	-5.43896	1.52163
H	0.12485	-4.92042	2.20942
H	0.35511	-6.40752	1.27981
C	-3.38147	-1.79308	-0.26286
C	-3.82721	-1.57645	1.06524
C	-3.87847	-0.97098	-1.30988
C	-4.74805	-0.55015	1.31303
C	-4.80979	0.02771	-1.00146
C	-5.26188	0.26064	0.30022
H	-5.09533	-0.39083	2.33156
H	-5.19775	0.63990	-1.81050
C	4.05822	-0.32214	0.40008
C	4.47154	-0.13801	-0.94235
C	4.10766	0.77107	1.30602
C	4.88700	1.13329	-1.35495
C	4.53971	2.01611	0.83566
C	4.92251	2.22750	-0.49155
H	5.20254	1.27454	-2.38563
H	4.58045	2.84892	1.53208
C	-3.39491	-2.44980	2.23891
C	-2.68864	-1.64663	3.35600

C	-4.57869	-3.25714	2.82537
H	-2.67298	-3.18796	1.87544
C	-2.23999	-2.55654	4.50958
H	-1.82771	-1.11507	2.93633
H	-3.37440	-0.88280	3.75002
C	-4.12731	-4.16511	3.97991
H	-5.04507	-3.85493	2.03183
H	-5.35261	-2.56561	3.18775
C	-3.41079	-3.36955	5.08124
H	-1.77152	-1.95541	5.29964
H	-1.46368	-3.24565	4.14402
H	-4.99108	-4.69993	4.39598
H	-3.44476	-4.93420	3.58804
H	-3.05766	-4.04556	5.87089
H	-4.12873	-2.68366	5.55581
C	-6.30656	1.32200	0.60737
C	-7.69542	0.93597	0.04315
C	-5.90812	2.73301	0.11946
H	-6.40696	1.37387	1.70243
C	-8.76520	1.98686	0.37760
H	-7.98913	-0.04677	0.43296
H	-7.61970	0.82638	-1.04841
C	-6.97886	3.78216	0.45656
H	-4.94678	3.02342	0.56098
H	-5.75586	2.71289	-0.96888
C	-8.35350	3.38634	-0.10221
H	-9.72589	1.69756	-0.06766
H	-8.92137	2.01011	1.46649
H	-7.04987	3.88826	1.54938
H	-6.67242	4.76213	0.06950
H	-9.11054	4.12649	0.18732
H	-8.31285	3.39408	-1.20176
C	-3.45843	-1.13428	-2.76907
C	-4.60291	-1.71345	-3.63817
C	-2.94135	0.17771	-3.40407
H	-2.62576	-1.84417	-2.80850
C	-4.15877	-1.93078	-5.09310
H	-5.45636	-1.02007	-3.61585
H	-4.96702	-2.65637	-3.21082
C	-2.48526	-0.04267	-4.85453
H	-3.73630	0.93727	-3.39548
H	-2.11583	0.56868	-2.80324
C	-3.60743	-0.64013	-5.71590
H	-4.99821	-2.31457	-5.68794
H	-3.37844	-2.70598	-5.11742
H	-1.62008	-0.72128	-4.86078
H	-2.13544	0.90500	-5.28234
H	-4.42370	0.09257	-5.80676
H	-3.24741	-0.83334	-6.73483
C	3.76017	0.63964	2.78836
C	5.03970	0.64639	3.66339
C	2.78744	1.72304	3.31020
H	3.26145	-0.32365	2.93965
C	4.72103	0.43971	5.15209
H	5.55577	1.60812	3.52799
H	5.74038	-0.12366	3.31830
C	2.45051	1.50462	4.79429
H	3.23748	2.71932	3.19621
H	1.87097	1.72019	2.71341
C	3.71525	1.48019	5.66467
H	5.64574	0.47917	5.74284
H	4.30307	-0.56816	5.29339
H	1.76556	2.28953	5.14081
H	1.91322	0.55140	4.90538
H	4.18488	2.47517	5.64647
H	3.45593	1.27677	6.71184
C	4.56406	-1.28654	-1.94239
C	3.78331	-1.03120	-3.25142
C	6.04066	-1.63358	-2.25659
H	4.12927	-2.18193	-1.48666
C	3.89562	-2.22493	-4.21248
H	4.17415	-0.13392	-3.75032
H	2.73326	-0.82432	-3.01930
C	6.15256	-2.82217	-3.22341
H	6.53451	-0.75601	-2.69782
H	6.57426	-1.85207	-1.32255
C	5.35997	-2.57652	-4.51584
H	3.35510	-2.00734	-5.14260
H	3.40007	-3.09922	-3.76287
H	5.76618	-3.72653	-2.72972
H	7.20758	-3.02089	-3.45370
H	5.82256	-1.74624	-5.07029
H	5.41476	-3.45673	-5.16985
P	0.30792	-0.84133	-0.04415
O	-0.32382	-0.15377	-1.20714
O	0.71156	0.04510	1.18969
H	0.35187	0.97128	-2.30332
H	0.23994	0.94733	1.21827
Cl	0.76169	1.94946	-3.10475
O	-0.51166	2.33059	1.26446
C	-1.85169	2.37920	0.67094
C	-0.05701	3.42209	0.40153
C	-1.48074	3.62373	-0.17647
H	-2.60880	2.52750	1.44536
H	-2.06479	1.47457	0.09644
H	0.34402	4.24517	0.99981
H	0.68790	3.07518	-0.31982
H	-1.52322	3.42972	-1.25049
C	-2.18734	4.91592	0.15036
C	-2.79326	5.66747	-0.86391
C	-2.25743	5.39263	1.46898
C	-3.45292	6.86355	-0.57322
H	-2.74567	5.31254	-1.89077
C	-2.91394	6.58695	1.76236
H	-1.79356	4.82448	2.27283
C	-3.51486	7.32713	0.74109
H	-3.91536	7.43271	-1.37535
H	-2.95695	6.94029	2.78931
H	-4.02642	8.25820	0.96957
C	5.37381	3.59141	-0.98581

C	4.25788	4.65670	-0.87940
C	6.65597	4.08643	-0.27690
H	5.61598	3.48626	-2.05422
C	4.71772	6.02179	-1.41366
H	3.95896	4.76169	0.17386
H	3.37037	4.31171	-1.42431
C	7.11411	5.45139	-0.81314
H	6.46505	4.16637	0.80310
H	7.45319	3.34178	-0.39585
C	5.99830	6.50221	-0.71417
H	3.91600	6.76170	-1.29221
H	4.90501	5.94153	-2.49475
H	8.00549	5.78851	-0.26831
H	7.41524	5.34293	-1.86576
H	6.33306	7.45510	-1.14401
H	5.77960	6.69751	0.34656

There are no imaginary frequencies.

SCF energy: -4055.693742 hartree
zero-point correction: +1.539990 hartree
enthalpy correction: +1.616052 hartree
free energy correction: +1.418251 hartree
quasiharmonic free energy correction: +1.448947 hartree

RC_C4

C	1.04846	-4.49212	0.15003
O	1.66965	-1.51536	-0.42039
O	-0.66627	-1.96692	0.58627
C	-1.09788	-2.97856	-0.28393
C	-0.24838	-4.05466	-0.52708
C	-2.37976	-2.89458	-0.86008
C	-0.61633	-5.00368	-1.49390
C	-2.74670	-3.92274	-1.74444
C	-1.86794	-4.94771	-2.09653
H	-3.73906	-3.89312	-2.18294
H	-2.16619	-5.69308	-2.82959
C	2.42695	-2.24079	0.51388
C	2.05947	-3.55192	0.80461
C	3.55302	-1.63151	1.10186
C	2.74702	-4.23582	1.82083
C	4.26590	-2.38909	2.04493
C	3.85381	-3.66339	2.43609
H	5.15299	-1.95152	2.49131
H	4.39928	-4.19991	3.20851
C	0.50760	-5.99013	-1.72573
H	0.69544	-6.16591	-2.79108
H	0.28118	-6.96915	-1.28090
C	1.69948	-5.31044	-1.01636
H	2.19266	-4.61383	-1.70420
H	2.45465	-6.01828	-0.66118
C	2.10333	-5.57803	2.09060
H	2.70705	-6.40138	1.68399
H	1.98302	-5.77658	3.16173
C	0.75346	-5.45232	1.35315
H	0.01518	-4.97731	2.00978
H	0.34215	-6.41348	1.03018
C	-3.35243	-1.79206	-0.55116
C	-3.91351	-1.68209	0.74563
C	-3.78037	-0.90574	-1.57589
C	-4.88032	-0.69681	0.98479
C	-4.75861	0.05056	-1.27826
C	-5.32761	0.17565	-0.00782
H	-5.31804	-0.62071	1.97769
H	-5.09033	0.71525	-2.07109
C	4.02142	-0.25370	0.73028
C	4.54824	-0.01758	-0.56579
C	4.00359	0.79847	1.68173
C	5.01464	1.26106	-0.88666
C	4.49542	2.05444	1.30380
C	4.99617	2.31614	0.02833
H	5.41339	1.43414	-1.88246
H	4.48819	2.86235	2.03147
C	-3.55877	-2.62934	1.88791
C	-2.96896	-1.89413	3.11404
C	-4.76976	-3.49601	2.31089
H	-2.78993	-3.32503	1.53685
C	-2.60530	-2.87474	4.23973
H	-2.08582	-1.32275	2.80783
H	-3.70176	-1.16853	3.49555
C	-4.40413	-4.47236	3.43975
H	-5.14960	-4.04566	1.44019
H	-5.58860	-2.84405	2.64693
C	-3.80601	-3.73979	4.64978
H	-2.21880	-2.32297	5.10642
H	-1.78753	-3.52761	3.89864
H	-5.29022	-5.04656	3.74045
H	-3.67322	-5.20353	3.06275
H	-3.51117	-4.46043	5.42368
H	-4.57730	-3.09680	5.10018
C	-6.41132	1.20051	0.28672
C	-7.70000	0.93729	-0.52789
C	-5.93668	2.65626	0.07405
H	-6.67574	1.09860	1.35040
C	-8.80303	1.95697	-0.20422
H	-8.05386	-0.08332	-0.33514
H	-7.46380	0.98601	-1.60064
C	-7.04026	3.67488	0.39791
H	-5.05237	2.85371	0.69229
H	-5.62023	2.78537	-0.97099
C	-8.31796	3.40007	-0.40802
H	-9.68769	1.76006	-0.82348
H	-9.12016	1.82694	0.84136
H	-7.27327	3.62521	1.47212
H	-6.67395	4.69140	0.20689
H	-9.10638	4.11015	-0.12698
H	-8.11465	3.56556	-1.47669
C	-3.23590	-0.95738	-3.00170

C	-4.28714	-1.49708	-4.00324
C	-2.70287	0.40651	-3.49900
H	-2.38447	-1.64581	-3.01708
C	-3.71901	-1.60073	-5.42749
H	-5.15888	-0.82644	-4.00482
H	-4.65874	-2.47598	-3.67473
C	-2.11993	0.29738	-4.91611
H	-3.51612	1.14650	-3.50801
H	-1.94253	0.77261	-2.80442
C	-3.14937	-0.25877	-5.91021
H	-4.49722	-1.95649	-6.11574
H	-2.92076	-2.35777	-5.44083
H	-1.24032	-0.36208	-4.89356
H	-1.75894	1.27929	-5.24618
H	-3.97301	0.46297	-6.02010
H	-2.69989	-0.37249	-6.90529
C	3.49885	0.61893	3.11229
C	4.66561	0.56703	4.13098
C	2.49248	1.70545	3.55900
H	2.96935	-0.33828	3.16923
C	4.16504	0.30813	5.56081
H	5.20983	1.52224	4.09869
H	5.38940	-0.20445	3.84170
C	1.97112	1.43615	4.97913
H	2.97485	2.69292	3.54343
H	1.65686	1.75251	2.85544
C	3.11945	1.34634	5.99406
H	5.01169	0.30497	6.25998
H	3.71837	-0.69624	5.60712
H	1.26463	2.22325	5.27351
H	1.40555	0.49292	4.98226
H	3.60343	2.33104	6.07928
H	2.73167	1.10252	6.99174
C	4.69366	-1.11879	-1.61212
C	3.96912	-0.79815	-2.93931
C	6.18255	-1.45125	-1.87918
H	4.24104	-2.03473	-1.21868
C	4.12636	-1.93885	-3.95670
H	4.37807	0.12499	-3.37264
H	2.90936	-0.60519	-2.74258
C	6.33794	-2.58781	-2.90145
H	6.69602	-0.55355	-2.25216
H	6.67494	-1.71924	-0.93544
C	5.60328	-2.27372	-4.21291
H	3.62723	-1.67142	-4.89692
H	3.61298	-2.83603	-3.57760
H	5.93124	-3.51634	-2.47325
H	7.40233	-2.77547	-3.09479
H	6.08798	-1.41490	-4.70114
H	5.68945	-3.11774	-4.90982
P	0.29344	-0.79224	0.01303
O	-0.26257	-0.03687	-1.14639
O	0.58729	0.01562	1.32956
H	0.46423	1.17626	-2.10630
H	0.11585	0.91664	1.36840
Cl	0.90220	2.21835	-2.80545
O	-0.66191	2.28744	1.44651
C	-1.97725	2.33986	0.80181
C	-0.21420	3.45987	0.69315
C	-1.63373	3.68603	0.11317
H	-2.77208	2.36458	1.55168
H	-2.11836	1.49648	0.12144
H	0.16435	4.23173	1.36898
H	0.54466	3.19063	-0.04682
H	-1.65706	3.62579	-0.97715
C	-2.38666	4.90401	0.58902
C	-3.01262	5.75564	-0.32930
C	-2.48385	5.20677	1.95652
C	-3.71871	6.88066	0.10258
H	-2.94474	5.53601	-1.39229
C	-3.18728	6.32914	2.39069
H	-2.00542	4.55731	2.68681
C	-3.80810	7.17075	1.46424
H	-4.19563	7.53026	-0.62665
H	-3.25116	6.54738	3.45352
H	-4.35612	8.04594	1.80259
C	5.50756	3.69898	-0.34002
C	7.01320	3.69699	-0.69299
C	4.69039	4.34286	-1.48421
H	5.38506	4.34025	0.54644
C	7.52210	5.10403	-1.04266
H	7.18195	3.02747	-1.54866
H	7.58712	3.27980	0.14423
C	5.20168	5.74923	-1.83249
H	4.75018	3.70323	-2.37579
H	3.63002	4.37792	-1.20578
C	6.69916	5.73879	-2.17363
H	8.58325	5.06030	-1.32054
H	7.46083	5.74306	-0.14891
H	4.62246	6.16055	-2.66913
H	5.03145	6.41991	-0.97669
H	7.05219	6.75832	-2.37571
H	6.85422	5.16448	-3.09917

There are no imaginary frequencies.

SCF energy: -4055.693320 hartree
zero-point correction: +1.539664 hartree
enthalpy correction: +1.615842 hartree
free energy correction: +1.417680 hartree
quasiharmonic free energy correction: +1.448541 hartree

RC_D1

C	0.41596	-4.06158	1.34375
O	-1.02329	-1.37015	0.87764
O	1.37300	-1.49294	-0.08911
C	2.08399	-2.01881	1.00489
C	1.54149	-3.09466	1.69873

C	3.31934	-1.44432	1.36016	H	6.44553	-4.57489	-2.43976
C	2.14236	-3.49661	2.90149	H	4.94789	-4.78036	-1.53750
C	3.94332	-1.95234	2.51164	H	4.50897	-5.10362	-3.95802
C	3.34605	-2.93163	3.30807	H	5.21438	-3.53251	-4.32597
H	4.90691	-1.54264	2.79750	C	6.00271	2.67206	-1.83419
H	3.82677	-3.25083	4.22933	C	5.23809	3.02953	-3.12943
C	-1.48638	-2.54021	0.26115	C	7.46530	2.29188	-2.16404
C	-0.77756	-3.72561	0.44939	H	6.03870	3.58393	-1.21860
C	-2.68381	-2.49815	-0.47982	C	5.95119	4.12941	-3.93111
C	-1.20927	-4.88395	-0.21787	H	4.21565	3.34003	-2.87883
C	-3.11929	-3.70083	-1.05991	H	5.14344	2.13001	-3.75431
C	-2.38176	-4.88006	-0.96346	C	8.17644	3.39304	-2.96558
H	-4.05549	-3.69561	-1.60855	H	8.00861	2.08378	-1.23374
H	-2.72604	-5.78247	-1.46243	H	7.47395	1.35733	-2.74353
C	1.29802	-4.55003	3.58734	C	7.40551	3.74790	-4.24546
H	1.14453	-4.32951	4.64964	H	5.94045	5.06462	-3.35127
H	1.76966	-5.54119	3.53587	H	5.40140	4.33344	-4.85914
C	-0.02037	-4.50729	2.77906	H	8.27000	4.29289	-2.33934
H	-0.68826	-3.74660	3.19847	H	9.19889	3.07789	-3.21083
H	-0.55745	-5.46098	2.77571	H	7.90702	4.56587	-4.77854
C	-0.24188	-6.02371	0.00706	H	7.41329	2.88158	-4.92380
H	-0.64273	-6.75001	0.72812	C	3.85937	1.31023	2.51221
H	-0.02606	-6.57940	-0.91256	C	5.12375	1.44714	3.39802
C	0.99536	-5.29689	0.56975	C	3.02585	2.61228	2.58275
H	1.61722	-4.93332	-0.25668	H	3.23803	0.51938	2.94498
H	1.62280	-5.92973	1.20433	C	4.77891	1.83178	4.84443
C	3.97714	-0.37299	0.53832	H	5.78221	2.21448	2.96542
C	4.40467	-0.66548	-0.78504	H	5.69798	0.51174	3.38175
C	4.23074	0.91100	1.08517	C	2.68643	2.99773	4.03164
C	5.04972	0.32815	-1.52764	H	3.58232	3.43847	2.11840
C	4.88475	1.86275	0.29083	H	2.10659	2.47868	2.00308
C	5.29753	1.60363	-1.01510	C	3.94732	3.12094	4.89832
H	5.37818	0.09211	-2.53630	H	5.70057	1.94430	5.43082
H	5.08279	2.84669	0.70854	H	4.20839	1.01479	5.31006
C	-3.53508	-1.26762	-0.63247	H	2.02422	2.23466	4.46232
C	-4.28780	-0.79844	0.47214	H	2.12203	3.93914	4.03972
C	-3.68916	-0.64911	-1.90186	H	4.56016	3.96129	4.53743
C	-5.17685	0.26710	0.28134	H	3.67580	3.35551	5.93583
C	-4.59888	0.40788	-2.03168	C	-2.94172	-1.12320	-3.14794
C	-5.36003	0.88038	-0.95822	C	-3.86783	-1.91964	-4.10197
H	-5.76990	0.61373	1.12396	C	-2.26497	0.01836	-3.94320
H	-4.72898	0.86404	-3.00930	H	-2.14112	-1.79850	-2.82669
C	4.24913	-2.04200	-1.42600	C	-3.10270	-2.46759	-5.31667
C	3.44443	-2.00325	-2.74599	H	-4.67709	-1.25899	-4.44617
C	5.61954	-2.72688	-1.65022	H	-4.35335	-2.74169	-3.56345
H	3.69535	-2.68732	-0.73748	C	-1.47963	-0.52822	-5.14604
C	3.28706	-3.40594	-3.35318	H	-3.02717	0.71961	-4.31127
H	2.46272	-1.55351	-2.56210	H	-1.60037	0.59058	-3.28998
H	3.95816	-1.35793	-3.47262	C	-2.37815	-1.35054	-6.08125
C	5.45887	-4.12769	-2.26130	H	-3.79211	-3.00135	-5.98405
H	6.16104	-2.78699	-0.69749	H	-2.36581	-3.20818	-4.97214
H	6.23444	-2.10660	-2.31776	H	-1.01536	0.30038	-5.69645
C	4.64693	-4.08810	-3.56426	H	-0.65659	-1.15938	-4.78043
H	2.73960	-3.34426	-4.30275	H	-3.12441	-0.68496	-6.54091
H	2.67244	-4.02413	-2.68108	H	-1.78856	-1.77325	-6.90513

C	-4.24658	-1.47303	1.83985
C	-4.02981	-0.49004	3.01192
C	-5.52225	-2.31975	2.07574
H	-3.40252	-2.16915	1.85920
C	-3.98491	-1.22601	4.35988
H	-4.84368	0.24804	3.03880
H	-3.09928	0.06797	2.85961
C	-5.48145	-3.04784	3.42798
H	-6.40297	-1.66211	2.03963
H	-5.64107	-3.04231	1.25802
C	-5.24696	-2.07076	4.58927
H	-3.85491	-0.50174	5.17363
H	-3.09897	-1.87685	4.38469
H	-4.67059	-3.79128	3.41233
H	-6.41364	-3.60774	3.58025
H	-6.11786	-1.40404	4.68078
H	-5.17314	-2.61824	5.53799
P	0.16402	-0.47126	0.24579
O	0.46499	0.62546	1.21526
O	-0.24720	-0.04745	-1.20924
H	0.09173	0.40697	2.89948
H	-0.38218	0.95534	-1.32674
Cl	-0.21136	0.26880	4.18429
O	-0.64112	2.48753	-1.55085
C	0.19297	3.48313	-0.87315
C	-1.85041	3.06011	-0.96090
C	-1.05983	4.28646	-0.43819
H	0.75357	3.02606	-0.05375
H	0.87370	3.96574	-1.58039
H	-2.60974	3.23962	-1.72547
H	-2.25578	2.41038	-0.17893
H	-1.21113	5.14952	-1.09315
C	-1.21742	4.70735	1.00090
C	-1.03661	3.79548	2.05247
C	-1.55996	6.02964	1.31081
C	-1.19512	4.19956	3.37807
H	-0.76414	2.76441	1.84208
C	-1.71920	6.43661	2.63658
H	-1.70360	6.74773	0.50593
C	-1.53709	5.52159	3.67386
H	-1.04980	3.47544	4.17471
H	-1.98474	7.46744	2.85648
H	-1.66009	5.83541	4.70704
C	-6.37940	1.99655	-1.12464
C	-5.73710	3.34425	-1.52631
C	-7.50308	1.62230	-2.11990
H	-6.85588	2.14892	-0.14435
C	-6.78306	4.46160	-1.66358
H	-5.20926	3.22154	-2.48371
H	-4.98083	3.62537	-0.78232
C	-8.54783	2.74096	-2.25281
H	-7.06133	1.42051	-3.10625
H	-7.98065	0.68848	-1.79797
C	-7.89862	4.07612	-2.64606
H	-6.29756	5.39271	-1.98344
H	-7.22433	4.66441	-0.67658
H	-9.31030	2.45568	-2.98894
H	-9.07165	2.86295	-1.29309
H	-8.65550	4.86952	-2.69239
H	-7.47510	3.98826	-3.65784

There are no imaginary frequencies.

SCF energy: -4055.694710 hartree
zero-point correction: +1.540444 hartree
enthalpy correction: +1.616320 hartree
free energy correction: +1.421790 hartree
quasiharmonic free energy correction: +1.449081 hartree

RC_D2 (lowest-energy reactant-complex)

C	-0.49466	-3.61396	-2.17716
O	0.99021	-1.17596	-1.01063
O	-1.47027	-1.40198	-0.24036
C	-2.12085	-1.63135	-1.46771
C	-1.56349	-2.54010	-2.36054
C	-3.31175	-0.93602	-1.75280
C	-2.09029	-2.62300	-3.65890
C	-3.86683	-1.13152	-3.02815
C	-3.24398	-1.92398	-3.99456
H	-4.79537	-0.62345	-3.26886
H	-3.66699	-1.99642	-4.99332
C	1.37298	-2.47609	-0.65542
C	0.64298	-3.55168	-1.15848
C	2.51472	-2.66274	0.14857
C	0.99142	-4.85199	-0.75771
C	2.87122	-3.98617	0.45580
C	2.10779	-5.07552	0.03884
H	3.76497	-4.15155	1.04873
H	2.38878	-6.08397	0.33198
C	-1.23093	-3.52277	-4.52193
H	-0.99695	-3.06530	-5.48968
H	-1.73332	-4.47620	-4.73663
C	0.02791	-3.73005	-3.64725
H	0.74537	-2.92283	-3.83260
H	0.53583	-4.68097	-3.83624
C	0.00869	-5.86247	-1.30400
H	0.43751	-6.41722	-2.15037
H	-0.28762	-6.60730	-0.55670
C	-1.16371	-4.96858	-1.75384
H	-1.83117	-4.78091	-0.90457
H	-1.76339	-5.40640	-2.55721
C	-3.99949	-0.06485	-0.74152
C	-4.53151	-0.64890	0.43953
C	-4.18206	1.32181	-0.97605
C	-5.20409	0.16289	1.35778
C	-4.87519	2.07963	-0.02213
C	-5.38768	1.53224	1.15270
H	-5.60935	-0.29518	2.25601

H	-5.02174	3.14147	-0.20343
C	3.38583	-1.54280	0.64643
C	4.22462	-0.84888	-0.26253
C	3.46686	-1.25696	2.03403
C	5.12047	0.10609	0.23292
C	4.38837	-0.29494	2.47013
C	5.22826	0.39673	1.59519
H	5.77247	0.61839	-0.46915
H	4.46673	-0.08655	3.53459
C	-4.47082	-2.14656	0.72950
C	-3.77924	-2.47643	2.07262
C	-5.87837	-2.78958	0.67472
H	-3.88279	-2.63251	-0.05508
C	-3.72622	-3.99172	2.32399
H	-2.76969	-2.05100	2.07665
H	-4.32701	-1.99950	2.89770
C	-5.82143	-4.30362	0.93017
H	-6.33800	-2.58495	-0.30065
H	-6.52592	-2.31781	1.42742
C	-5.12302	-4.62726	2.25899
H	-3.26009	-4.19377	3.29719
H	-3.07910	-4.46175	1.56767
H	-6.83523	-4.72486	0.91931
H	-5.27447	-4.78834	0.10751
H	-5.05562	-5.71406	2.39933
H	-5.73303	-4.24271	3.09024
C	-6.11432	2.40232	2.16479
C	-5.34817	2.50052	3.50493
C	-7.56994	1.94499	2.41367
H	-6.16350	3.41913	1.74605
C	-6.07017	3.40693	4.51375
H	-4.33092	2.86821	3.31956
H	-5.23986	1.49318	3.93213
C	-8.29030	2.85345	3.42222
H	-8.11545	1.92094	1.46194
H	-7.56602	0.91400	2.79541
C	-7.51848	2.95199	4.74660
H	-6.07333	4.43980	4.13431
H	-5.51892	3.42623	5.46284
H	-8.39729	3.85986	2.99054
H	-9.30792	2.48259	3.60057
H	-8.02802	3.63905	5.43441
H	-7.51332	1.96641	5.23577
C	-3.69027	2.04033	-2.23153
C	-4.87671	2.44671	-3.14201
C	-2.82129	3.28178	-1.91526
H	-3.05629	1.35407	-2.80240
C	-4.40970	3.16405	-4.41749
H	-5.54890	3.10994	-2.57841
H	-5.47216	1.56180	-3.40173
C	-2.35941	3.99921	-3.19385
H	-3.39229	3.99059	-1.29920
H	-1.95486	2.96776	-1.32374
C	-3.54573	4.38915	-4.08657
H	-5.27944	3.45834	-5.01989
H	-3.82361	2.46536	-5.03216
H	-1.68660	3.33809	-3.75602
H	-1.77202	4.88740	-2.92725
H	-4.16409	5.13825	-3.56858
H	-3.18864	4.86341	-5.01002
C	2.62475	-1.98401	3.08129
C	3.46985	-3.00167	3.88916
C	1.90009	-1.03596	4.06617
H	1.84577	-2.54841	2.55670
C	2.61301	-3.78853	4.89281
H	4.26165	-2.46067	4.42767
H	3.98129	-3.69455	3.21058
C	1.02582	-1.82035	5.05732
H	2.63864	-0.45345	4.63521
H	1.28956	-0.31563	3.51506
C	1.84750	-2.85395	5.84049
H	3.24638	-4.47844	5.46588
H	1.89412	-4.41081	4.33962
H	0.53134	-1.12542	5.74846
H	0.22464	-2.33193	4.50447
H	2.56654	-2.32771	6.48629
H	1.19738	-3.43570	6.50679
C	4.25393	-1.15633	-1.75643
C	4.00835	0.08866	-2.63879
C	5.57683	-1.85262	-2.16137
H	3.44953	-1.86316	-1.98234
C	4.03467	-0.26546	-4.13330
H	4.77983	0.84571	-2.43813
H	3.04515	0.54074	-2.37822
C	5.60314	-2.19885	-3.65799
H	6.42281	-1.19086	-1.92585
H	5.71516	-2.75902	-1.55786
C	5.34511	-0.96094	-4.52958
H	3.88350	0.64084	-4.73232
H	3.18670	-0.92760	-4.36056
H	4.83071	-2.95417	-3.86644
H	6.56564	-2.65819	-3.91902
H	6.18124	-0.25503	-4.41094
H	5.32323	-1.24140	-5.59075
P	-0.21162	-0.38714	-0.26589
O	-0.40613	0.90801	-0.98635
O	0.10461	-0.30815	1.27042
H	-0.03515	1.01589	-2.67680
H	0.36021	0.62469	1.58845
Cl	0.27292	1.13176	-3.96347
O	0.77170	2.04738	2.12177
C	0.06512	3.24274	1.65608
C	2.05246	2.60120	1.68486
C	1.40541	3.98351	1.41373
H	-0.51093	3.02590	0.75274
H	-0.58745	3.63837	2.43976
H	2.79531	2.53930	2.48378
H	2.42360	2.08769	0.79265
H	1.61792	4.67711	2.23266
C	1.65750	4.66504	0.09266

C	1.40491	4.01369	-1.12467
C	2.16756	5.96914	0.06233
C	1.65741	4.65289	-2.33836
H	1.00369	3.00352	-1.13207
C	2.42158	6.61101	-1.15106
H	2.36789	6.48729	0.99804
C	2.16732	5.95352	-2.35501
H	1.45358	4.12720	-3.26694
H	2.81660	7.62366	-1.15345
H	2.36376	6.45087	-3.30114
C	6.25504	1.38610	2.12422
C	7.69586	0.83565	1.99238
C	6.15855	2.78320	1.47012
H	6.05823	1.51759	3.19950
C	8.73867	1.80982	2.56104
H	7.91005	0.64886	0.93014
H	7.76375	-0.13603	2.49737
C	7.19979	3.75629	2.04474
H	6.31269	2.69163	0.38596
H	5.14741	3.18906	1.60299
C	8.62500	3.19888	1.91591
H	9.74818	1.40356	2.41771
H	8.59197	1.90281	3.64757
H	7.12257	4.72743	1.53938
H	6.97819	3.93873	3.10707
H	9.34671	3.89032	2.36936
H	8.88900	3.12537	0.85040

There are no imaginary frequencies.

SCF energy: -4055.696127 hartree
zero-point correction: +1.540486 hartree
enthalpy correction: +1.616245 hartree
free energy correction: +1.423311 hartree
quasiharmonic free energy correction: +1.449119 hartree

RC_D3

C	0.30339	-4.09856	1.37158
O	-1.03698	-1.35927	0.88538
O	1.30499	-1.62290	-0.18533
C	2.04380	-2.14762	0.89089
C	1.48688	-3.17497	1.64378
C	3.31864	-1.61948	1.17026
C	2.12446	-3.56621	2.83100
C	3.97152	-2.11702	2.31018
C	3.36875	-3.04283	3.16473
H	4.96398	-1.74202	2.54005
H	3.87638	-3.35362	4.07436
C	-1.57922	-2.52480	0.32816
C	-0.91418	-3.73478	0.52074
C	-2.80766	-2.45049	-0.35765
C	-1.42635	-4.89111	-0.09069
C	-3.31965	-3.64787	-0.88349
C	-2.62971	-4.85545	-0.78456
H	-4.27925	-3.61684	-1.38921
H	-3.03471	-5.75516	-1.24101
C	1.26601	-4.55714	3.58881
H	1.17129	-4.29567	4.64864
H	1.69013	-5.57020	3.55034
C	-0.08501	-4.47935	2.83862
H	-0.69816	-3.67596	3.26210
H	-0.66329	-5.40713	2.89062
C	-0.50127	-6.06692	0.12646
H	-0.90099	-6.75309	0.88637
H	-0.35189	-6.65814	-0.78415
C	0.79116	-5.38152	0.61201
H	1.39131	-5.07182	-0.25168
H	1.41746	-6.02323	1.23871
C	3.98221	-0.61104	0.27736
C	4.32773	-0.97216	-1.05100
C	4.31805	0.68223	0.75792
C	4.96978	-0.03236	-1.86529
C	4.96418	1.57598	-0.10479
C	5.29396	1.24911	-1.42155
H	5.23746	-0.31288	-2.88137
H	5.21800	2.56350	0.27034
C	-3.61465	-1.18886	-0.50000
C	-4.30034	-0.66947	0.62533
C	-3.79637	-0.58598	-1.77328
C	-5.15041	0.43069	0.45215
C	-4.66548	0.50627	-1.88506
C	-5.36073	1.02923	-0.79005
H	-5.68924	0.81803	1.31355
H	-4.81700	0.95035	-2.86510
C	4.09913	-2.36878	-1.62293
C	3.25910	-2.36442	-2.92108
C	5.43924	-3.11060	-1.85017
H	3.54241	-2.96126	-0.89046
C	3.03980	-3.78855	-3.45579
H	2.29796	-1.87371	-2.73198
H	3.77146	-1.77203	-3.69222
C	5.21690	-4.53219	-2.38924
H	6.00475	-3.14399	-0.91020
H	6.05476	-2.54313	-2.56265
C	4.37043	-4.52531	-3.67045
H	2.46800	-3.75315	-4.39227
H	2.42480	-4.35380	-2.73887
H	6.18339	-5.01950	-2.57299
H	4.70624	-5.13364	-1.62225
H	4.18808	-5.55250	-4.01246
H	4.93394	-4.02489	-4.47228
C	5.97687	2.24362	-2.34598
C	7.34802	2.71450	-1.80985
C	5.07601	3.46188	-2.65766
H	6.16246	1.72765	-3.30050
C	8.02860	3.70432	-2.76834
H	7.99335	1.84421	-1.63654
H	7.20836	3.19709	-0.83211

C	5.75868	4.45126	-3.61482
H	4.12476	3.11431	-3.08078
H	4.82921	3.97578	-1.71741
C	7.12348	4.90623	-3.07749
H	8.27549	3.18724	-3.70763
H	8.98116	4.04425	-2.34179
H	5.89887	3.96848	-4.59348
H	5.10758	5.31830	-3.78642
H	7.61214	5.57569	-3.79709
H	6.97338	5.49183	-2.15811
C	4.03857	1.15051	2.18541
C	5.35157	1.28111	2.99798
C	3.24930	2.48049	2.24307
H	3.41723	0.39939	2.68380
C	5.09635	1.73985	4.44173
H	6.01204	2.00520	2.49896
H	5.89224	0.32562	2.99398
C	2.99837	2.93595	3.68928
H	3.80512	3.26872	1.71606
H	2.29755	2.35191	1.71756
C	4.30717	3.05632	4.48159
H	6.05132	1.84789	4.97306
H	4.52776	0.96290	4.97338
H	2.33924	2.21184	4.18663
H	2.46198	3.89357	3.68651
H	4.92370	3.86043	4.05122
H	4.09980	3.34377	5.52058
C	-3.12105	-1.11329	-3.03841
C	-4.11433	-1.89722	-3.93392
C	-2.43848	-0.01718	-3.89094
H	-2.33216	-1.81023	-2.73483
C	-3.41854	-2.50546	-5.16114
H	-4.91100	-1.21459	-4.26448
H	-4.60863	-2.68605	-3.35526
C	-1.72204	-0.62335	-5.10817
H	-3.18996	0.70160	-4.24770
H	-1.72787	0.54829	-3.28175
C	-2.68501	-1.43737	-5.98470
H	-4.15250	-3.03130	-5.78594
H	-2.69585	-3.26315	-4.82377
H	-1.25143	0.17310	-5.69912
H	-0.90772	-1.27388	-4.75729
H	-3.42474	-0.75776	-6.43439
H	-2.14343	-1.90372	-6.81793
C	-4.21865	-1.30846	2.00768
C	-3.78826	-0.31841	3.11326
C	-5.55223	-1.99656	2.39031
H	-3.45983	-2.09680	1.98088
C	-3.69900	-1.01002	4.48210
H	-4.51223	0.50657	3.17727
H	-2.82121	0.12668	2.85532
C	-5.46421	-2.68222	3.76259
H	-6.35668	-1.24701	2.40752
H	-5.82504	-2.72630	1.61697
C	-5.01746	-1.70199	4.85737
H	-3.41708	-0.27900	5.24978
H	-2.88972	-1.75420	4.45624
H	-4.74329	-3.51141	3.70435
H	-6.43300	-3.12993	4.02064
H	-5.79891	-0.94020	5.00036
H	-4.91463	-2.22549	5.81690
P	0.16320	-0.53565	0.17853
O	0.55832	0.56515	1.10892
O	-0.29138	-0.12212	-1.26648
H	0.29873	0.38374	2.81930
H	-0.39400	0.88315	-1.39638
Cl	0.08082	0.28210	4.12466
O	-0.60615	2.42010	-1.63452
C	0.29459	3.39377	-1.01186
C	-1.76412	3.04356	-0.99500
C	-0.90663	4.24857	-0.53213
H	0.87534	2.92763	-0.21201
H	0.95913	3.84037	-1.75703
H	-2.55438	3.23788	-1.72369
H	-2.15164	2.41972	-0.18346
H	-1.05868	5.10561	-1.19479
C	-0.98060	4.69899	0.90474
C	-0.78571	3.79882	1.96388
C	-1.25785	6.03870	1.20518
C	-0.86765	4.23144	3.28746
H	-0.56182	2.75463	1.76097
C	-1.34002	6.47419	2.52890
H	-1.41112	6.74803	0.39432
C	-1.14508	5.57054	3.57377
H	-0.71289	3.51620	4.09030
H	-1.55566	7.51816	2.74124
H	-1.20802	5.90633	4.60546
C	-6.33950	2.18421	-0.93764
C	-5.65585	3.49899	-1.37861
C	-7.50836	1.84247	-1.89091
H	-6.77708	2.36802	0.05529
C	-6.65945	4.65636	-1.50359
H	-5.16264	3.34060	-2.34919
H	-4.86663	3.75956	-0.66181
C	-8.50971	3.00174	-2.01193
H	-7.10670	1.60700	-2.88683
H	-8.01392	0.93470	-1.53874
C	-7.81747	4.30178	-2.44724
H	-6.14606	5.56183	-1.85219
H	-7.06318	4.89194	-0.50779
H	-9.30533	2.73697	-2.72010
H	-8.99873	3.16132	-1.03941
H	-8.54182	5.12532	-2.48655
H	-7.42698	4.17924	-3.46863

There are no imaginary frequencies.

SCF energy: -4055.695306 hartree
zero-point correction: +1.540508 hartree
enthalpy correction: +1.616306 hartree

free energy correction: +1.422673 hartree
quasiharmonic free energy correction: +1.449193 hartree

RC_D4

C	-0.19428	-3.94546	-1.82789
O	1.08729	-1.27256	-0.95076
O	-1.28261	-1.68712	-0.01328
C	-1.98200	-2.09013	-1.16507
C	-1.38880	-3.01441	-2.01704
C	-3.25437	-1.54359	-1.41908
C	-1.98814	-3.27184	-3.25969
C	-3.87325	-1.92136	-2.62239
C	-3.23516	-2.73554	-3.56082
H	-4.86491	-1.53500	-2.83531
H	-3.71584	-2.94652	-4.51277
C	1.61961	-2.49387	-0.51662
C	0.98655	-3.67767	-0.89379
C	2.80900	-2.49257	0.23852
C	1.49832	-4.89672	-0.41809
C	3.32795	-3.74091	0.61851
C	2.67265	-4.93552	0.32362
H	4.26153	-3.76177	1.17150
H	3.07889	-5.88218	0.67106
C	-1.08681	-4.14292	-4.10953
H	-0.97357	-3.74979	-5.12602
H	-1.48444	-5.16245	-4.20791
C	0.24350	-4.12703	-3.31898
H	0.84381	-3.26120	-3.62015
H	0.84899	-5.02602	-3.47146
C	0.60638	-6.04795	-0.82415
H	1.04539	-6.61832	-1.65470
H	0.43921	-6.75898	-0.00715
C	-0.68232	-5.32397	-1.25927
H	-1.31485	-5.13915	-0.38301
H	-1.27666	-5.88667	-1.98508
C	-3.93801	-0.62116	-0.45173
C	-4.29282	-1.08833	0.84028
C	-4.27217	0.70774	-0.82813
C	-4.94126	-0.21742	1.72344
C	-4.92452	1.52846	0.09964
C	-5.26203	1.09620	1.38353
H	-5.21295	-0.57915	2.71240
H	-5.17838	2.54256	-0.19598
C	3.56018	-1.24608	0.61835
C	4.29291	-0.53858	-0.36764
C	3.63006	-0.83659	1.97506
C	5.07889	0.55196	0.02288
C	4.43939	0.25842	2.30571
C	5.17639	0.96572	1.35387
H	5.65122	1.07737	-0.73670
H	4.51037	0.56493	3.34654
C	-4.05630	-2.52268	1.30538
C	-3.20966	-2.60489	2.59714
C	-5.38809	-3.29152	1.48659
H	-3.49976	-3.05603	0.52848
C	-2.96913	-4.06170	3.02172
H	-2.25632	-2.08835	2.44314
H	-3.72776	-2.07916	3.41174
C	-5.14705	-4.74689	1.91759
H	-5.96061	-3.26160	0.55074
H	-6.00377	-2.78530	2.24370
C	-4.28968	-4.82775	3.18952
H	-2.39088	-4.08968	3.95454
H	-2.35274	-4.56331	2.26012
H	-6.10724	-5.25644	2.07178
H	-4.63720	-5.28441	1.10399
H	-4.09423	-5.87600	3.45089
H	-4.85163	-4.39560	4.03118
C	-5.94945	2.01341	2.38153
C	-7.32735	2.50933	1.88612
C	-5.05911	3.21423	2.77912
H	-6.12622	1.42657	3.29587
C	-8.01306	3.41904	2.91764
H	-7.96489	1.64789	1.65087
H	-7.19564	3.06406	0.94609
C	-5.74710	4.12389	3.80889
H	-4.10298	2.84518	3.17264
H	-4.82095	3.79926	1.87907
C	-7.11802	4.60375	3.31008
H	-8.25053	2.83180	3.81731
H	-8.97079	3.78000	2.52102
H	-5.87920	3.56951	4.75002
H	-5.10363	4.98233	4.04176
H	-7.61001	5.21520	4.07740
H	-6.97626	5.25494	2.43456
C	-3.99143	1.28905	-2.21352
C	-5.30605	1.46276	-3.01583
C	-3.22012	2.62978	-2.17164
H	-3.36019	0.58633	-2.76669
C	-5.05607	2.02518	-4.42309
H	-5.97355	2.14252	-2.46637
H	-5.83774	0.50443	-3.07987
C	-2.97313	3.19044	-3.58172
H	-3.78756	3.37159	-1.59232
H	-2.26775	2.47837	-1.65306
C	-4.28210	3.34959	-4.36779
H	-6.01185	2.16024	-4.94671
H	-4.47865	1.29426	-5.00792
H	-2.30149	2.51346	-4.12676
H	-2.45092	4.15312	-3.50854
H	-4.90914	4.11410	-3.88394
H	-4.07580	3.71229	-5.38323
C	2.88682	-1.56099	3.09616
C	3.83384	-2.44517	3.94684
C	2.10905	-0.61476	4.04169
H	2.14602	-2.22329	2.63461
C	3.06404	-3.23928	5.01426
H	4.58109	-1.80056	4.43258

H	4.39456	-3.13271	3.30309
C	1.31513	-1.40612	5.09221
H	2.81093	0.05087	4.56364
H	1.43555	0.02620	3.46724
C	2.23007	-2.32041	5.91938
H	3.76378	-3.83420	5.61595
H	2.39665	-3.95545	4.51253
H	0.77419	-0.71411	5.75072
H	0.55199	-2.01345	4.58419
H	2.90764	-1.69992	6.52502
H	1.63911	-2.91735	6.62621
C	4.32694	-0.96901	-1.83077
C	3.96826	0.16983	-2.81208
C	5.69734	-1.58880	-2.20070
H	3.58021	-1.75565	-1.97833
C	4.00436	-0.30956	-4.27088
H	4.67721	1.00161	-2.69387
H	2.97450	0.56387	-2.57272
C	5.73320	-2.06091	-3.66230
H	6.48868	-0.84266	-2.03809
H	5.91723	-2.42548	-1.52503
C	5.36237	-0.92891	-4.63181
H	3.77332	0.52700	-4.94184
H	3.20968	-1.05361	-4.42492
H	5.02394	-2.89228	-3.78986
H	6.72727	-2.46081	-3.90220
H	6.13892	-0.15001	-4.59001
H	5.35057	-1.30142	-5.66446
P	-0.15202	-0.54751	-0.20583
O	-0.53136	0.64644	-1.02087
O	0.23473	-0.29384	1.29484
H	-0.17070	0.67307	-2.71848
H	0.34326	0.68923	1.53539
Cl	0.12310	0.73386	-4.01175
O	0.48130	2.19089	1.98073
C	-0.47296	3.17153	1.45638
C	1.60799	2.98670	1.49793
C	0.67145	4.17126	1.14728
H	-0.99108	2.77705	0.57857
H	-1.19336	3.46242	2.22638
H	2.34115	3.14558	2.29340
H	2.09012	2.51310	0.63719
H	0.72600	4.94775	1.91586
C	0.76289	4.80192	-0.21918
C	0.68537	4.02768	-1.38730
C	0.93815	6.18619	-0.34224
C	0.78023	4.62583	-2.64378
H	0.54273	2.95198	-1.32283
C	1.03354	6.78729	-1.59852
H	1.00024	6.79938	0.55454
C	0.95465	6.00779	-2.75290
H	0.71590	4.00573	-3.53342
H	1.16857	7.86325	-1.67307
H	1.02824	6.47307	-3.73228
C	6.08488	2.11165	1.77042
C	7.57980	1.75277	1.59258
C	5.76787	3.43832	1.04436
H	5.92120	2.28359	2.84551
C	8.50385	2.89266	2.04774
H	7.77034	1.52935	0.53301
H	7.80429	0.83326	2.14762
C	6.69066	4.57773	1.50450
H	5.88187	3.29753	-0.03958
H	4.71743	3.71021	1.21011
C	8.17184	4.21016	1.33203
H	9.55194	2.61700	1.87369
H	8.39574	3.03431	3.13353
H	6.45770	5.49513	0.94884
H	6.49416	4.79717	2.56478
H	8.81118	5.01960	1.70703
H	8.39553	4.10616	0.25982

There are no imaginary frequencies.

SCF energy: -4055.695545 hartree
zero-point correction: +1.540246 hartree
enthalpy correction: +1.616157 hartree
free energy correction: +1.420937 hartree
quasiharmonic free energy correction: +1.449051 hartree

TS(*R*)_A1 (lowest-energy TS(*R*))

C	-0.71732	-4.53100	-0.00796
O	-1.52718	-1.59969	0.52095
O	0.80326	-1.88125	-0.57330
C	1.32209	-2.83690	0.31302
C	0.57230	-3.97560	0.59852
C	2.60705	-2.63136	0.85220
C	1.05869	-4.87528	1.56221
C	3.09354	-3.61163	1.73171
C	2.32080	-4.70638	2.11868
H	4.09279	-3.48964	2.13690
H	2.70607	-5.41612	2.84647
C	-2.30911	-2.41719	-0.31208
C	-1.84831	-3.69686	-0.60605
C	-3.53940	-1.93263	-0.79671
C	-2.55235	-4.46869	-1.54437
C	-4.26322	-2.78397	-1.64768
C	-3.76472	-4.02165	-2.05750
H	-5.22646	-2.44533	-2.01579
H	-4.32556	-4.62728	-2.76512
C	0.03616	-5.95076	1.85509
H	0.32248	-6.91114	1.40413
H	-0.08306	-6.13140	2.92937
C	-1.23957	-5.37959	1.20189
H	-1.75021	-4.71200	1.90559
H	-1.95446	-6.14867	0.89467

C	-1.80207	-5.74693	-1.85153	H	7.78835	3.01519	-3.16687
H	-2.29293	-6.62059	-1.40065	C	3.35540	-0.61995	2.96780
H	-1.73906	-5.94453	-2.92780	C	4.50905	-1.06492	3.90275
C	-0.41942	-5.48493	-1.21415	C	2.72720	0.67922	3.52472
H	0.22650	-4.96098	-1.92840	H	2.57699	-1.38838	3.01880
H	0.09717	-6.39928	-0.90687	C	4.02930	-1.25308	5.35075
C	3.45701	-1.44108	0.51074	H	5.30359	-0.30475	3.87504
C	3.96156	-1.28305	-0.80617	H	4.96383	-1.99277	3.53385
C	3.81830	-0.50680	1.51644	C	2.22825	0.48699	4.96506
C	4.79586	-0.19509	-1.08957	H	3.47488	1.48592	3.51864
C	4.66504	0.55600	1.17317	H	1.90016	1.00627	2.88886
C	5.16665	0.73744	-0.11631	C	3.35368	0.01423	5.89540
H	5.18970	-0.09073	-2.09737	H	4.87402	-1.54240	5.98997
H	4.95345	1.26665	1.94380	H	3.31260	-2.08712	5.38395
C	-4.06766	-0.57845	-0.42485	H	1.41562	-0.25394	4.96751
C	-4.39635	-0.29332	0.92453	H	1.79183	1.42370	5.33227
C	-4.26298	0.41800	-1.41867	H	4.10621	0.81202	5.98799
C	-4.86442	0.98391	1.25118	H	2.96625	-0.16684	6.90645
C	-4.73794	1.67551	-1.02910	C	-4.00527	0.17602	-2.90517
C	-5.02909	1.99038	0.30065	C	-5.33052	0.07360	-3.70163
H	-5.10670	1.20550	2.28740	C	-3.09724	1.24180	-3.55937
H	-4.87843	2.43702	-1.79117	H	-3.48416	-0.78068	-3.01438
C	3.69775	-2.29455	-1.91824	C	-5.08462	-0.22962	-5.18798
C	3.03911	-1.66887	-3.16927	H	-5.87812	1.02228	-3.60512
C	4.99014	-3.05054	-2.31389	H	-5.97823	-0.69536	-3.26171
H	3.00229	-3.05134	-1.54277	C	-2.83488	0.92673	-5.04019
C	2.77475	-2.72359	-4.25556	H	-3.56590	2.23296	-3.48752
H	2.10093	-1.18038	-2.88184	H	-2.15393	1.29786	-3.01016
H	3.69486	-0.88893	-3.58225	C	-4.14574	0.80209	-5.83021
C	4.72356	-4.10171	-3.40236	H	-6.04035	-0.26334	-5.72729
H	5.42396	-3.52526	-1.42463	H	-4.63810	-1.23085	-5.28125
H	5.73787	-2.33139	-2.67741	H	-2.19728	1.70417	-5.48117
C	4.05555	-3.48020	-4.63761	H	-2.27434	-0.01681	-5.11532
H	2.33423	-2.24730	-5.14105	H	-4.64712	1.78129	-5.85392
H	2.02705	-3.44117	-3.88535	H	-3.93991	0.53196	-6.87416
H	4.06896	-4.88609	-2.99404	C	-5.48584	3.37786	0.71680
H	5.66238	-4.59614	-3.68388	C	-4.36871	4.43197	0.52785
H	3.83276	-4.25596	-5.38161	C	-6.78023	3.83382	0.00632
H	4.75900	-2.78200	-5.11565	H	-5.70664	3.33613	1.79399
C	6.10241	1.89379	-0.43105	C	-4.81593	5.82564	0.99401
C	5.52059	2.86132	-1.48705	H	-4.09670	4.47503	-0.53779
C	7.50697	1.41021	-0.86278	H	-3.47086	4.11427	1.07189
H	6.23045	2.47106	0.49683	C	-7.22567	5.22677	0.47823
C	6.47187	4.03172	-1.78278	H	-7.57643	3.09864	0.18001
H	4.55398	3.24503	-1.13688	H	-6.61166	3.85836	-1.08005
H	5.32671	2.30753	-2.41736	C	-6.11170	6.26908	0.29810
C	8.45420	2.58467	-1.15435	H	-4.97747	5.80648	2.08189
H	7.92790	0.76367	-0.08258	H	-4.01636	6.55581	0.81383
H	7.41339	0.78751	-1.76415	H	-7.50340	5.17549	1.54159
C	7.86448	3.53940	-2.20242	H	-8.12896	5.53552	-0.06402
H	6.56385	4.65606	-0.88202	H	-6.43763	7.24437	0.68241
H	6.04248	4.67460	-2.56196	H	-5.91691	6.40585	-0.77646
H	8.63866	3.14011	-0.22279	C	-4.32434	-1.33532	2.03683
H	9.42861	2.20533	-1.48808	C	-3.44286	-0.89494	3.22838
H	8.53707	4.39169	-2.36276	C	-5.73664	-1.72864	2.53583

H	-3.87830	-2.24924	1.63066
C	-3.37671	-1.98319	4.31083
H	-3.85115	0.02306	3.67239
H	-2.43779	-0.64497	2.87406
C	-5.67241	-2.81163	3.62468
H	-6.24199	-0.83832	2.93623
H	-6.34425	-2.07588	1.69016
C	-4.77675	-2.38524	4.79742
H	-2.76590	-1.63415	5.15325
H	-2.86623	-2.86987	3.90391
H	-5.27562	-3.74001	3.18663
H	-6.68426	-3.04488	3.98156
H	-5.23879	-1.52875	5.31076
H	-4.70892	-3.19301	5.53799
P	-0.28364	-0.78365	-0.11167
O	0.33546	-0.08122	1.14805
O	-0.61863	0.05105	-1.30573
H	-0.11213	0.75430	1.55198
H	-0.17877	1.52044	-2.04348
Cl	-0.63371	2.53459	2.20106
O	0.09949	2.48113	-2.09762
C	-0.22368	2.89839	-0.35773
C	1.52276	2.54412	-1.70304
C	1.30378	2.94750	-0.23227
H	-0.79718	2.01381	-0.16706
H	-0.78758	3.82238	-0.41640
H	1.99895	1.57287	-1.84876
H	2.00406	3.29802	-2.32559
H	1.64718	2.17286	0.45215
C	1.87113	4.28998	0.18222
C	1.68390	5.43422	-0.60707
C	2.59131	4.40712	1.37648
C	2.20791	6.66528	-0.21350
H	1.11884	5.37072	-1.53541
C	3.11910	5.63748	1.77062
H	2.72011	3.53237	2.00663
C	2.93007	6.76935	0.97703
H	2.05108	7.54227	-0.83587
H	3.67196	5.71138	2.70320
H	3.33886	7.72795	1.28496

1 imaginary frequency: -394.21 cm^{-1}.

SCF energy: -4055.670375 hartree
zero-point correction: +1.542783 hartree
enthalpy correction: +1.617752 hartree
free energy correction: +1.427000 hartree
quasiharmonic free energy correction: +1.452685 hartree

SCF energy (other methods):
B3LYP/6-31G(d): -4054.313146
B3LYP-D3(BJ)/6-311+G(d,p): -4055.658375
B3LYP-D3(BJ)/6-311+G(d,p)/SMD(benzene): -4055.727397
B3LYP-D3(BJ)/def2-TZVP/CPCM(benzene): -4056.040033
B3LYP-D3(BJ)/def2-TZVPP/CPCM(benzene): -4056.077734
B3LYP/6-311+G(d,p)/CPCM(benzene): -4055.209402
M06-2X/6-311+G(d,p)/CPCM (benzene): -4053.802975
ωB97X-D/6-311+G(d,p)/CPCM (benzene): -4054.249057

TS(*R*)_A2

C	-0.73852	-4.47137	0.41633
O	-1.54903	-1.49241	0.57178
O	0.82543	-1.90766	-0.37442
C	1.30505	-2.76703	0.62452
C	0.53191	-3.85992	1.00781
C	2.57721	-2.51902	1.17571
C	0.97449	-4.65360	2.07956
C	3.02291	-3.40345	2.17128
C	2.22227	-4.43923	2.65262
H	4.01147	-3.25006	2.59175
H	2.57594	-5.06932	3.46488
C	-2.29272	-2.39565	-0.20586
C	-1.83447	-3.70524	-0.32325
C	-3.48656	-1.96215	-0.81389
C	-2.50026	-4.57707	-1.20047
C	-4.17839	-2.90406	-1.59336
C	-3.67869	-4.18599	-1.82507
H	-5.11674	-2.60403	-2.04846
H	-4.21110	-4.86744	-2.48402
C	-0.07172	-5.68095	2.45196
H	0.22022	-6.68847	2.12415
H	-0.23323	-5.73772	3.53442
C	-1.31577	-5.17805	1.69013
H	-1.84744	-4.43473	2.29540
H	-2.02516	-5.97239	1.43998
C	-1.75135	-5.88650	-1.32167
H	-2.26929	-6.69774	-0.79139
H	-1.64516	-6.21095	-2.36315
C	-0.39555	-5.55569	-0.66083
H	0.28098	-5.11448	-1.40216
H	0.10498	-6.42864	-0.23113
C	3.45095	-1.37894	0.73699
C	3.98128	-1.35098	-0.57949
C	3.80660	-0.35700	1.65566
C	4.83852	-0.30668	-0.94676
C	4.67555	0.65705	1.23095
C	5.20590	0.70864	-0.05865
H	5.25301	-0.30407	-1.95172
H	4.95855	1.43287	1.93792
C	-4.02347	-0.57047	-0.65014
C	-4.44884	-0.11676	0.62560
C	-4.15363	0.28404	-1.77581

C	-4.96429	1.17713	0.74888	H	2.89089	0.54423	6.96857
C	-4.68076	1.56785	-1.58798	C	-3.76931	-0.13432	-3.19402
C	-5.08228	2.04382	-0.33966	C	-5.01670	-0.37062	-4.08154
H	-5.28601	1.51587	1.72951	C	-2.82615	0.86754	-3.89815
H	-4.78091	2.22648	-2.44768	H	-3.22421	-1.08239	-3.13778
C	3.71440	-2.45286	-1.60082	C	-4.63446	-0.85362	-5.48947
C	3.07152	-1.92683	-2.90563	H	-5.58476	0.56794	-4.15719
C	4.99596	-3.25906	-1.92552	H	-5.69026	-1.09395	-3.60529
H	3.00657	-3.16512	-1.16600	C	-2.42678	0.37693	-5.29825
C	2.78882	-3.06734	-3.89549	H	-3.31795	1.84534	-3.99335
H	2.14249	-1.39606	-2.66834	H	-1.93699	1.02082	-3.28143
H	3.74568	-1.20014	-3.38223	C	-3.65902	0.11385	-6.17598
C	4.71278	-4.39743	-2.91796	H	-5.53766	-0.98134	-6.10053
H	5.42268	-3.66070	-0.99764	H	-4.16586	-1.84619	-5.41411
H	5.75497	-2.58669	-2.35044	H	-1.76813	1.11234	-5.77865
C	4.05590	-3.87773	-4.20554	H	-1.84248	-0.55036	-5.20369
H	2.35846	-2.66276	-4.82075	H	-4.17331	1.06716	-6.36956
H	2.02709	-3.73520	-3.46563	H	-3.35579	-0.28112	-7.15435
H	4.04473	-5.13183	-2.44359	C	-5.63178	3.45167	-0.18532
H	5.64343	-4.93036	-3.15237	C	-7.12077	3.46203	0.23373
H	3.82025	-4.71335	-4.87724	C	-4.79619	4.31068	0.79169
H	4.77142	-3.23734	-4.74308	H	-5.57353	3.93336	-1.17376
C	6.17061	1.81406	-0.45711	C	-7.67049	4.89242	0.34832
C	5.64089	2.68189	-1.62168	H	-7.22548	2.95199	1.20226
C	7.57906	1.26858	-0.79180	H	-7.71122	2.88221	-0.48725
H	6.27985	2.47862	0.41311	C	-5.34452	5.74135	0.89981
C	6.62219	3.80410	-1.99491	H	-3.74605	4.32148	0.47656
H	4.67042	3.11172	-1.34356	H	-4.80670	3.84417	1.78630
H	5.46789	2.04318	-2.50039	C	-6.82668	5.74972	1.30362
C	8.55649	2.39516	-1.16083	H	-7.67195	5.35823	-0.64871
H	7.96176	0.69344	0.06060	H	-8.71658	4.86698	0.68044
H	7.50368	0.56412	-1.63268	H	-5.23214	6.24847	-0.07064
C	8.01927	3.25310	-2.31561	H	-4.74933	6.31542	1.62116
H	6.69423	4.51084	-1.15536	H	-7.20979	6.77817	1.33007
H	6.23121	4.37480	-2.84707	H	-6.92446	5.35371	2.32552
H	8.71960	3.03497	-0.28081	C	-4.43143	-1.00086	1.86922
H	9.53461	1.97148	-1.42258	C	-3.63285	-0.38497	3.04167
H	8.71221	4.07583	-2.53351	C	-5.86627	-1.35955	2.32900
H	7.96623	2.63935	-3.22740	H	-3.94481	-1.94884	1.61788
C	3.31774	-0.32371	3.10265	C	-3.62142	-1.31637	4.26338
C	4.45890	-0.66968	4.09325	H	-4.07898	0.57623	3.33069
C	2.67751	1.02309	3.51326	H	-2.61017	-0.16423	2.71926
H	2.53897	-1.08441	3.21855	C	-5.85573	-2.28387	3.55664
C	3.96503	-0.70430	5.54775	H	-6.41221	-0.43695	2.57238
H	5.25500	0.08281	3.99547	H	-6.41155	-1.83243	1.50188
H	4.91643	-1.63100	3.82755	C	-5.04387	-1.68152	4.71289
C	2.16688	0.98198	4.96191	H	-3.07055	-0.84428	5.08690
H	3.41937	1.83059	3.42652	H	-3.07355	-2.23765	4.01161
H	1.85447	1.27265	2.83790	H	-5.41790	-3.25330	3.27454
C	3.28586	0.61389	5.94671	H	-6.88483	-2.49063	3.87890
H	4.80376	-0.92255	6.22204	H	-5.55061	-0.77454	5.07512
H	3.24804	-1.53058	5.66404	H	-5.01149	-2.37973	5.55966
H	1.35723	0.24160	5.03667	P	-0.26193	-0.75642	-0.07194
H	1.72466	1.95055	5.22478	O	0.30636	0.05534	1.14454
H	4.03783	1.41748	5.95650	O	-0.52387	-0.03808	-1.35646

H	-0.13349	0.94373	1.43088
H	-0.02811	1.33271	-2.22902
Cl	-0.64437	2.78531	1.85535
O	0.26424	2.27895	-2.37953
C	-0.12291	2.88492	-0.70770
C	1.67106	2.37320	-1.93640
C	1.39870	2.91488	-0.52026
H	-0.72933	2.03897	-0.45365
H	-0.65691	3.81119	-0.88746
H	2.14744	1.39185	-1.97310
H	2.18029	3.06476	-2.60710
H	1.69307	2.19972	0.24683
C	1.98107	4.27761	-0.20426
C	1.85708	5.34822	-1.10201
C	2.65385	4.48813	1.00471
C	2.39794	6.59786	-0.80034
H	1.32930	5.21299	-2.04450
C	3.19841	5.73697	1.30715
H	2.73212	3.67269	1.71720
C	3.07374	6.79449	0.40556
H	2.29069	7.41693	-1.50650
H	3.71393	5.88408	2.25236
H	3.49600	7.76751	0.64175

1 imaginary frequency: -395.46 cm^{-1}.

SCF energy: -4055.669727 hartree
zero-point correction: +1.542510 hartree
enthalpy correction: +1.617543 hartree
free energy correction: +1.426042 hartree
quasiharmonic free energy correction: +1.452397 hartree

TS(*R*)_A3

C	-0.78826	-4.52155	0.30736
O	0.75075	-1.96472	-0.54379
O	-1.51682	-1.54129	0.63731
C	-2.35023	-2.40303	-0.09591
C	-1.92744	-3.71177	-0.30776
C	-3.59105	-1.93037	-0.56480
C	-2.68501	-4.53746	-1.15421
C	-4.36540	-2.82717	-1.31910
C	-3.90791	-4.10304	-1.65278
H	-5.33811	-2.49783	-1.67022
H	-4.50929	-4.74801	-2.28874
C	1.29688	-2.85997	0.38840
C	0.53787	-3.94921	0.80766
C	2.61605	-2.64963	0.83418
C	1.05308	-4.77797	1.81860
C	3.12367	-3.56120	1.77368
C	2.34549	-4.59470	2.29582
H	4.14665	-3.43522	2.11334
H	2.75218	-5.24937	3.06254
C	-1.97466	-5.85383	-1.38705
H	-2.46324	-6.67564	-0.84532
H	-1.96220	-6.13983	-2.44503
C	-0.56110	-5.57396	-0.83063
H	0.06290	-5.12185	-1.61059
H	-0.04879	-6.47232	-0.47322
C	0.02474	-5.80265	2.24451
H	0.27336	-6.80260	1.86232
H	-0.04891	-5.89231	3.33424
C	-1.26956	-5.26001	1.60302
H	-1.73779	-4.52914	2.27252
H	-2.00947	-6.03678	1.38836
C	-4.08305	-0.54508	-0.26443
C	-4.29307	0.39205	-1.31109
C	-4.36647	-0.17333	1.07376
C	-4.73763	1.67870	-0.98592
C	-4.80472	1.12917	1.33535
C	-4.98355	2.07849	0.33019
H	-4.89237	2.39286	-1.78981
H	-5.01269	1.41690	2.36278
C	3.47901	-1.53263	0.32093
C	3.89536	-1.52956	-1.03414
C	3.94012	-0.51415	1.19792
C	4.74011	-0.50596	-1.48237
C	4.79454	0.47426	0.69388
C	5.20842	0.50411	-0.64095
H	5.07017	-0.51353	-2.51890
H	5.15569	1.24181	1.37252
C	-4.08785	0.05064	-2.78594
C	-5.44031	-0.10881	-3.52579
C	-3.21029	1.06969	-3.54707
H	-3.56643	-0.91032	-2.84757
C	-5.24453	-0.52297	-4.99248
H	-6.07175	-0.84197	-3.00853
H	-5.98529	0.84535	-3.48100
C	-2.99598	0.64635	-5.00855
H	-2.24936	1.17243	-3.03659
H	-3.68360	2.06128	-3.53366
C	-4.33169	0.45809	-5.74250
H	-6.21784	-0.59826	-5.49494
H	-4.79802	-1.52806	-5.02434
H	-2.43163	-0.29763	-5.03233
H	-2.37891	1.39156	-5.52747
H	-4.15894	0.10901	-6.76888
H	-4.83859	1.43132	-5.82477
C	-5.40911	3.49508	0.67548
C	-6.71216	3.93179	-0.03070
C	-4.28084	4.51853	0.40312
H	-5.60602	3.51789	1.75788
C	-7.12575	5.35587	0.37257
H	-7.51514	3.22050	0.20143
H	-6.56832	3.89321	-1.12022
C	-4.69590	5.94295	0.80149
H	-3.37541	4.21638	0.94352
H	-4.03342	4.49881	-0.66923
C	-6.00067	6.36874	0.11149

H	-7.38083	5.36763	1.44278
H	-8.03604	5.64904	-0.16661
H	-4.83224	5.98602	1.89213
H	-3.88982	6.64893	0.56331
H	-6.30319	7.36842	0.44947
H	-5.82864	6.44445	-0.97290
C	-4.28381	-1.14934	2.24371
C	-3.36376	-0.66166	3.38629
C	-5.69193	-1.48188	2.79644
H	-3.86621	-2.09482	1.88200
C	-3.29722	-1.68737	4.52838
H	-3.73832	0.29090	3.78502
H	-2.36223	-0.45815	2.99387
C	-5.62689	-2.50085	3.94476
H	-6.16898	-0.55849	3.15454
H	-6.32599	-1.86344	1.98569
C	-4.69378	-2.02837	5.06944
H	-2.65890	-1.30548	5.33541
H	-2.81652	-2.60798	4.16239
H	-5.26246	-3.46272	3.55335
H	-6.63497	-2.68801	4.33765
H	-5.12435	-1.13335	5.54284
H	-4.62486	-2.79333	5.85409
C	3.57683	-0.46518	2.68112
C	4.78126	-0.85182	3.57628
C	3.02221	0.90405	3.13916
H	2.78368	-1.19762	2.86386
C	4.40592	-0.86730	5.06663
H	5.59474	-0.13039	3.41060
H	5.17899	-1.83017	3.27835
C	2.62760	0.88256	4.62364
H	3.78422	1.68303	2.98925
H	2.15594	1.18211	2.53255
C	3.80716	0.47366	5.51655
H	5.28840	-1.11526	5.67129
H	3.67210	-1.66779	5.24299
H	2.24376	1.86690	4.91780
H	1.79807	0.17470	4.76454
H	4.58522	1.25060	5.46666
H	3.49236	0.41567	6.56657
C	6.16171	1.56820	-1.16111
C	5.59795	3.00034	-1.02306
C	7.55591	1.47522	-0.49605
H	6.30572	1.37939	-2.23613
C	6.56943	4.05735	-1.56987
H	5.39045	3.21244	0.03482
H	4.63367	3.06996	-1.54266
C	8.52510	2.53226	-1.04685
H	7.96476	0.46740	-0.64112
H	7.44732	1.61289	0.58935
C	7.95156	3.95012	-0.90868
H	6.67816	3.92212	-2.65657
H	6.14947	5.05992	-1.42039
H	8.72236	2.32411	-2.10916
H	9.49136	2.45901	-0.53140
H	8.64059	4.68444	-1.34529
H	7.86174	4.20135	0.15871
C	3.53555	-2.64177	-2.01477
C	2.81148	-2.13293	-3.28275
C	4.78283	-3.47166	-2.40603
H	2.84944	-3.33488	-1.51833
C	2.45367	-3.29023	-4.22889
H	3.45718	-1.42183	-3.81821
H	1.90627	-1.58748	-2.99233
C	4.42370	-4.62505	-3.35507
H	5.52039	-2.81718	-2.89193
H	5.26381	-3.86073	-1.49957
C	3.68972	-4.12018	-4.60615
H	1.96645	-2.89916	-5.13147
H	1.71632	-3.94216	-3.73652
H	3.78064	-5.34277	-2.82406
H	5.33143	-5.17283	-3.63979
H	4.37518	-3.49692	-5.20006
H	3.40204	-4.96404	-5.24656
P	-0.28407	-0.80811	-0.10808
O	0.41362	-0.03985	1.07059
O	-0.65478	-0.04538	-1.33921
H	-0.01907	0.80843	1.46205
H	-0.23098	1.38474	-2.16058
Cl	-0.53320	2.62146	2.04362
O	0.03697	2.34373	-2.27230
C	-0.23696	2.85503	-0.54744
C	1.47058	2.44539	-1.92656
C	1.29147	2.95801	-0.48530
H	-0.77409	1.96644	-0.28504
H	-0.83252	3.75638	-0.63743
H	1.94965	1.46808	-2.01013
H	1.92917	3.15047	-2.61976
H	1.68553	2.25221	0.24452
C	1.82202	4.34806	-0.19684
C	1.61228	5.40766	-1.09109
C	2.52483	4.59642	0.98771
C	2.10336	6.68331	-0.81294
H	1.05602	5.24374	-2.01231
C	3.01908	5.87134	1.26682
H	2.66401	3.78983	1.70107
C	2.81260	6.91751	0.36653
H	1.93084	7.49311	-1.51690
H	3.55973	6.04754	2.19281
H	3.19650	7.91052	0.58435

1 imaginary frequency: -394.45 cm^{-1}.

SCF energy: -4055.669228 hartree
zero-point correction: +1.542714 hartree
enthalpy correction: +1.617673 hartree
free energy correction: +1.427092 hartree
quasiharmonic free energy correction: +1.452658 hartree

TS(*R*)_A4

C	-0.82479	-4.43671	0.66434
O	-1.54553	-1.43177	0.65573
O	0.76738	-1.98247	-0.37467
C	1.27491	-2.79154	0.65241
C	0.48932	-3.82726	1.15081
C	2.58398	-2.55484	1.11418
C	0.96101	-4.55730	2.25472
C	3.05250	-3.38122	2.14847
C	2.24367	-4.34733	2.74718
H	4.06806	-3.23733	2.50289
H	2.61897	-4.92897	3.58544
C	-2.34804	-2.36111	-0.02781
C	-1.93047	-3.68847	-0.07900
C	-3.55776	-1.93362	-0.60760
C	-2.65876	-4.59542	-0.86607
C	-4.30720	-2.90216	-1.29616
C	-3.85192	-4.21006	-1.46585
H	-5.25772	-2.60535	-1.72752
H	-4.43113	-4.91656	-2.05526
C	-0.09779	-5.51660	2.75246
H	0.14669	-6.55585	2.49186
H	-0.20910	-5.48463	3.84225
C	-1.36143	-5.03074	2.01132
H	-1.84267	-4.22861	2.58286
H	-2.10406	-5.81857	1.85356
C	-1.95549	-5.93389	-0.92679
H	-2.47438	-6.68902	-0.32013
H	-1.90429	-6.33253	-1.94647
C	-0.56327	-5.60448	-0.34633
H	0.09526	-5.23930	-1.14326
H	-0.07295	-6.46232	0.12374
C	3.47442	-1.49217	0.53638
C	3.92579	-1.59402	-0.80366
C	3.92768	-0.41722	1.34830
C	4.80414	-0.62130	-1.29946
C	4.81562	0.51597	0.79954
C	5.27022	0.43844	-0.52000
H	5.16147	-0.70888	-2.32320
H	5.17048	1.32657	1.42996
C	-4.06042	-0.52384	-0.49611
C	-4.43151	-0.00091	0.76999
C	-4.22060	0.27478	-1.65775
C	-4.92619	1.30442	0.84646
C	-4.72726	1.57277	-1.51663
C	-5.07677	2.11592	-0.28010
H	-5.20471	1.69753	1.82000
H	-4.85202	2.18850	-2.40441
C	3.55654	-2.75683	-1.72010
C	2.84437	-2.30187	-3.01543
C	4.78924	-3.62830	-2.06461
H	2.85815	-3.41036	-1.18823
C	2.46631	-3.49847	-3.90234
H	1.94866	-1.72545	-2.75813
H	3.50626	-1.63227	-3.58352
C	4.40903	-4.82219	-2.95424
H	5.26118	-3.97930	-1.13808
H	5.54031	-3.01457	-2.58187
C	3.68745	-4.36928	-4.23215
H	1.98911	-3.14464	-4.82540
H	1.71514	-4.10992	-3.37995
H	3.75067	-5.49815	-2.38838
H	5.30635	-5.40187	-3.20697
H	3.38606	-5.24007	-4.82869
H	4.38556	-3.79028	-4.85529
C	6.26758	1.43775	-1.08411
C	7.64835	1.32759	-0.39366
C	5.75897	2.89561	-1.03209
H	6.41857	1.18486	-2.14492
C	8.66575	2.31450	-0.98621
H	8.01898	0.29822	-0.47732
H	7.53018	1.52838	0.68093
C	6.77782	3.88212	-1.62271
H	4.80334	2.97504	-1.56552
H	5.54947	3.17413	0.00978
C	8.14638	3.75890	-0.93671
H	8.87016	2.03944	-2.03183
H	9.62090	2.23346	-0.45153
H	6.89427	3.68252	-2.69865
H	6.39546	4.90678	-1.53497
H	8.86933	4.43996	-1.40378
H	8.05360	4.07387	0.11341
C	3.51858	-0.24712	2.81045
C	4.69288	-0.56481	3.77063
C	2.95624	1.15598	3.13875
H	2.71586	-0.95969	3.02594
C	4.27110	-0.46175	5.24444
H	5.51430	0.13986	3.57509
H	5.09547	-1.56426	3.56308
C	2.51965	1.25577	4.60854
H	3.72367	1.91989	2.94554
H	2.10775	1.38255	2.48696
C	3.66957	0.91393	5.56667
H	5.13205	-0.66524	5.89492
H	3.52606	-1.24215	5.45966
H	1.68233	0.56444	4.78158
H	2.13419	2.26223	4.81189
H	4.45493	1.67992	5.47818
H	3.32274	0.94274	6.60778
C	-3.88609	-0.21977	-3.06383
C	-5.16214	-0.49402	-3.89778
C	-2.96285	0.73883	-3.84973
H	-3.34330	-1.16677	-2.97400
C	-4.82627	-1.05355	-5.28930
H	-5.72718	0.44323	-4.00547
H	-5.82397	-1.18685	-3.36364
C	-2.60765	0.17167	-5.23277
H	-3.45614	1.71145	-3.98292
H	-2.05530	0.92315	-3.26926

C	-3.86749	-0.13134	-6.05688
H	-5.74874	-1.20739	-5.86458
H	-4.36114	-2.04406	-5.17526
H	-1.96145	0.87687	-5.77179
H	-2.02407	-0.75213	-5.10586
H	-4.38290	0.81312	-6.28723
H	-3.59634	-0.58144	-7.02076
C	-5.60935	3.53472	-0.17593
C	-7.08365	3.57616	0.29084
C	-4.73582	4.43158	0.73142
H	-5.58044	3.96881	-1.18744
C	-7.62045	5.01422	0.35822
H	-7.15898	3.11166	1.28473
H	-7.70122	2.96844	-0.38287
C	-5.27227	5.86957	0.79329
H	-3.69748	4.42049	0.37931
H	-4.71350	4.01051	1.74605
C	-6.73990	5.90669	1.24571
H	-7.65220	5.43482	-0.65824
H	-8.65504	5.01183	0.72547
H	-5.18999	6.33200	-0.20218
H	-4.64983	6.47122	1.46766
H	-7.11574	6.93812	1.23944
H	-6.80538	5.55668	2.28679
C	-4.37861	-0.82296	2.05435
C	-3.53316	-0.16186	3.16709
C	-5.79983	-1.14336	2.58010
H	-3.91034	-1.78721	1.83210
C	-3.48604	-1.03729	4.42888
H	-3.96037	0.81593	3.42798
H	-2.52128	0.03400	2.79766
C	-5.75406	-2.01147	3.84727
H	-6.32736	-0.20441	2.80068
H	-6.37911	-1.64663	1.79516
C	-4.89483	-1.36677	4.94489
H	-2.90172	-0.53465	5.21017
H	-2.95606	-1.97480	4.19981
H	-5.33636	-2.99753	3.59372
H	-6.77268	-2.19163	4.21551
H	-5.37965	-0.43894	5.28366
H	-4.83810	-2.02649	5.82074
P	-0.26802	-0.78059	-0.09030
O	0.38398	0.08167	1.04819
O	-0.56735	-0.12653	-1.40092
H	-0.04169	0.97832	1.32557
H	-0.05611	1.19535	-2.34509
Cl	-0.53555	2.84624	1.69265
O	0.25283	2.12833	-2.53833
C	-0.09745	2.82238	-0.88791
C	1.66724	2.21581	-2.11712
C	1.42854	2.88563	-0.75146
H	-0.68123	1.98096	-0.57376
H	-0.65272	3.72873	-1.10166
H	2.10866	1.21862	-2.06692
H	2.19490	2.82370	-2.85179
H	1.75775	2.25231	0.07104
C	1.98945	4.28320	-0.57948
C	1.90279	5.23703	-1.60379
C	2.59488	4.64708	0.62910
C	2.42126	6.52035	-1.42882
H	1.42306	4.98480	-2.54777
C	3.11603	5.92947	0.80523
H	2.63668	3.92547	1.43925
C	3.03399	6.86877	-0.22380
H	2.34548	7.24684	-2.23354
H	3.58045	6.19571	1.75087
H	3.43917	7.86770	-0.08647

1 imaginary frequency: -397.23 cm^{-1}.

SCF energy: -4055.668644 hartree
zero-point correction: +1.542329 hartree
enthalpy correction: +1.617443 hartree
free energy correction: +1.424813 hartree
quasiharmonic free energy correction: +1.452229 hartree

TS(*R*)_B1

C	0.34665	-4.60797	-0.35672
O	1.32240	-1.72807	-0.85858
O	-0.90033	-1.86468	0.45044
C	-1.60831	-2.78658	-0.33910
C	-0.97135	-3.94953	-0.76435
C	-2.95082	-2.50746	-0.66219
C	-1.63587	-4.78617	-1.67687
C	-3.61610	-3.44424	-1.46999
C	-2.96290	-4.55010	-2.01456
H	-4.66076	-3.27023	-1.70514
H	-3.49028	-5.21393	-2.69510
C	2.06988	-2.59599	-0.04685
C	1.57260	-3.87670	0.18890
C	3.30912	-2.17273	0.47279
C	2.29230	-4.73707	1.03549
C	4.04131	-3.10632	1.22489
C	3.53697	-4.36904	1.53136
H	5.01361	-2.80866	1.60541
H	4.10661	-5.04709	2.16199
C	-0.71052	-5.87623	-2.17374
H	-0.97613	-6.85631	-1.75414
H	-0.74526	-5.98243	-3.26397
C	0.66932	-5.40023	-1.66698
H	1.11936	-4.71463	-2.39398
H	1.37528	-6.21916	-1.49845
C	1.51528	-6.00786	1.29483
H	1.92217	-6.85238	0.72121
H	1.53718	-6.30415	2.34969
C	0.10226	-5.62826	0.80956
H	-0.44187	-5.11978	1.61411
H	-0.49683	-6.48739	0.49416

C	-3.66424	-1.27024	-0.19750	H	-6.08394	-0.09094	-3.17323
C	-3.88278	-1.04135	1.18639	H	-5.78449	-1.78960	-2.85341
C	-4.17346	-0.34310	-1.14647	C	-3.24733	0.49080	-4.86896
C	-4.57943	0.10447	1.58606	H	-4.11161	1.59147	-3.22909
C	-4.87668	0.77660	-0.68322	H	-2.47625	1.01065	-2.91457
C	-5.08965	1.02919	0.67203	C	-4.56193	0.07158	-5.54276
H	-4.74218	0.26797	2.64792	H	-6.15272	-1.39375	-5.29195
H	-5.27678	1.47957	-1.40956	H	-4.53399	-2.01889	-4.98869
C	3.84900	-0.78383	0.29719	H	-2.49447	-0.29736	-5.01345
C	4.26176	-0.32662	-0.97756	H	-2.84061	1.39319	-5.34084
C	4.00153	0.05828	1.43258	H	-5.27266	0.91124	-5.50523
C	4.79920	0.96220	-1.09139	H	-4.39578	-0.14808	-6.60546
C	4.54203	1.33702	1.25417	C	3.64863	-0.37694	2.85649
C	4.94796	1.81367	0.00401	C	4.92324	-0.53046	3.72385
H	5.12646	1.31041	-2.06770	C	2.63935	0.55897	3.56299
H	4.66031	1.97691	2.12480	H	3.17072	-1.36023	2.81068
C	-3.44081	-2.01967	2.27111	C	4.60047	-1.00701	5.14793
C	-2.49653	-1.37404	3.31155	H	5.44381	0.43661	3.77457
C	-4.64785	-2.67771	2.98310	H	5.62166	-1.22602	3.24123
H	-2.88286	-2.83437	1.79940	C	2.32305	0.08328	4.99074
C	-2.04004	-2.39263	4.36697	H	3.03767	1.58251	3.60439
H	-1.63072	-0.93936	2.80122	H	1.71544	0.59298	2.97768
H	-3.01726	-0.54856	3.81852	C	3.59332	-0.07579	5.83694
C	-4.19396	-3.69124	4.04612	H	5.52373	-1.07606	5.73796
H	-5.29116	-3.16775	2.24112	H	4.18164	-2.02348	5.10362
H	-5.26115	-1.89974	3.45965	H	1.62989	0.78588	5.47172
C	-3.23551	-3.05726	5.06537	H	1.79958	-0.88302	4.93985
H	-1.39085	-1.90309	5.10484	H	4.05668	0.91137	5.98484
H	-1.42738	-3.16624	3.87994	H	3.34240	-0.45585	6.83570
H	-3.68635	-4.53147	3.54873	C	5.56713	3.19173	-0.16446
H	-5.06817	-4.11563	4.55691	C	4.63543	4.33502	0.29724
H	-2.88913	-3.81276	5.78266	C	6.93856	3.30528	0.54350
H	-3.77925	-2.29912	5.64903	H	5.74714	3.33771	-1.24022
C	-5.83971	2.27276	1.12133	C	5.27562	5.71593	0.08838
C	-4.90351	3.30054	1.80053	H	4.39446	4.20313	1.36143
C	-7.04296	1.95528	2.03807	H	3.68305	4.27317	-0.24449
H	-6.24206	2.75481	0.21727	C	7.57818	4.68647	0.33519
C	-5.65720	4.56991	2.22688	H	7.60629	2.51530	0.17757
H	-4.08514	3.55800	1.11583	H	6.80455	3.12409	1.61989
H	-4.44152	2.83455	2.68356	C	6.64133	5.81765	0.78386
C	-7.79507	3.22805	2.45666	H	5.40434	5.89522	-0.98929
H	-7.72077	1.26012	1.52695	H	4.60175	6.50111	0.45527
H	-6.68884	1.43642	2.94027	H	7.81681	4.81667	-0.73084
C	-6.85696	4.24205	3.12772	H	8.53158	4.74312	0.87613
H	-6.01289	5.09551	1.32831	H	7.09916	6.79458	0.58257
H	-4.97259	5.25914	2.73800	H	6.49801	5.75790	1.87324
H	-8.24990	3.68941	1.56731	C	4.22482	-1.21361	-2.21789
H	-8.62264	2.96977	3.12984	C	3.52900	-0.55274	-3.42898
H	-7.40460	5.15895	3.38079	C	5.64813	-1.68423	-2.60885
H	-6.49263	3.82322	4.07791	H	3.65500	-2.11759	-1.97977
C	-4.01602	-0.51147	-2.65684	C	3.49844	-1.49592	-4.64086
C	-5.35611	-0.90006	-3.33238	H	4.06288	0.36479	-3.71206
C	-3.43454	0.73500	-3.36371	H	2.51348	-0.24288	-3.16140
H	-3.30784	-1.32568	-2.83952	C	5.62234	-2.61800	-3.82916
C	-5.18379	-1.14365	-4.83969	H	6.27073	-0.80569	-2.83188

H	6.11821	-2.18866	-1.75453
C	4.90759	-1.97077	-5.02484
H	3.01979	-0.99187	-5.48961
H	2.87242	-2.36999	-4.40544
H	5.10154	-3.54879	-3.55858
H	6.64641	-2.90377	-4.10364
H	5.49614	-1.10882	-5.37319
H	4.85962	-2.67547	-5.86541
P	0.13287	-0.82874	-0.22469
O	-0.60265	-0.27889	-1.49409
O	0.58396	0.13536	0.82351
H	-0.19094	0.45462	-2.09076
H	1.13932	1.74020	1.19854
Cl	0.34668	2.01451	-3.12246
O	1.09771	2.73300	1.10391
C	0.85903	2.78232	-0.68179
C	-0.33612	3.08785	1.17302
C	-0.60281	3.09985	-0.34471
H	1.21458	1.78708	-0.86006
H	1.52238	3.57728	-1.00067
H	-0.88115	2.33314	1.74086
H	-0.40531	4.06166	1.65761
H	-1.23829	2.26731	-0.64609
C	-1.15150	4.39694	-0.90032
C	-2.33263	4.39430	-1.65026
C	-0.51237	5.62062	-0.65481
C	-2.86587	5.58674	-2.14213
H	-2.82754	3.45075	-1.86075
C	-1.03963	6.81245	-1.15057
H	0.40888	5.64999	-0.07530
C	-2.22116	6.79873	-1.89468
H	-3.78181	5.56528	-2.72640
H	-0.52789	7.75110	-0.95538
H	-2.63334	7.72694	-2.28108

1 imaginary frequency: -381.36 cm^{-1}.

SCF energy: -4055.669313 hartree
zero-point correction: +1.542722 hartree
enthalpy correction: +1.617667 hartree
free energy correction: +1.426757 hartree
quasiharmonic free energy correction: +1.452625 hartree

TS(*R*)_B2

C	0.37965	-4.53404	-0.83706
O	1.37721	-1.61674	-0.88323
O	-0.93136	-1.91704	0.23794
C	-1.57577	-2.71700	-0.72139
C	-0.90655	-3.81797	-1.24944
C	-2.88903	-2.38247	-1.10726
C	-1.49962	-4.51870	-2.31325
C	-3.48889	-3.19268	-2.08487
C	-2.79537	-4.22369	-2.71934
H	-4.51099	-2.97549	-2.37730
H	-3.26741	-4.78433	-3.52234
C	2.07401	-2.59036	-0.15036
C	1.56463	-3.88746	-0.11940
C	3.27741	-2.24850	0.49849
C	2.22875	-4.85696	0.65104
C	3.96198	-3.27960	1.16288
C	3.43983	-4.56778	1.26769
H	4.90790	-3.04214	1.63996
H	3.96863	-5.32738	1.83802
C	-0.54019	-5.54371	-2.87884
H	-0.83786	-6.56760	-2.61330
H	-0.49257	-5.50555	-3.97309
C	0.79760	-5.15257	-2.21267
H	1.30050	-4.38213	-2.80822
H	1.48914	-5.99329	-2.10149
C	1.43506	-6.14311	0.69520
H	1.87863	-6.91315	0.04863
H	1.38604	-6.56933	1.70366
C	0.05751	-5.69251	0.16927
H	-0.53926	-5.28550	0.99405
H	-0.51967	-6.49920	-0.29202
C	-3.63078	-1.21069	-0.53194
C	-3.94804	-1.17174	0.85129
C	-4.05491	-0.14933	-1.37565
C	-4.64408	-0.07040	1.36072
C	-4.76306	0.91806	-0.80756
C	-5.06161	0.99038	0.55310
H	-4.88184	-0.05217	2.42101
H	-5.09611	1.72683	-1.45316
C	3.82194	-0.85103	0.54921
C	4.30290	-0.21957	-0.62516
C	3.90853	-0.17658	1.79621
C	4.83420	1.07269	-0.53261
C	4.46119	1.10985	1.82597
C	4.93047	1.75759	0.68159
H	5.20232	1.54629	-1.43782
H	4.53855	1.62533	2.78046
C	-3.62844	-2.31865	1.80585
C	-2.78190	-1.88453	3.02459
C	-4.91587	-3.03818	2.27786
H	-3.04153	-3.06769	1.26544
C	-2.45925	-3.07791	3.93737
H	-1.85862	-1.40800	2.67775
H	-3.33108	-1.13114	3.60749
C	-4.59535	-4.22735	3.19671
H	-5.48984	-3.37598	1.40558
H	-5.55824	-2.32546	2.81451
C	-3.73380	-3.80272	4.39524
H	-1.87989	-2.73958	4.80640
H	-1.81573	-3.78456	3.39178
H	-4.05797	-4.99470	2.61948
H	-5.52608	-4.69538	3.54311
H	-3.47804	-4.67617	5.00915
H	-4.31935	-3.12921	5.03903

C	-5.80900	2.18544	1.12150
C	-4.91863	3.03620	2.05762
C	-7.11954	1.79065	1.83989
H	-6.08803	2.82880	0.27309
C	-5.66651	4.25965	2.60991
H	-4.01995	3.35614	1.51423
H	-4.57580	2.40911	2.89389
C	-7.86519	3.01909	2.38396
H	-7.76098	1.22744	1.15050
H	-6.88908	1.11185	2.67359
C	-6.97259	3.85748	3.31054
H	-5.89667	4.94520	1.78091
H	-5.01822	4.81537	3.29977
H	-8.19821	3.64301	1.54101
H	-8.77311	2.70222	2.91313
H	-7.51113	4.75039	3.65299
H	-6.73518	3.27111	4.21102
C	-3.80155	-0.11499	-2.88201
C	-5.10276	-0.36015	-3.68751
C	-3.14191	1.19605	-3.37019
H	-3.10526	-0.92123	-3.13276
C	-4.83797	-0.39658	-5.20110
H	-5.82084	0.44135	-3.45988
H	-5.58112	-1.29428	-3.36619
C	-2.85821	1.15253	-4.87911
H	-3.80712	2.04759	-3.16397
H	-2.21076	1.37867	-2.82715
C	-4.13470	0.88008	-5.68652
H	-5.78173	-0.54453	-5.74274
H	-4.20544	-1.26673	-5.43211
H	-2.12007	0.36343	-5.08275
H	-2.39433	2.09472	-5.19418
H	-4.82188	1.73301	-5.57731
H	-3.90366	0.80201	-6.75692
C	3.46776	-0.79610	3.12375
C	4.68225	-1.08075	4.04313
C	2.42022	0.05095	3.88472
H	2.98943	-1.75790	2.91535
C	4.26301	-1.74097	5.36539
H	5.20189	-0.13599	4.25744
H	5.40834	-1.71412	3.51778
C	2.00549	-0.60952	5.20969
H	2.82292	1.05200	4.09308
H	1.53765	0.18083	3.25137
C	3.21557	-0.89982	6.10814
H	5.14470	-1.90142	5.99953
H	3.84393	-2.73632	5.15517
H	1.28528	0.03118	5.73527
H	1.48192	-1.55248	4.99312
H	3.67162	0.05128	6.42187
H	2.89671	-1.41065	7.02592
C	5.51835	3.15683	0.77806
C	6.90268	3.28734	0.10387
C	4.55136	4.23160	0.22724
H	5.66043	3.37394	1.84793
C	7.47712	4.70493	0.25123
H	6.81441	3.04892	-0.96526
H	7.59162	2.54808	0.53152
C	5.12837	5.64958	0.36059
H	3.59503	4.16068	0.76178
H	4.34027	4.01700	-0.83036
C	6.51067	5.76400	-0.29889
H	7.67162	4.90895	1.31489
H	8.44611	4.77048	-0.25997
H	5.21616	5.90428	1.42750
H	4.43508	6.37878	-0.07809
H	6.92132	6.77063	-0.14849
H	6.40540	5.62786	-1.38539
C	4.35505	-0.93207	-1.97318
C	3.70063	-0.13562	-3.12378
C	5.81067	-1.31114	-2.34415
H	3.80408	-1.87433	-1.88779
C	3.75964	-0.91513	-4.44614
H	4.21810	0.82452	-3.25754
H	2.66398	0.11109	-2.87322
C	5.87667	-2.07838	-3.67394
H	6.41540	-0.39573	-2.41924
H	6.25387	-1.90981	-1.53765
C	5.20017	-1.30119	-4.81301
H	3.30687	-0.31879	-5.24792
H	3.15122	-1.82800	-4.35578
H	5.37558	-3.05070	-3.55324
H	6.92216	-2.29778	-3.92800
H	5.77675	-0.38663	-5.01847
H	5.21557	-1.89289	-5.73775
P	0.14532	-0.80584	-0.21251
O	-0.49999	-0.07756	-1.44072
O	0.52002	0.00122	0.98764
H	-0.04329	0.71934	-1.90922
H	1.03450	1.54153	1.59709
Cl	0.55971	2.39330	-2.69942
O	0.99578	2.53909	1.62843
C	0.88259	2.82164	-0.14479
C	-0.44093	2.89098	1.64382
C	-0.59886	3.11014	0.12673
H	1.24574	1.85363	-0.42770
H	1.57027	3.64165	-0.31106
H	-1.02206	2.06926	2.06348
H	-0.54811	3.79015	2.25020
H	-1.21473	2.33467	-0.32823
C	-1.09955	4.47747	-0.28818
C	-2.20468	4.59157	-1.13852
C	-0.48940	5.64841	0.18418
C	-2.69177	5.84651	-1.50737
H	-2.67500	3.69170	-1.52387
C	-0.97099	6.90318	-0.18698
H	0.37394	5.58699	0.84472
C	-2.07689	7.00546	-1.03332
H	-3.54837	5.91643	-2.17232
H	-0.48269	7.80007	0.18477

H	-2.45358	7.98263	-1.32320

1 imaginary frequency: -377.40 cm^{-1}.

SCF energy: -4055.669950 hartree
zero-point correction: +1.542720 hartree
enthalpy correction: +1.617617 hartree
free energy correction: +1.427503 hartree
quasiharmonic free energy correction: +1.452606 hartree

TS(*R*)_B3

C	0.42412	-4.55711	-0.75187
O	-0.83862	-1.95169	0.41151
O	1.30210	-1.61576	-0.99665
C	2.11211	-2.53936	-0.31704
C	1.65947	-3.85178	-0.19379
C	3.36553	-2.13516	0.18313
C	2.44470	-4.77456	0.51789
C	4.15931	-3.11953	0.79458
C	3.70395	-4.42276	0.98809
H	5.14187	-2.83351	1.15707
H	4.32311	-5.14591	1.51307
C	-1.57033	-2.80833	-0.42899
C	-0.93083	-3.89887	-1.01257
C	-2.93555	-2.53739	-0.64495
C	-1.62558	-4.65132	-1.97433
C	-3.62330	-3.40141	-1.51284
C	-2.97514	-4.42033	-2.21145
H	-4.68419	-3.23678	-1.66850
H	-3.52421	-5.02179	-2.93167
C	1.71551	-6.08953	0.67653
H	2.11406	-6.85491	-0.00411
H	1.80032	-6.49582	1.69081
C	0.26968	-5.70507	0.30603
H	-0.24446	-5.30386	1.18729
H	-0.32301	-6.54343	-0.07119
C	-0.70295	-5.65130	-2.63832
H	-0.91963	-6.67937	-2.31701
H	-0.79721	-5.63806	-3.73014
C	0.69136	-5.19046	-2.15739
H	1.08011	-4.41462	-2.82670
H	1.42742	-5.99938	-2.11961
C	3.85806	-0.71860	0.12770
C	4.03234	0.01214	1.33401
C	4.20566	-0.12596	-1.11048
C	4.53102	1.31823	1.26389
C	4.69338	1.18713	-1.11699
C	4.86492	1.93058	0.05236
H	4.67230	1.86944	2.18960
H	4.96649	1.64149	-2.06592
C	-3.65094	-1.38138	-0.00680
C	-3.80706	-1.32096	1.40108
C	-4.22457	-0.36307	-0.81803
C	-4.51551	-0.25024	1.96082
C	-4.92438	0.67841	-0.19840
C	-5.08254	0.76182	1.18729
H	-4.63985	-0.20974	3.04065
H	-5.36526	1.44934	-0.82429
C	3.75226	-0.57592	2.71852
C	5.07017	-0.79980	3.50187
C	2.77123	0.26389	3.57051
H	3.28185	-1.55564	2.58947
C	4.82650	-1.43243	4.88016
H	5.75228	-1.42640	2.91352
H	5.58042	0.16556	3.63092
C	2.53203	-0.36927	4.95160
H	1.81844	0.34947	3.03900
H	3.16292	1.28200	3.70473
C	3.84399	-0.59893	5.71418
H	5.77949	-1.54745	5.41299
H	4.41908	-2.44568	4.74670
H	2.01670	-1.33239	4.82053
H	1.85601	0.26565	5.53924
H	3.64593	-1.08992	6.67576
H	4.30270	0.37364	5.94801
C	5.45033	3.33285	-0.00326
C	6.90509	3.36675	0.52575
C	4.59632	4.38943	0.73213
H	5.48698	3.62733	-1.06303
C	7.51897	4.77129	0.42395
H	7.51387	2.64221	-0.02939
H	6.91129	3.03789	1.57530
C	5.20816	5.79452	0.62221
H	3.57487	4.38540	0.33098
H	4.50961	4.11783	1.79354
C	6.65486	5.82121	1.13777
H	7.61712	5.04569	-0.63692
H	8.53509	4.76733	0.83904
H	5.19272	6.11529	-0.42996
H	4.59326	6.51581	1.17613
H	7.08670	6.82192	1.00874
H	6.65678	5.61688	2.21902
C	4.16210	-0.90185	-2.42280
C	3.45637	-0.15347	-3.57432
C	5.58659	-1.32994	-2.85705
H	3.59877	-1.82584	-2.25688
C	3.41979	-1.00751	-4.85112
H	3.98700	0.78307	-3.79533
H	2.44204	0.13301	-3.27732
C	5.55848	-2.17198	-4.14216
H	6.19918	-0.43111	-3.01945
H	6.06803	-1.89170	-2.04597
C	4.82788	-1.44559	-5.28124
H	2.93053	-0.44707	-5.65737
H	2.80043	-1.89962	-4.67264
H	5.04849	-3.12478	-3.93550
H	6.58257	-2.42729	-4.44521
H	5.40792	-0.55704	-5.57256

H	4.77549	-2.08846	-6.16973
C	-4.14322	-0.35863	-2.34421
C	-5.50948	-0.71328	-2.98522
C	-3.63529	0.97478	-2.94012
H	-3.42506	-1.12474	-2.65275
C	-5.41989	-0.78653	-4.51727
H	-6.24668	0.05094	-2.69789
H	-5.88725	-1.66219	-2.58409
C	-3.53083	0.90201	-4.47149
H	-4.32399	1.78990	-2.67329
H	-2.65836	1.22745	-2.51823
C	-4.87135	0.51713	-5.11449
H	-6.40713	-1.01624	-4.93978
H	-4.75813	-1.61942	-4.79810
H	-3.17496	1.86254	-4.86287
H	-2.76721	0.15932	-4.74317
H	-5.60015	1.32463	-4.94566
H	-4.76092	0.42031	-6.20243
C	-5.85548	1.89855	1.83574
C	-5.22665	3.28292	1.55520
C	-7.34828	1.89740	1.43122
H	-5.81611	1.74108	2.92457
C	-6.00844	4.41808	2.23426
H	-5.20276	3.45899	0.47053
H	-4.18112	3.28684	1.88957
C	-8.12794	3.03304	2.11161
H	-7.79433	0.92558	1.67724
H	-7.42560	2.00680	0.33992
C	-7.49096	4.40245	1.83289
H	-5.92961	4.30904	3.32639
H	-5.55473	5.38560	1.98424
H	-8.14770	2.85800	3.19773
H	-9.17317	3.02309	1.77662
H	-8.03747	5.19247	2.36379
H	-7.57750	4.62951	0.75976
C	-3.27318	-2.39266	2.34671
C	-2.28222	-1.82089	3.38769
C	-4.41093	-3.16321	3.06017
H	-2.72411	-3.13435	1.75853
C	-1.72762	-2.92212	4.30370
H	-2.79420	-1.06912	4.00533
H	-1.46498	-1.30613	2.87179
C	-3.85627	-4.26128	3.98224
H	-5.01529	-2.46212	3.65313
H	-5.08603	-3.59930	2.31277
C	-2.85527	-3.69680	5.00149
H	-1.04769	-2.48531	5.04701
H	-1.12447	-3.62000	3.70353
H	-3.35471	-5.02606	3.37046
H	-4.68135	-4.76922	4.49853
H	-3.38407	-3.02074	5.69002
H	-2.44127	-4.50659	5.61638
P	0.12378	-0.82258	-0.21691
O	-0.69934	-0.18251	-1.38734
O	0.60396	0.05965	0.88931
H	-0.31156	0.57385	-1.97056
H	1.21452	1.63496	1.31821
Cl	0.20483	2.18370	-2.93919
O	1.18697	2.63212	1.27853
C	0.86505	2.78857	-0.48927
C	-0.23325	3.01077	1.43697
C	-0.56737	3.13277	-0.06262
H	1.53928	3.57892	-0.79654
H	1.17955	1.79460	-0.73718
H	-0.76958	2.22842	1.97499
H	-0.25954	3.94941	1.99046
H	-1.24770	2.34564	-0.38679
C	-1.08655	4.48254	-0.51115
C	-0.40112	5.66454	-0.19654
C	-2.28163	4.57036	-1.23304
C	-0.89761	6.90486	-0.59618
H	0.53254	5.62292	0.36197
C	-2.78349	5.81068	-1.62966
H	-2.81215	3.66022	-1.49693
C	-2.09357	6.98113	-1.31271
H	-0.35059	7.81050	-0.34794
H	-3.71066	5.86013	-2.19419
H	-2.48201	7.94684	-1.62471

1 imaginary frequency: -381.01 cm^{-1}.

SCF energy: -4055.669271 hartree
zero-point correction: +1.542766 hartree
enthalpy correction: +1.617696 hartree
free energy correction: +1.427004 hartree
quasiharmonic free energy correction: +1.452648 hartree

TS(*R*)_B4

C	0.33617	-4.44945	-1.19270
O	1.30991	-1.53276	-1.00518
O	-0.94328	-1.96412	0.19228
C	-1.63065	-2.68494	-0.80070
C	-0.97566	-3.71497	-1.46985
C	-2.96810	-2.34232	-1.07991
C	-1.61236	-4.31561	-2.56901
C	-3.60584	-3.05849	-2.10582
C	-2.93061	-4.00385	-2.87883
H	-4.64545	-2.83419	-2.32124
H	-3.43522	-4.48724	-3.71170
C	2.03925	-2.56124	-0.38804
C	1.54335	-3.86192	-0.46237
C	3.26009	-2.26715	0.25073
C	2.24531	-4.89197	0.18640
C	3.97631	-3.34665	0.79340
C	3.47259	-4.64623	0.78959
H	4.93431	-3.14211	1.26130
H	4.02854	-5.44968	1.26635
C	-0.66844	-5.26145	-3.28058

H	-0.94017	-6.31179	-3.10653	H	-8.18966	2.79787	3.13823
H	-0.67444	-5.11211	-4.36627	H	-9.02548	3.33801	1.68630
C	0.69553	-4.91713	-2.64160	H	-5.86647	3.92763	3.74818
H	1.15949	-4.08114	-3.17732	H	-5.23506	5.17346	2.67554
H	1.40234	-5.75246	-2.64853	H	-7.75121	5.21433	2.77802
C	1.47077	-6.18898	0.12791	H	-7.16964	4.89566	1.14650
H	1.90019	-6.88105	-0.60998	C	-3.99180	0.10318	-2.52221
H	1.46585	-6.71664	1.08841	C	-5.32258	-0.08229	-3.29469
C	0.06896	-5.71025	-0.29807	C	-3.38442	1.47953	-2.88002
H	-0.50007	-5.39977	0.58606	H	-3.28897	-0.64890	-2.89405
H	-0.51533	-6.47527	-0.81758	C	-5.12915	0.06796	-4.81167
C	-3.70153	-1.26475	-0.33481	H	-6.04708	0.66606	-2.94127
C	-3.96209	-1.40774	1.05136	H	-5.76350	-1.06094	-3.06591
C	-4.17933	-0.11496	-1.02159	C	-3.17372	1.62497	-4.39457
C	-4.66662	-0.39740	1.71706	H	-4.05456	2.28256	-2.53887
C	-4.87896	0.85941	-0.30008	H	-2.42977	1.61434	-2.36400
C	-5.12935	0.74790	1.06984	C	-4.48116	1.41345	-5.17074
H	-4.87059	-0.51165	2.77928	H	-6.09403	-0.04193	-5.32442
H	-5.24104	1.73545	-0.83115	H	-4.48820	-0.74962	-5.17380
C	3.79990	-0.87577	0.41136	H	-2.42738	0.88857	-4.72456
C	4.27900	-0.15464	-0.71089	H	-2.74699	2.61062	-4.61501
C	3.89697	-0.30690	1.70852	H	-5.18283	2.22626	-4.92833
C	4.82750	1.11886	-0.51510	H	-4.29966	1.47114	-6.25186
C	4.46261	0.96751	1.84110	C	3.46611	-1.03750	2.98145
C	4.93731	1.69985	0.75145	C	4.69461	-1.42749	3.84252
H	5.20064	1.66023	-1.37938	C	2.45194	-0.24918	3.84417
H	4.54953	1.40250	2.83397	H	2.96512	-1.96688	2.69295
C	-3.56167	-2.64368	1.85128	C	4.29283	-2.20672	5.10339
C	-2.66709	-2.30938	3.06765	H	5.23284	-0.51465	4.13584
C	-4.79898	-3.45794	2.30245	H	5.40003	-2.01629	3.24280
H	-2.97898	-3.30551	1.20306	C	2.05363	-1.02969	5.10770
C	-2.26238	-3.57722	3.83546	H	2.87990	0.71884	4.14070
H	-1.77784	-1.76717	2.72872	H	1.55855	-0.04136	3.24761
H	-3.20802	-1.63872	3.75052	C	3.27647	-1.42486	5.94701
C	-4.39351	-4.72258	3.07568	H	5.18492	-2.44127	5.69880
H	-5.40357	-3.72506	1.42631	H	3.85235	-3.17060	4.80762
H	-5.43735	-2.83017	2.94033	H	1.35520	-0.43285	5.70885
C	-3.48974	-4.39078	4.27236	H	1.50958	-1.93892	4.81166
H	-1.65206	-3.30886	4.70779	H	3.75610	-0.51577	6.34018
H	-1.62471	-4.20137	3.19115	H	2.96706	-2.01643	6.81838
H	-3.85836	-5.40409	2.39755	C	5.55872	3.07222	0.95792
H	-5.28971	-5.26016	3.41200	C	6.97772	3.18840	0.35608
H	-3.17704	-5.31251	4.78018	C	4.65714	4.21161	0.42723
H	-4.06497	-3.80889	5.00826	H	5.65714	3.22269	2.04392
C	-5.86870	1.82980	1.83923	C	7.59339	4.57345	0.60817
C	-7.29628	2.08131	1.30180	H	6.93142	3.00965	-0.72728
C	-5.07365	3.15595	1.88856	H	7.61926	2.40210	0.77335
H	-5.97279	1.47828	2.87725	C	5.27636	5.59722	0.66918
C	-8.02937	3.16148	2.11217	H	3.67430	4.14639	0.91214
H	-7.86353	1.14217	1.31320	H	4.48998	4.06717	-0.65006
H	-7.23832	2.39613	0.25005	C	6.69035	5.69708	0.07841
C	-5.80884	4.23803	2.69405	H	7.74645	4.71119	1.68907
H	-4.08011	2.97078	2.31750	H	8.58631	4.63123	0.14408
H	-4.90499	3.51579	0.86350	H	5.32419	5.78658	1.75205
C	-7.22981	4.47202	2.16013	H	4.62955	6.37577	0.24458

H	7.12843	6.67755	0.30485
H	6.62996	5.62681	-1.01776
C	4.31728	-0.76101	-2.11035
C	3.73608	0.15627	-3.20852
C	5.75774	-1.19491	-2.48115
H	3.71044	-1.67230	-2.10776
C	3.78470	-0.52271	-4.58577
H	4.31131	1.09142	-3.25987
H	2.70867	0.44340	-2.96138
C	5.81410	-1.86066	-3.86488
H	6.41261	-0.31143	-2.47200
H	6.14722	-1.87775	-1.71485
C	5.21054	-0.95991	-4.95265
H	3.38452	0.15776	-5.34752
H	3.12531	-1.40386	-4.57966
H	5.25671	-2.80890	-3.83087
H	6.85180	-2.11954	-4.11367
H	5.84192	-0.06647	-5.07165
H	5.21677	-1.47709	-5.92111
P	0.09223	-0.80169	-0.22382
O	-0.62204	-0.00259	-1.36799
O	0.50708	-0.06877	1.01061
H	-0.16229	0.78248	-1.85162
H	1.16204	1.42989	1.61432
Cl	0.47649	2.45242	-2.62849
O	1.18386	2.42692	1.66807
C	0.99052	2.77080	-0.09161
C	-0.22465	2.86436	1.77351
C	-0.44676	3.15804	0.27708
H	1.26680	1.78816	-0.41802
H	1.72699	3.54330	-0.27514
H	-0.83306	2.06017	2.18861
H	-0.24657	3.74010	2.42196
H	-1.14618	2.45224	-0.17068
C	-0.85554	4.57663	-0.06035
C	-1.97859	4.81180	-0.86049
C	-0.13766	5.67571	0.43224
C	-2.37885	6.11476	-1.15984
H	-2.53145	3.96802	-1.26256
C	-0.53269	6.97874	0.13087
H	0.74255	5.52009	1.05395
C	-1.65777	7.20186	-0.66526
H	-3.25118	6.27858	-1.78675
H	0.03822	7.81861	0.51785
H	-1.96708	8.21658	-0.90078

1 imaginary frequency: -382.04 cm^{-1}.

SCF energy: -4055.669566 hartree
zero-point correction: +1.542909 hartree
enthalpy correction: +1.617786 hartree
free energy correction: +1.427407 hartree
quasiharmonic free energy correction: +1.452839 hartree

TS(*R*)_C3

C	-0.89072	-3.88926	-1.91711
O	0.78695	-1.39963	-1.21598
O	-1.57147	-1.42174	-0.14344
C	-2.40630	-1.81881	-1.20396
C	-1.97209	-2.82275	-2.06456
C	-3.65664	-1.19097	-1.36725
C	-2.68366	-3.05621	-3.25183
C	-4.39940	-1.55077	-2.50511
C	-3.90236	-2.42534	-3.47322
H	-5.37906	-1.10441	-2.64132
H	-4.47584	-2.62063	-4.37607
C	1.15450	-2.66265	-0.72540
C	0.35666	-3.76236	-1.04436
C	2.34624	-2.80462	0.01282
C	0.71604	-5.02780	-0.55012
C	2.70405	-4.10238	0.41464
C	1.89512	-5.20730	0.16151
H	3.63473	-4.22964	0.95802
H	2.18142	-6.19121	0.52451
C	-1.93534	-4.03512	-4.13397
H	-2.44857	-5.00475	-4.18954
H	-1.84105	-3.67315	-5.16440
C	-0.56646	-4.15948	-3.42180
H	0.11770	-3.38304	-3.78315
H	-0.08429	-5.12942	-3.57836
C	-0.33253	-6.05976	-0.89358
H	-0.00830	-6.69756	-1.72819
H	-0.55568	-6.72829	-0.05447
C	-1.53120	-5.18000	-1.29071
H	-2.09115	-4.89324	-0.39291
H	-2.22978	-5.67150	-1.97398
C	-4.21706	-0.21673	-0.37209
C	-4.49515	-0.63904	0.95355
C	-4.54365	1.11027	-0.76060
C	-5.06671	0.27165	1.84957
C	-5.12238	1.97074	0.17883
C	-5.38707	1.58083	1.49315
H	-5.27947	-0.05583	2.86438
H	-5.37225	2.98270	-0.12790
C	3.25408	-1.66776	0.38632
C	4.09065	-1.07729	-0.58918
C	3.36100	-1.26595	1.74387
C	4.99677	-0.08355	-0.19288
C	4.29251	-0.28015	2.08075
C	5.11805	0.33178	1.13489
H	5.65261	0.36044	-0.93981
H	4.37201	0.02190	3.11999
C	-4.26496	-2.06491	1.44593
C	-3.33320	-2.13447	2.67815
C	-5.60264	-2.78678	1.74112
H	-3.77881	-2.63803	0.65036
C	-3.10768	-3.58504	3.13231
H	-2.37784	-1.65369	2.44216

H	-3.77571	-1.56676	3.50883
C	-5.37469	-4.23549	2.20012
H	-6.14920	-2.23977	2.52238
H	-6.23815	-2.76651	0.84637
C	-4.43509	-4.30511	3.41293
H	-2.46810	-3.60215	4.02444
H	-2.55883	-4.12815	2.34783
H	-4.93768	-4.81240	1.37097
H	-6.33648	-4.71033	2.43453
H	-4.25201	-5.35074	3.69313
H	-4.92609	-3.83223	4.27673
C	-5.99640	2.53614	2.50516
C	-7.39902	3.03379	2.08639
C	-5.06980	3.73700	2.80890
H	-6.11994	1.97776	3.44564
C	-8.00731	3.97542	3.13724
H	-8.05905	2.17402	1.91504
H	-7.32377	3.56410	1.12611
C	-5.68017	4.67891	3.85800
H	-4.09175	3.37143	3.14474
H	-4.88933	4.29653	1.87966
C	-7.07794	5.16016	3.44154
H	-8.18923	3.41210	4.06464
H	-8.98633	4.33598	2.79579
H	-5.75177	4.15032	4.82019
H	-5.01466	5.53572	4.02353
H	-7.51297	5.79320	4.22562
H	-6.99059	5.79052	2.54378
C	-4.30614	1.65165	-2.16869
C	-5.63330	1.85671	-2.94048
C	-3.49882	2.96992	-2.18047
H	-3.71216	0.91878	-2.72500
C	-5.39099	2.35669	-4.37295
H	-6.25299	2.58554	-2.39846
H	-6.21046	0.92393	-2.95944
C	-3.23980	3.46143	-3.61331
H	-4.04589	3.75058	-1.63482
H	-2.55695	2.82167	-1.64201
C	-4.55305	3.64314	-4.38841
H	-6.35034	2.52066	-4.88089
H	-4.86544	1.57604	-4.94291
H	-2.60636	2.73262	-4.14036
H	-2.67450	4.40154	-3.59075
H	-5.13327	4.45695	-3.92827
H	-4.34781	3.95216	-5.42158
C	2.53958	-1.90178	2.86450
C	3.40867	-2.85379	3.72542
C	1.83777	-0.87875	3.78861
H	1.74797	-2.50632	2.40754
C	2.58198	-3.56019	4.81089
H	4.21303	-2.27024	4.19672
H	3.90432	-3.59759	3.08974
C	0.99594	-1.58512	4.86341
H	2.58622	-0.24746	4.28697
H	1.21236	-0.20635	3.19667
C	1.84069	-2.55423	5.70283
H	3.23215	-4.20401	5.41822
H	1.84977	-4.22359	4.32668
H	0.51907	-0.83786	5.51046
H	0.18005	-2.14119	4.37742
H	2.57661	-1.97988	6.28549
H	1.21072	-3.08250	6.43060
C	6.14752	1.37472	1.54102
C	5.54479	2.53796	2.36111
C	7.33146	0.73734	2.30758
H	6.56204	1.80460	0.61495
C	6.61017	3.57985	2.73387
H	5.10025	2.13996	3.28337
H	4.72067	3.00242	1.80900
C	8.39414	1.77827	2.69317
H	7.77964	-0.05924	1.69976
H	6.94580	0.25377	3.21675
C	7.78606	2.94305	3.48885
H	6.98691	4.06159	1.81819
H	6.15632	4.37663	3.33656
H	8.86203	2.17170	1.77792
H	9.19643	1.29883	3.26926
H	8.55482	3.69574	3.70762
H	7.42954	2.56918	4.46021
C	4.09661	-1.54053	-2.04281
C	3.73488	-0.41398	-3.03652
C	5.44522	-2.19170	-2.43374
H	3.33232	-2.31678	-2.15815
C	3.73649	-0.90973	-4.49119
H	4.45190	0.41346	-2.93581
H	2.74725	-0.01687	-2.77264
C	5.44019	-2.68597	-3.88852
H	6.25694	-1.46268	-2.30071
H	5.66075	-3.02215	-1.74967
C	5.07650	-1.55911	-4.86664
H	3.51270	-0.07871	-5.17365
H	2.92884	-1.64545	-4.62180
H	4.71003	-3.50253	-3.99126
H	6.41961	-3.11069	-4.14404
H	5.86691	-0.79387	-4.84650
H	5.03931	-1.94242	-5.89454
P	-0.32993	-0.45244	-0.51778
O	0.14428	-0.05908	0.91977
O	-0.65209	0.62945	-1.49759
H	0.64526	0.82696	1.08563
H	-0.47675	2.08766	-2.34159
Cl	1.47854	2.55847	1.52052
O	-0.08808	2.99394	-2.51616
C	0.61933	3.23456	-0.89273
C	1.30911	2.78950	-2.95616
C	1.96934	3.00293	-1.57859
H	0.08252	2.43544	-0.42444
H	0.31821	4.23827	-0.61439
H	1.42120	1.79407	-3.38813
H	1.53336	3.55699	-3.69687

H	2.42512	2.09125	-1.19136
C	2.96189	4.14411	-1.51300
C	4.27890	3.90274	-1.10910
C	2.60076	5.44471	-1.89314
C	5.21674	4.93655	-1.08565
H	4.56466	2.90074	-0.80208
C	3.53418	6.48025	-1.86500
H	1.58211	5.65817	-2.21290
C	4.84726	6.22789	-1.46238
H	6.23522	4.73157	-0.76711
H	3.23588	7.48342	-2.15764
H	5.57569	7.03386	-1.44058

1 imaginary frequency: -384.25 cm^{-1}.

SCF energy: -4055.662939 hartree
zero-point correction: +1.542689 hartree
enthalpy correction: +1.617515 hartree
free energy correction: +1.428713 hartree
quasiharmonic free energy correction: +1.452307 hartree

TS(*R*)_C4

C	-1.02075	-3.82988	-1.96196
O	0.76561	-1.42018	-1.25036
O	-1.62001	-1.29376	-0.25311
C	-2.44089	-1.66498	-1.33331
C	-2.03730	-2.70890	-2.16110
C	-3.65068	-0.97500	-1.54588
C	-2.72747	-2.92987	-3.36340
C	-4.38007	-1.32071	-2.69680
C	-3.90430	-2.24105	-3.63226
H	-5.33080	-0.82736	-2.86960
H	-4.46273	-2.42603	-4.54664
C	1.05400	-2.69284	-0.73352
C	0.20874	-3.75418	-1.05887
C	2.21651	-2.88498	0.03892
C	0.48829	-5.02901	-0.53784
C	2.49831	-4.19420	0.46339
C	1.63995	-5.25970	0.20337
H	3.40685	-4.36111	1.03290
H	1.86601	-6.25188	0.58582
C	-2.01041	-3.96646	-4.20432
H	-2.57507	-4.90740	-4.25549
H	-1.86831	-3.63209	-5.23859
C	-0.67084	-4.14998	-3.45134
H	0.06505	-3.42051	-3.80884
H	-0.23884	-5.14804	-3.57396
C	-0.60802	-6.00787	-0.88842
H	-0.30151	-6.67837	-1.70392
H	-0.88680	-6.64702	-0.04306
C	-1.74666	-5.07014	-1.32899
H	-2.30959	-4.73534	-0.45000
H	-2.45620	-5.53464	-2.01974
C	-4.18737	0.05340	-0.59270
C	-4.52320	-0.31638	0.73767
C	-4.43871	1.38067	-1.02726
C	-5.07933	0.64215	1.59071
C	-5.00441	2.29244	-0.12736
C	-5.32770	1.95533	1.18599
H	-5.33560	0.34683	2.60452
H	-5.19895	3.30844	-0.46202
C	3.16118	-1.78675	0.43383
C	4.03732	-1.22102	-0.52155
C	3.25322	-1.39341	1.79514
C	4.96666	-0.25877	-0.10231
C	4.20826	-0.43877	2.15499
C	5.07242	0.14950	1.22896
H	5.65207	0.16633	-0.83345
H	4.27506	-0.14221	3.19671
C	-4.36435	-1.73450	1.27841
C	-3.46087	-1.79939	2.53184
C	-5.73437	-2.39563	1.56804
H	-3.88580	-2.35205	0.51245
C	-3.29740	-3.24177	3.03443
H	-2.48436	-1.36027	2.30224
H	-3.89982	-1.19092	3.33517
C	-5.56865	-3.83689	2.07487
H	-6.27480	-1.80495	2.32127
H	-6.35151	-2.37959	0.66042
C	-4.65608	-3.90396	3.30845
H	-2.67708	-3.25415	3.94014
H	-2.75323	-3.82843	2.27863
H	-5.13656	-4.45365	1.27221
H	-6.55149	-4.26980	2.30307
H	-4.51799	-4.94671	3.62308
H	-5.14615	-3.38753	4.14753
C	-5.92386	2.98662	2.12871
C	-5.00047	3.28413	3.33341
C	-7.33766	2.59879	2.61993
H	-6.02668	3.92444	1.56138
C	-5.59779	4.35439	4.25975
H	-4.01321	3.59740	2.97247
H	-4.84138	2.35759	3.90341
C	-7.93306	3.67070	3.54590
H	-7.99437	2.43105	1.75686
H	-7.28409	1.64269	3.16009
C	-7.00696	3.97003	4.73445
H	-5.64678	5.31250	3.72096
H	-4.93578	4.51564	5.12002
H	-8.09330	4.59541	2.97145
H	-8.92102	3.35154	3.90240
H	-7.43159	4.76915	5.35567
H	-6.94153	3.07769	5.37486
C	-4.13623	1.87326	-2.44059
C	-5.43017	2.11115	-3.25835
C	-3.27793	3.15856	-2.46369
H	-3.55596	1.10204	-2.95823
C	-5.12401	2.55480	-4.69713

H	-6.03167	2.88314	-2.75712
H	-6.04826	1.20495	-3.26731
C	-2.95300	3.59423	-3.90127
H	-3.81217	3.97583	-1.96041
H	-2.36010	2.99248	-1.89040
C	-4.23194	3.80398	-4.72581
H	-6.05984	2.74268	-5.23957
H	-4.61586	1.73495	-5.22642
H	-2.33289	2.82423	-4.38388
H	-2.35083	4.51145	-3.88766
H	-4.79143	4.65606	-4.31156
H	-3.98053	4.06966	-5.76084
C	2.39098	-2.00547	2.89846
C	3.22078	-2.96876	3.78487
C	1.68541	-0.96240	3.79698
H	1.59899	-2.59785	2.42694
C	2.35621	-3.65072	4.85630
H	4.02623	-2.39923	4.27113
H	3.71554	-3.72609	3.16444
C	0.80864	-1.64466	4.85970
H	2.43193	-0.33625	4.30452
H	1.08308	-0.28831	3.18300
C	1.61710	-2.62256	5.72428
H	2.97950	-4.30301	5.48247
H	1.62110	-4.30283	4.36113
H	0.33205	-0.88359	5.49065
H	-0.00691	-2.18994	4.36088
H	2.35229	-2.05762	6.31702
H	0.96210	-3.13180	6.44347
C	6.12289	1.16098	1.65949
C	5.53544	2.33849	2.47021
C	7.27332	0.49009	2.44810
H	6.56822	1.58143	0.74338
C	6.62038	3.35071	2.86706
H	5.06236	1.95050	3.38247
H	4.73474	2.82506	1.90295
C	8.35561	1.50168	2.85672
H	7.71209	-0.31718	1.84757
H	6.85731	0.01561	3.34869
C	7.76349	2.68086	3.64336
H	7.02770	3.82488	1.96062
H	6.17582	4.15762	3.46313
H	8.85128	1.88444	1.95163
H	9.13359	0.99991	3.44696
H	8.54781	3.41195	3.87944
H	7.37762	2.31459	4.60637
C	4.05644	-1.67647	-1.97755
C	3.73255	-0.53633	-2.96926
C	5.39658	-2.35284	-2.35430
H	3.27843	-2.43649	-2.10882
C	3.74229	-1.02424	-4.42652
H	4.46817	0.27293	-2.85420
H	2.75074	-0.11855	-2.71625
C	5.39960	-2.83986	-3.81160
H	6.22167	-1.64165	-2.20766
H	5.58641	-3.19097	-1.67201
C	5.07240	-1.70073	-4.78859
H	3.54575	-0.18496	-5.10739
H	2.92012	-1.74086	-4.57157
H	4.65325	-3.63983	-3.92762
H	6.37281	-3.28440	-4.05693
H	5.87892	-0.95294	-4.75500
H	5.03981	-2.07842	-5.81872
P	-0.31254	-0.40177	-0.59379
O	0.13999	-0.02742	0.85556
O	-0.53857	0.68995	-1.58934
H	0.66444	0.84129	1.04174
H	-0.27473	2.14138	-2.41923
Cl	1.53611	2.53960	1.52038
O	0.14131	3.03967	-2.57203
C	0.79156	3.25214	-0.92106
C	1.54975	2.81105	-2.96096
C	2.16127	2.99463	-1.55651
H	0.21907	2.46209	-0.48071
H	0.50203	4.26008	-0.64581
H	1.65926	1.81944	-3.40231
H	1.81734	3.58351	-3.68190
H	2.57966	2.06797	-1.16235
C	3.17980	4.10868	-1.44284
C	4.48044	3.82462	-1.01426
C	2.86207	5.42537	-1.80573
C	5.44454	4.83211	-0.94952
H	4.73266	2.80958	-0.72085
C	3.82150	6.43484	-1.73593
H	1.85736	5.67179	-2.14513
C	5.11782	6.13988	-1.30872
H	6.44977	4.59378	-0.61265
H	3.55653	7.45102	-2.01542
H	5.86647	6.92551	-1.25447

1 imaginary frequency: -383.85 cm^{-1}.

SCF energy: -4055.662726 hartree
zero-point correction: +1.542535 hartree
enthalpy correction: +1.617483 hartree
free energy correction: +1.427522 hartree
quasiharmonic free energy correction: +1.452090 hartree

TS(*S*)_A1 (lowest-energy TS(*S*))

C	-1.14936	-4.25413	-0.87006
O	-1.71373	-1.36011	0.13867
O	0.63302	-1.73209	-0.90165
C	0.98670	-2.83937	-0.11721
C	0.13340	-3.94357	-0.09734
C	2.21176	-2.83820	0.57776
C	0.46708	-5.04174	0.71349

C	2.54398	-3.99810	1.29832	H	1.50097	-1.38807	6.93660
C	1.67715	-5.08407	1.39468	H	2.81525	-0.35234	6.38703
H	3.49786	-4.02250	1.81629	C	6.32512	1.31627	0.84028
H	1.94430	-5.94624	2.00056	C	7.54357	0.73937	1.60163
C	-2.55526	-1.99030	-0.79807	C	5.90889	2.67194	1.45259
C	-2.18376	-3.22475	-1.31953	H	6.65482	1.51714	-0.19019
C	-3.74515	-1.34272	-1.18125	C	8.71441	1.73339	1.64732
C	-2.91567	-3.74936	-2.39742	H	7.85793	-0.20096	1.13173
C	-4.51215	-1.96678	-2.17828	H	7.23705	0.48634	2.62723
C	-4.08512	-3.12986	-2.82201	C	7.08085	3.66497	1.49440
H	-5.44714	-1.50288	-2.47495	H	5.08087	3.09824	0.87387
H	-4.66852	-3.54436	-3.64039	H	5.53784	2.51347	2.47555
C	-0.64242	-6.06823	0.71534	C	8.28901	3.08364	2.24254
H	-0.38484	-6.93723	0.09366	H	9.09272	1.89231	0.62652
H	-0.85615	-6.45202	1.71937	H	9.54538	1.30652	2.22356
C	-1.81852	-5.27475	0.11572	H	7.37500	3.91624	0.46488
H	-2.32844	-4.71447	0.90820	H	6.75803	4.60420	1.96151
H	-2.56448	-5.90288	-0.37943	H	9.12802	3.79086	2.21945
C	-2.23848	-4.98786	-2.94605	H	8.02617	2.94537	3.30215
H	-2.80379	-5.89891	-2.70592	C	3.76421	-2.07654	-1.87149
H	-2.14407	-4.95744	-4.03752	C	3.54560	-1.13563	-3.07769
C	-0.86644	-4.96780	-2.23269	C	4.96713	-3.01636	-2.13375
H	-0.15490	-4.36410	-2.80744	H	2.87805	-2.71571	-1.80897
H	-0.43105	-5.96314	-2.10116	C	3.36743	-1.93075	-4.38036
C	3.17333	-1.68502	0.60754	H	4.41148	-0.46736	-3.19101
C	3.42467	-1.01644	1.83476	H	2.67540	-0.49245	-2.90510
C	3.92152	-1.34194	-0.54437	C	4.79874	-3.80319	-3.44294
C	4.42751	-0.03962	1.88043	H	5.88922	-2.41889	-2.18099
C	4.90530	-0.34916	-0.43951	H	5.08756	-3.70636	-1.28852
C	5.18824	0.30855	0.75978	C	4.55478	-2.87023	-4.63835
H	4.63251	0.44797	2.82999	H	3.23517	-1.23904	-5.22136
H	5.49558	-0.10101	-1.31846	H	2.44202	-2.52269	-4.31748
C	-4.20028	-0.05759	-0.55147	H	3.94542	-4.49044	-3.34189
C	-4.55563	-0.03479	0.82323	H	5.68295	-4.42956	-3.61988
C	-4.32738	1.12430	-1.32614	H	5.45873	-2.26845	-4.81710
C	-4.99338	1.16448	1.39324	H	4.38699	-3.45772	-5.55043
C	-4.78046	2.29277	-0.69903	C	-4.02760	1.18121	-2.82246
C	-5.10815	2.34523	0.65524	C	-5.33178	1.26418	-3.65567
H	-5.26487	1.17151	2.44564	C	-3.08776	2.34107	-3.22594
H	-4.87889	3.19941	-1.29068	H	-3.51464	0.25581	-3.10413
C	2.66899	-1.33347	3.12513	C	-5.04865	1.25506	-5.16587
C	3.59385	-1.95745	4.19892	H	-5.86732	2.18749	-3.38989
C	1.93176	-0.10664	3.71282	H	-6.00528	0.43850	-3.39275
H	1.89609	-2.07420	2.89743	C	-2.79256	2.32508	-4.73343
C	2.82465	-2.31540	5.47990	H	-3.54737	3.30527	-2.96523
H	4.08784	-2.84972	3.79394	H	-2.14912	2.27364	-2.66857
H	4.39766	-1.24822	4.44364	C	-4.08144	2.37895	-5.56528
C	1.16342	-0.46654	4.99460	H	-5.99070	1.34224	-5.72361
H	1.24041	0.28677	2.96070	H	-4.60990	0.28486	-5.44302
H	2.65628	0.68821	3.94345	H	-2.13171	3.16173	-4.98869
C	2.08068	-1.09935	6.05039	H	-2.23318	1.41165	-4.97934
H	3.51424	-2.72756	6.22810	H	-4.57566	3.35007	-5.40870
H	2.09822	-3.10997	5.25356	H	-3.84916	2.31732	-6.63653
H	0.67583	0.42919	5.40082	C	-5.56677	3.64505	1.29594
H	0.35723	-1.17160	4.74420	C	-6.97462	3.53919	1.92575

C	-4.55025	4.16699	2.33826
H	-5.62690	4.39985	0.49706
C	-7.42255	4.86879	2.55249
H	-6.96824	2.75908	2.70050
H	-7.69418	3.21320	1.16419
C	-5.00100	5.49469	2.96662
H	-4.42773	3.41300	3.12916
H	-3.56649	4.28104	1.86570
C	-6.40389	5.38108	3.58140
H	-8.40906	4.74986	3.01895
H	-7.54287	5.62056	1.75812
H	-5.00823	6.27730	2.19315
H	-4.27616	5.81554	3.72606
H	-6.72365	6.35106	3.98353
H	-6.36956	4.68544	4.43327
C	-4.55651	-1.28483	1.69815
C	-3.67695	-1.15064	2.96267
C	-5.99682	-1.69818	2.08835
H	-4.14604	-2.11640	1.11664
C	-3.69124	-2.44105	3.79708
H	-4.04470	-0.32193	3.58452
H	-2.65278	-0.89494	2.66946
C	-6.01060	-2.98505	2.92722
H	-6.46773	-0.88532	2.65939
H	-6.60082	-1.82903	1.18145
C	-5.12079	-2.85885	4.17286
H	-3.08238	-2.30958	4.70122
H	-3.21778	-3.24999	3.21982
H	-5.65101	-3.82190	2.30964
H	-7.03987	-3.23355	3.21737
H	-5.55073	-2.10376	4.84809
H	-5.10899	-3.80450	4.73049
P	-0.39505	-0.59120	-0.38399
O	-0.83234	0.09987	-1.72386
O	0.14386	0.26405	0.71759
H	-0.17512	0.66337	-2.28088
H	0.24248	1.93227	1.17317
Cl	0.83277	2.07466	-3.17757
O	0.53778	2.88551	1.09759
C	0.67128	2.93342	-0.71854
C	2.01602	2.87120	1.05786
C	2.17648	2.80871	-0.47218
H	0.24791	3.89909	-0.97155
H	0.03303	2.08883	-0.86812
H	2.35413	3.80097	1.51536
H	2.40476	2.01211	1.60376
H	2.51591	1.82367	-0.79272
C	3.03795	3.88074	-1.10757
C	2.88554	5.23398	-0.77331
C	4.00962	3.52749	-2.05128
C	3.68712	6.20993	-1.36552
H	2.13091	5.53789	-0.04998
C	4.81601	4.50125	-2.64145
H	4.11655	2.48522	-2.33608
C	4.65775	5.84509	-2.30011
H	3.55218	7.25435	-1.09717
H	5.56147	4.20934	-3.37622
H	5.28295	6.60433	-2.76217

1 imaginary frequency: -388.63 cm^{-1}.

SCF energy: -4055.666773 hartree
zero-point correction: +1.542294 hartree
enthalpy correction: +1.617435 hartree
free energy correction: +1.425589 hartree
quasiharmonic free energy correction: +1.452065 hartree

SCF energy (other methods):
B3LYP/6-31G(d): -4054.310828
B3LYP-D3(BJ)/6-311+G(d,p): -4055.655138
B3LYP-D3(BJ)/6-311+G(d,p)/SMD(benzene): -4055.723399
B3LYP-D3(BJ)/def2-TZVP/CPCM(benzene): -4056.036733
B3LYP-D3(BJ)/def2-TZVPP/CPCM(benzene): -4056.074433
B3LYP/6-311+G(d,p)/CPCM(benzene): -4055.206638
M06-2X/6-311+G(d,p)/CPCM (benzene): -4053.800227
ωB97X-D/6-311+G(d,p)/CPCM (benzene): -4054.245285

TS(*S*)_A2

C	-1.15741	-4.17516	-1.18912
O	-1.73301	-1.35335	0.00500
O	0.66556	-1.69656	-0.92391
C	0.95162	-2.86591	-0.20486
C	0.08082	-3.95081	-0.31998
C	2.13127	-2.94240	0.56023
C	0.34855	-5.11491	0.42042
C	2.40150	-4.16120	1.20606
C	1.51481	-5.23394	1.16593
H	3.32189	-4.24396	1.77575
H	1.73248	-6.14594	1.71609
C	-2.53301	-1.89804	-1.01830
C	-2.15026	-3.09554	-1.61280
C	-3.69226	-1.20404	-1.41295
C	-2.82598	-3.52207	-2.76777
C	-4.40960	-1.73597	-2.49675
C	-3.96160	-2.85146	-3.20664
H	-5.31968	-1.23300	-2.80660
H	-4.50256	-3.19029	-4.08666
C	-0.77187	-6.11820	0.27338
H	-0.48796	-6.93876	-0.40051
H	-1.05131	-6.57769	1.22829
C	-1.89857	-5.25887	-0.32928
H	-2.44855	-4.75429	0.47384

H	-2.62162	-5.83378	-0.91498	H	8.92005	4.04336	1.58967
C	-2.13364	-4.72494	-3.37397	H	7.66427	3.91562	0.35980
H	-2.72135	-5.64299	-3.23653	C	3.85680	-2.01886	-1.71241
H	-1.97805	-4.61144	-4.45285	C	3.75511	-0.96434	-2.83747
C	-0.80398	-4.78241	-2.58635	C	5.03594	-2.98553	-1.98547
H	-0.05446	-4.14536	-3.06955	H	2.94427	-2.62059	-1.76512
H	-0.38765	-5.79174	-2.51126	C	3.63556	-1.62695	-4.21844
C	3.11212	-1.82007	0.74569	H	4.65047	-0.32593	-2.83179
C	3.30016	-1.26791	2.04164	H	2.89879	-0.30332	-2.66224
C	3.95201	-1.41244	-0.31609	C	4.92429	-3.63980	-3.37132
C	4.34237	-0.35631	2.23897	H	5.98314	-2.43095	-1.91683
C	4.97312	-0.48350	-0.05991	H	5.06953	-3.75523	-1.20353
C	5.20416	0.04531	1.21100	C	4.80048	-2.59122	-4.48663
H	4.51033	0.03666	3.23973	H	3.58814	-0.85518	-4.99642
H	5.62807	-0.20426	-0.87797	H	2.68572	-2.17958	-4.27231
C	-4.17253	0.03530	-0.71434	H	4.03854	-4.29235	-3.38987
C	-4.60227	-0.03686	0.63730	H	5.79185	-4.28855	-3.55014
C	-4.25440	1.27031	-1.40877	H	5.73758	-2.01743	-4.54810
C	-5.07699	1.12019	1.26243	H	4.67332	-3.08450	-5.45909
C	-4.74294	2.39335	-0.72771	C	-3.85387	1.43622	-2.87319
C	-5.14945	2.35064	0.60526	C	-5.09380	1.59436	-3.78920
H	-5.40653	1.05476	2.29604	C	-2.88378	2.61552	-3.11910
H	-4.80288	3.34123	-1.25652	H	-3.32553	0.53053	-3.18867
C	2.43251	-1.64726	3.24138	C	-4.69876	1.69406	-5.27074
C	3.23561	-2.40403	4.32734	H	-5.64274	2.50101	-3.49490
C	1.71240	-0.43130	3.87155	H	-5.78907	0.75847	-3.63960
H	1.64444	-2.32296	2.89403	C	-2.47762	2.71183	-4.59725
C	2.34952	-2.81811	5.51217	H	-3.35974	3.56051	-2.82051
H	3.71685	-3.28803	3.89034	H	-1.98969	2.49807	-2.49986
H	4.04996	-1.76132	4.69116	C	-3.70239	2.83680	-5.51436
C	0.82590	-0.84757	5.05624	H	-5.59613	1.82864	-5.88940
H	1.10331	0.05797	3.10450	H	-4.24207	0.74355	-5.58449
H	2.45498	0.30153	4.21978	H	-1.79943	3.56145	-4.73888
C	1.62224	-1.61200	6.12339	H	-1.90076	1.81716	-4.86963
H	2.95677	-3.32436	6.27389	H	-4.20433	3.79760	-5.32233
H	1.60614	-3.55208	5.16746	H	-3.39279	2.85261	-6.56754
H	0.35132	0.03902	5.49649	C	-5.64177	3.60316	1.31167
H	0.00928	-1.48507	4.68656	C	-7.11261	3.48953	1.77480
H	0.95899	-1.93778	6.93504	C	-4.73334	3.99233	2.50118
H	2.36232	-0.93545	6.57671	H	-5.59490	4.42858	0.58508
C	6.35421	0.99644	1.53210	C	-7.59320	4.77121	2.47395
C	5.85042	2.41057	1.91274	H	-7.20969	2.64098	2.46726
C	7.42592	1.10718	0.43114	H	-7.75231	3.26051	0.91320
H	6.85366	0.58958	2.42669	C	-5.21732	5.27186	3.20072
C	7.00203	3.33690	2.33351	H	-4.71795	3.16696	3.22726
H	5.11387	2.33892	2.72340	H	-3.70095	4.11406	2.14996
H	5.33073	2.84470	1.04753	C	-6.68091	5.14991	3.64993
C	8.58491	2.02226	0.85699	H	-8.62782	4.64519	2.81830
H	7.80604	0.11050	0.17330	H	-7.60542	5.59673	1.74665
H	6.97078	1.51822	-0.48161	H	-5.12158	6.12177	2.50855
C	8.08390	3.42019	1.24740	H	-4.57180	5.49679	4.05967
H	7.44999	2.95693	3.26398	H	-7.01909	6.08852	4.10752
H	6.61192	4.33737	2.56011	H	-6.75664	4.37664	4.42908
H	9.10800	1.57059	1.71304	C	-4.62079	-1.33689	1.43692
H	9.32047	2.09352	0.04567	C	-3.77648	-1.25679	2.72986

C	-6.06468	-1.78918	1.76510
H	-4.18357	-2.13094	0.82336
C	-3.79457	-2.58561	3.50114
H	-4.17195	-0.46384	3.38034
H	-2.74874	-0.97443	2.47708
C	-6.08092	-3.11551	2.54154
H	-6.56551	-1.01297	2.36108
H	-6.64074	-1.88528	0.83591
C	-5.22822	-3.03772	3.81642
H	-3.21231	-2.48962	4.42711
H	-3.29444	-3.36001	2.89962
H	-5.69192	-3.91688	1.89540
H	-7.11394	-3.39198	2.79005
H	-5.68674	-2.32055	4.51377
H	-5.21995	-4.00860	4.32890
P	-0.37605	-0.57544	-0.39043
O	-0.72926	0.20880	-1.70358
O	0.11201	0.19731	0.79269
H	-0.03646	0.78980	-2.19404
H	0.28256	1.82849	1.35549
Cl	1.03806	2.23191	-2.96109
O	0.62383	2.76877	1.34626
C	0.81643	2.92519	-0.45844
C	2.10093	2.68959	1.34933
C	2.31222	2.77274	-0.17404
H	0.40522	3.90617	-0.66817
H	0.18124	2.09293	-0.67405
H	2.46709	3.54745	1.91285
H	2.43101	1.75949	1.81102
H	2.66519	1.82344	-0.57677
C	3.18940	3.90102	-0.67746
C	3.04977	5.20833	-0.19016
C	4.16171	3.64837	-1.65264
C	3.86813	6.23609	-0.65915
H	2.29348	5.43548	0.55905
C	4.98408	4.67409	-2.12099
H	4.25591	2.64619	-2.05987
C	4.84159	5.97043	-1.62386
H	3.74415	7.24362	-0.27114
H	5.72930	4.46057	-2.88246
H	5.47990	6.77013	-1.98969

1 imaginary frequency: -387.43 cm^{-1}.

SCF energy: -4055.665544 hartree
zero-point correction: +1.543114 hartree
enthalpy correction: +1.617967 hartree
free energy correction: +1.427587 hartree
quasiharmonic free energy correction: +1.453078 hartree

TS(*S*)_A3

C	-1.00373	-4.25452	-1.18130
O	-1.63318	-1.52323	0.17451
O	0.65999	-1.65284	-1.03210
C	1.11344	-2.82234	-0.40523
C	0.31256	-3.96436	-0.45880
C	2.38291	-2.83770	0.20471
C	0.74885	-5.12803	0.19747
C	2.81431	-4.05298	0.76333
C	2.00407	-5.18536	0.78981
H	3.80235	-4.08701	1.21192
H	2.34977	-6.09555	1.27336
C	-2.50321	-2.08844	-0.77731
C	-2.11070	-3.23886	-1.45307
C	-3.74212	-1.46484	-1.01893
C	-2.88507	-3.68290	-2.53730
C	-4.54237	-2.01923	-2.03109
C	-4.10644	-3.08383	-2.82180
H	-5.51373	-1.57420	-2.22032
H	-4.72225	-3.43888	-3.64438
C	-0.31170	-6.20384	0.15136
H	-0.06017	-6.98312	-0.58166
H	-0.43871	-6.70844	1.11589
C	-1.55971	-5.41005	-0.27750
H	-2.03844	-4.96737	0.60394
H	-2.30979	-6.01683	-0.79272
C	-2.18886	-4.81854	-3.25781
H	-2.69432	-5.77879	-3.08525
H	-2.16715	-4.66727	-4.34307
C	-0.77621	-4.80152	-2.62937
H	-0.13218	-4.10227	-3.17481
H	-0.28731	-5.78063	-2.63557
C	3.29424	-1.64868	0.30920
C	3.59754	-1.11334	1.58936
C	3.95126	-1.14102	-0.83711
C	4.56245	-0.10328	1.68952
C	4.90008	-0.12195	-0.67546
C	5.23620	0.40426	0.57357
H	4.80988	0.28205	2.67555
H	5.42140	0.25306	-1.55306
C	-4.21514	-0.27251	-0.23864
C	-4.47965	-0.39319	1.14923
C	-4.45212	0.96791	-0.89051
C	-4.94478	0.72480	1.85183
C	-4.92518	2.04632	-0.13442
C	-5.17168	1.95596	1.23741
H	-5.14995	0.62908	2.91570
H	-5.10525	2.99073	-0.63963
C	2.93884	-1.61282	2.87507
C	3.95010	-2.33332	3.80093
C	2.21250	-0.49605	3.66067
H	2.17182	-2.34558	2.60557
C	3.27312	-2.88343	5.06532
H	4.44722	-3.14512	3.25529
H	4.74309	-1.62866	4.09018
C	1.53707	-1.04301	4.92896
H	1.46412	-0.03332	3.00911
H	2.93070	0.28622	3.94724

C	2.53428	-1.77983	5.83526
H	4.01882	-3.36578	5.71064
H	2.55581	-3.66621	4.77725
H	1.05554	-0.22377	5.47852
H	0.73347	-1.73473	4.63635
H	2.01685	-2.20342	6.70572
H	3.26805	-1.06008	6.22862
C	6.33400	1.44850	0.70483
C	7.59333	0.87439	1.39757
C	5.87348	2.73694	1.42315
H	6.63005	1.73773	-0.31484
C	8.72039	1.91456	1.49215
H	7.93792	-0.01447	0.85435
H	7.32341	0.53501	2.40826
C	7.00131	3.77633	1.51533
H	5.01496	3.16651	0.89368
H	5.53242	2.48636	2.43838
C	8.25089	3.19788	2.19382
H	9.06725	2.16374	0.47826
H	9.58254	1.48490	2.01836
H	7.26029	4.11585	0.50185
H	6.64804	4.66305	2.05703
H	9.05763	3.94189	2.20596
H	8.01919	2.97061	3.24529
C	3.73079	-1.71687	-2.23152
C	3.33061	-0.65145	-3.27724
C	4.96956	-2.50832	-2.71895
H	2.90536	-2.43397	-2.18166
C	3.08828	-1.28405	-4.65587
H	4.13006	0.09832	-3.36842
H	2.43575	-0.11262	-2.94761
C	4.73496	-3.13252	-4.10339
H	5.83692	-1.83402	-2.76471
H	5.22030	-3.28775	-1.98770
C	4.31057	-2.07912	-5.13773
H	2.82712	-0.50363	-5.38101
H	2.21853	-1.95552	-4.59588
H	3.94834	-3.89779	-4.02387
H	5.64190	-3.65350	-4.43741
H	5.14718	-1.38529	-5.31093
H	4.09982	-2.55846	-6.10265
C	-4.24315	1.18140	-2.38834
C	-5.59387	1.28368	-3.14218
C	-3.37887	2.41888	-2.72452
H	-3.70883	0.31356	-2.78823
C	-5.39181	1.42706	-4.65878
H	-6.14967	2.15357	-2.76212
H	-6.21943	0.40811	-2.92612
C	-3.16088	2.55435	-4.23874
H	-3.86991	3.33082	-2.35517
H	-2.41141	2.35044	-2.21943
C	-4.49249	2.62453	-4.99948
H	-6.36493	1.52267	-5.15888
H	-4.93029	0.50667	-5.04683
H	-2.54923	3.44030	-4.44565
H	-2.57775	1.69372	-4.59528
H	-5.01639	3.55468	-4.73075
H	-4.31430	2.66956	-6.08187
C	-5.67331	3.14684	2.03787
C	-4.65406	4.30979	2.05846
C	-7.05177	3.64999	1.55125
H	-5.80083	2.81086	3.07842
C	-5.15813	5.49974	2.88975
H	-4.46538	4.64171	1.02740
H	-3.69371	3.94898	2.44807
C	-7.55334	4.84099	2.38285
H	-6.97506	3.95189	0.49696
H	-7.77651	2.82684	1.58546
C	-6.53092	5.98688	2.40353
H	-4.42802	6.31870	2.85370
H	-5.23488	5.19758	3.94504
H	-7.74348	4.50791	3.41424
H	-8.51491	5.19483	1.98900
H	-6.89097	6.80695	3.03809
H	-6.42927	6.39885	1.38832
C	-4.34826	-1.71005	1.90869
C	-3.37101	-1.62869	3.10453
C	-5.72642	-2.23503	2.37979
H	-3.94963	-2.46751	1.22634
C	-3.24703	-2.98237	3.82144
H	-3.72840	-0.87692	3.82260
H	-2.39016	-1.29006	2.75373
C	-5.60273	-3.58536	3.10266
H	-6.18598	-1.50065	3.05643
H	-6.39982	-2.32558	1.51799
C	-4.61494	-3.51161	4.27684
H	-2.56865	-2.89143	4.67996
H	-2.78575	-3.71167	3.13795
H	-5.25719	-4.34693	2.38743
H	-6.58925	-3.91494	3.45410
H	-5.02160	-2.84086	5.04852
H	-4.50697	-4.49798	4.74670
P	-0.38440	-0.63347	-0.32693
O	-0.93533	0.18205	-1.54954
O	0.18221	0.11700	0.83559
H	-0.34637	0.84837	-2.06697
H	0.24473	1.72169	1.48513
Cl	0.52738	2.41495	-2.84431
O	0.48951	2.69178	1.50762
C	0.49013	2.96433	-0.29380
C	1.95994	2.76619	1.37041
C	2.01369	2.90893	-0.16177
H	-0.00526	3.92303	-0.39965
H	-0.10650	2.10297	-0.50444
H	2.28631	3.64642	1.92409
H	2.42756	1.86742	1.77115
H	2.38445	1.99722	-0.63051
C	2.76154	4.10905	-0.70561
C	2.56898	5.39177	-0.17293
C	3.66345	3.95024	-1.76448

C	3.26481	6.48810	-0.68243
H	1.86538	5.54608	0.64322
C	4.36423	5.04453	-2.27271
H	3.79769	2.96596	-2.20284
C	4.16827	6.31627	-1.73261
H	3.10032	7.47537	-0.25899
H	5.05682	4.90320	-3.09799
H	4.71158	7.16932	-2.13004

1 imaginary frequency: -392.38 cm^{-1}.

SCF energy: -4055.666522 hartree
zero-point correction: +1.542588 hartree
enthalpy correction: +1.617641 hartree
free energy correction: +1.426218 hartree
quasiharmonic free energy correction: +1.452395 hartree

TS(*S*)_A4

C	-0.86908	-4.23113	-1.32215
O	-1.60668	-1.55501	0.09298
O	0.75861	-1.63293	-0.97570
C	1.18854	-2.82322	-0.37190
C	0.39707	-3.96395	-0.50887
C	2.42640	-2.85932	0.29882
C	0.79830	-5.14893	0.13069
C	2.82993	-4.09319	0.83774
C	2.02047	-5.22545	0.78682
H	3.79510	-4.14346	1.33215
H	2.34245	-6.15092	1.25759
C	-2.40214	-2.08372	-0.94246
C	-1.95619	-3.20562	-1.63438
C	-3.62698	-1.45924	-1.24453
C	-2.64857	-3.60747	-2.78841
C	-4.34571	-1.96991	-2.33796
C	-3.84685	-2.99748	-3.13949
H	-5.30388	-1.52053	-2.57726
H	-4.39835	-3.31935	-4.01933
C	-0.25587	-6.22262	-0.01364
H	0.04201	-6.97887	-0.75332
H	-0.44106	-6.75665	0.92531
C	-1.47745	-5.41612	-0.49423
H	-2.01178	-5.00306	0.36945
H	-2.19142	-6.00773	-1.07447
C	-1.90406	-4.71997	-3.49606
H	-2.42219	-5.68333	-3.39156
H	-1.80505	-4.53317	-4.57145
C	-0.54055	-4.72952	-2.76841
H	0.14118	-4.01407	-3.24238
H	-0.05270	-5.70913	-2.77328
C	3.33406	-1.67750	0.48103
C	3.59578	-1.19379	1.78890
C	4.03039	-1.12651	-0.62385
C	4.56059	-0.19071	1.95550
C	4.98065	-0.12387	-0.39498
C	5.27663	0.35182	0.88583
H	4.78171	0.16390	2.96022
H	5.52894	0.27309	-1.24470
C	-4.19025	-0.32365	-0.43926
C	-4.58811	-0.54160	0.90413
C	-4.40692	0.94709	-1.03658
C	-5.17762	0.51005	1.61565
C	-5.00539	1.95680	-0.27408
C	-5.39825	1.76669	1.05252
H	-5.49061	0.33969	2.64337
H	-5.17121	2.92504	-0.73748
C	2.89793	-1.73786	3.03502
C	3.88295	-2.48722	3.96612
C	2.14412	-0.64995	3.83526
H	2.14161	-2.46218	2.71662
C	3.17272	-3.07881	5.19276
H	4.39740	-3.28001	3.40873
H	4.66602	-1.79189	4.30133
C	1.43568	-1.23991	5.06563
H	1.41115	-0.17054	3.17815
H	2.84918	0.12712	4.16561
C	2.41025	-2.00117	5.97604
H	3.90211	-3.57938	5.84281
H	2.46588	-3.85398	4.86133
H	0.93441	-0.44062	5.62680
H	0.64455	-1.92544	4.72806
H	1.87095	-2.45201	6.81906
H	3.13092	-1.29164	6.41023
C	6.38102	1.36850	1.12878
C	6.20465	2.67758	0.32799
C	7.77811	0.76027	0.85468
H	6.35033	1.63605	2.19631
C	7.33462	3.67943	0.61105
H	5.23391	3.13155	0.56086
H	6.18844	2.44912	-0.74721
C	8.90800	1.76314	1.13270
H	7.91033	-0.14334	1.46294
H	7.82587	0.43709	-0.19520
C	8.71619	3.06565	0.34171
H	7.28007	3.99875	1.66262
H	7.18944	4.58259	0.00517
H	8.93055	1.99327	2.20846
H	9.87803	1.30930	0.89219
H	9.50770	3.78356	0.59200
H	8.81472	2.85339	-0.73335
C	3.84821	-1.64149	-2.04776
C	3.49187	-0.52587	-3.05677
C	5.09312	-2.42576	-2.53106
H	3.01495	-2.35069	-2.05565
C	3.28774	-1.09349	-4.46939
H	4.30030	0.21835	-3.08815
H	2.59289	0.00817	-2.73045
C	4.89530	-2.98486	-3.94884
H	5.96910	-1.76135	-2.51965

H	5.31201	-3.23999	-1.82802
C	4.51673	-1.88061	-4.94741
H	3.05850	-0.27840	-5.16670
H	2.40958	-1.75667	-4.46791
H	4.09715	-3.74196	-3.92859
H	5.80601	-3.50276	-4.27735
H	5.36612	-1.19020	-5.06113
H	4.33280	-2.31321	-5.93953
C	-4.04370	1.26287	-2.48610
C	-5.30510	1.38549	-3.37764
C	-3.18313	2.53894	-2.64016
H	-3.44306	0.43549	-2.87790
C	-4.94136	1.64093	-4.84846
H	-5.92702	2.21306	-3.00578
H	-5.92226	0.48195	-3.29339
C	-2.80727	2.79006	-4.10801
H	-3.73579	3.41098	-2.26165
H	-2.27435	2.45138	-2.03779
C	-4.05069	2.88249	-5.00330
H	-5.85574	1.74678	-5.44752
H	-4.40855	0.76289	-5.24309
H	-2.20554	3.70309	-4.18373
H	-2.16076	1.97309	-4.45719
H	-4.63107	3.77712	-4.72989
H	-3.75819	3.01085	-6.05370
C	-6.04918	2.87717	1.86062
C	-5.09375	4.06965	2.09955
C	-7.37393	3.36988	1.23391
H	-6.29616	2.45958	2.84878
C	-5.75357	5.17152	2.94306
H	-4.78904	4.48735	1.12919
H	-4.17660	3.71330	2.58541
C	-8.03198	4.47175	2.07870
H	-7.17530	3.75884	0.22509
H	-8.05927	2.52207	1.10958
C	-7.07359	5.64787	2.31883
H	-5.06249	6.01571	3.06444
H	-5.95153	4.78339	3.95345
H	-8.33764	4.05083	3.04832
H	-8.94995	4.82159	1.58901
H	-7.54815	6.40180	2.96006
H	-6.86136	6.14207	1.35900
C	-4.46725	-1.89448	1.59961
C	-3.62314	-1.83385	2.89333
C	-5.85671	-2.51299	1.88947
H	-3.95912	-2.58965	0.92418
C	-3.50680	-3.21430	3.55865
H	-4.08528	-1.13411	3.60392
H	-2.62876	-1.43690	2.66065
C	-5.73556	-3.89143	2.55747
H	-6.42838	-1.84017	2.54425
H	-6.42571	-2.59198	0.95433
C	-4.88694	-3.82909	3.83581
H	-2.93043	-3.13446	4.48971
H	-2.93765	-3.88663	2.89856
H	-5.27195	-4.59588	1.85043
H	-6.73402	-4.28919	2.78147
H	-5.40998	-3.21781	4.58656
H	-4.77893	-4.83133	4.27078
P	-0.32438	-0.64848	-0.27814
O	-0.79613	0.23652	-1.48622
O	0.17155	0.03091	0.95796
H	-0.18963	0.94212	-1.91941
H	0.26454	1.59979	1.74029
Cl	0.71698	2.57846	-2.55241
O	0.52222	2.56286	1.80417
C	0.55561	2.94470	0.02939
C	1.99818	2.64286	1.69203
C	2.05741	3.14125	0.23774
H	-0.10502	3.79860	-0.06300
H	0.15489	1.99584	-0.24936
H	2.35387	3.34120	2.44963
H	2.43580	1.65649	1.84324
H	2.61134	2.45899	-0.40738
C	2.53741	4.56256	0.02000
C	2.17672	5.60053	0.89105
C	3.33143	4.86386	-1.09334
C	2.61053	6.90646	0.66138
H	1.54464	5.39673	1.75322
C	3.76775	6.16922	-1.32342
H	3.58688	4.07284	-1.79212
C	3.41131	7.19372	-0.44545
H	2.32124	7.69871	1.34677
H	4.38068	6.38532	-2.19426
H	3.75050	8.21045	-0.62444

1 imaginary frequency: -390.27 cm^{-1}.

SCF energy: -4055.662697 hartree
zero-point correction: +1.542747 hartree
enthalpy correction: +1.617756 hartree
free energy correction: +1.427345 hartree
quasiharmonic free energy correction: +1.452382 hartree

TS(*S*)_B1

C	-0.93467	-4.43795	-0.64279
O	0.75339	-1.86949	-0.87360
O	-1.56535	-1.51243	0.23066
C	-2.41033	-2.21638	-0.64751
C	-2.01446	-3.46606	-1.11387
C	-3.63350	-1.63013	-1.02319
C	-2.76288	-4.07233	-2.13599
C	-4.40993	-2.33273	-1.95971
C	-3.96520	-3.51457	-2.55426
H	-5.36933	-1.91581	-2.24824
H	-4.56096	-3.99253	-3.32791
C	1.18003	-2.92356	-0.05183
C	0.36345	-4.04845	0.06359

C	2.43434	-2.84890	0.58359
C	0.76194	-5.08927	0.91924
C	2.83001	-3.95589	1.35363
C	1.99959	-5.05724	1.54998
H	3.80623	-3.92640	1.82771
H	2.31786	-5.87506	2.19164
C	-2.06716	-5.32123	-2.63520
H	-2.59616	-6.23174	-2.32158
H	-2.01025	-5.35365	-3.72921
C	-0.67413	-5.22028	-1.97219
H	-0.00048	-4.63047	-2.60424
H	-0.20416	-6.19332	-1.79934
C	-0.31555	-6.14486	1.01968
H	-0.05446	-7.03954	0.43717
H	-0.48138	-6.47800	2.05048
C	-1.53674	-5.42007	0.42205
H	-2.03443	-4.83052	1.20097
H	-2.28049	-6.09638	-0.00899
C	-4.12748	-0.33096	-0.45460
C	-4.44446	-0.23411	0.92649
C	-4.35199	0.78522	-1.30173
C	-4.97174	0.96292	1.42146
C	-4.88390	1.95604	-0.74565
C	-5.20181	2.07395	0.60666
H	-5.22041	1.02340	2.47779
H	-5.05924	2.81056	-1.39467
C	3.36199	-1.67193	0.48993
C	3.65855	-0.91674	1.65575
C	4.02980	-1.38085	-0.72385
C	4.62373	0.09497	1.57749
C	4.98480	-0.35586	-0.74078
C	5.31100	0.38687	0.39430
H	4.86415	0.65448	2.47835
H	5.51270	-0.14688	-1.66795
C	-4.27902	-1.39469	1.90358
C	-3.32714	-1.05122	3.07323
C	-5.63779	-1.89755	2.44839
H	-3.83216	-2.23974	1.37112
C	-3.14865	-2.24425	4.02476
H	-2.35827	-0.73252	2.67390
H	-3.73250	-0.20069	3.63954
C	-5.45821	-3.08757	3.40493
H	-6.28972	-2.17749	1.61106
H	-6.14687	-1.07980	2.97787
C	-4.49739	-2.75253	4.55536
H	-2.49128	-1.96468	4.85865
H	-2.63945	-3.05951	3.48844
H	-6.43305	-3.40078	3.80105
H	-5.06145	-3.94596	2.84215
H	-4.35025	-3.63169	5.19627
H	-4.95092	-1.97631	5.18992
C	-5.78704	3.36357	1.15742
C	-4.88687	4.01514	2.23277
C	-7.22033	3.17284	1.70637
H	-5.85484	4.07423	0.31964
C	-5.48085	5.33294	2.75395
H	-3.88413	4.18423	1.82061
H	-4.76343	3.31638	3.07260
C	-7.81343	4.49075	2.22809
H	-7.86067	2.74978	0.92217
H	-7.19961	2.43475	2.52124
C	-6.90876	5.13996	3.28601
H	-5.49581	6.07066	1.93779
H	-4.83526	5.75065	3.53736
H	-7.94051	5.18720	1.38588
H	-8.81585	4.31442	2.63921
H	-7.32850	6.10169	3.60806
H	-6.87833	4.49769	4.17898
C	-4.06246	0.77412	-2.80121
C	-5.37035	0.76917	-3.63218
C	-3.16603	1.94765	-3.26154
H	-3.51552	-0.14394	-3.03930
C	-5.09246	0.70780	-5.14208
H	-5.94124	1.68092	-3.40353
H	-6.00966	-0.07102	-3.33194
C	-2.87645	1.87650	-4.76857
H	-3.65876	2.90511	-3.03942
H	-2.22436	1.93805	-2.70498
C	-4.17073	1.84973	-5.59384
H	-6.03952	0.73618	-5.69739
H	-4.61890	-0.25591	-5.38198
H	-2.28885	0.97181	-4.97899
H	-2.24555	2.72336	-5.06350
H	-4.69924	2.80762	-5.47232
H	-3.94212	1.75346	-6.66329
C	3.81440	-2.19177	-1.99723
C	3.42816	-1.32176	-3.21487
C	5.05269	-3.06071	-2.32872
H	2.98487	-2.88575	-1.82867
C	3.19603	-2.18291	-4.46590
H	4.22973	-0.60036	-3.42618
H	2.53480	-0.73010	-2.98799
C	4.82672	-3.91460	-3.58641
H	5.92392	-2.40767	-2.48249
H	5.29406	-3.70273	-1.47157
C	4.41930	-3.05289	-4.79079
H	2.94697	-1.53839	-5.31800
H	2.32232	-2.83171	-4.30160
H	5.73322	-4.49005	-3.81607
H	4.03413	-4.65065	-3.38407
H	5.26120	-2.40123	-5.06888
H	4.21688	-3.68902	-5.66235
C	6.41528	1.43157	0.34655
C	5.93232	2.84830	0.72857
C	7.62741	1.02669	1.21900
H	6.76873	1.48346	-0.69414
C	7.06770	3.88168	0.65769
H	5.52455	2.82960	1.75046
H	5.11188	3.14827	0.06457
C	8.76040	2.06205	1.14763

H	7.29905	0.91902	2.26294
H	7.99024	0.03983	0.90570
C	8.26626	3.46678	1.52302
H	7.39391	3.98547	-0.38746
H	6.69630	4.86802	0.96448
H	9.16760	2.08320	0.12584
H	9.58586	1.75901	1.80453
H	9.07925	4.19699	1.42200
H	7.96884	3.47420	2.58251
C	2.99718	-1.18149	3.00849
C	4.00680	-1.72501	4.04897
C	2.26690	0.05580	3.58140
H	2.23067	-1.95064	2.87031
C	3.33554	-2.03084	5.39670
H	4.80521	-0.98437	4.20044
H	4.49768	-2.62564	3.65929
C	1.59445	-0.25313	4.92849
H	2.98215	0.87963	3.72148
H	1.51707	0.39000	2.85757
C	2.59746	-0.80399	5.95157
H	4.08560	-2.38368	6.11652
H	2.61855	-2.85463	5.26416
H	0.79444	-0.99121	4.77030
H	1.10892	0.65065	5.31916
H	3.33146	-0.02143	6.19648
H	2.08693	-1.05755	6.88955
P	-0.27666	-0.73568	-0.34751
O	-0.76547	-0.08286	-1.69141
O	0.27518	0.15342	0.71973
H	-0.15466	0.52185	-2.24194
H	0.28201	1.85226	1.23267
Cl	0.80454	2.02119	-3.15716
O	0.45824	2.82642	1.11462
C	0.59262	2.85456	-0.71346
C	1.91972	3.04196	1.05060
C	2.01112	3.34775	-0.45608
H	0.40718	1.80755	-0.77869
H	-0.20751	3.52412	-1.00071
H	2.44315	2.13343	1.34954
H	2.16070	3.86384	1.72389
H	2.71791	2.68564	-0.96589
C	2.28935	4.79428	-0.84208
C	1.75262	5.33137	-2.02114
C	3.13357	5.59831	-0.06460
C	2.03611	6.64514	-2.39543
H	1.13189	4.70959	-2.65943
C	3.42026	6.91164	-0.44175
H	3.58492	5.20494	0.84249
C	2.86689	7.44235	-1.60660
H	1.60834	7.04280	-3.31188
H	4.07567	7.51757	0.17837
H	3.08609	8.46537	-1.90024

1 imaginary frequency: -391.63 cm^{-1}.

SCF energy: -4055.659885 hartree
zero-point correction: +1.542989 hartree
enthalpy correction: +1.618118 hartree
free energy correction: +1.426120 hartree
quasiharmonic free energy correction: +1.452582 hartree

TS(*S*)_B2

C	-1.05025	-4.30693	-0.95358
O	0.69949	-1.77048	-0.86168
O	-1.69146	-1.43881	0.08918
C	-2.47537	-2.05289	-0.90617
C	-2.06894	-3.27464	-1.43279
C	-3.64970	-1.40579	-1.33527
C	-2.74159	-3.78005	-2.55753
C	-4.35673	-2.00933	-2.38772
C	-3.88908	-3.15587	-3.03244
H	-5.27713	-1.54228	-2.72287
H	-4.42511	-3.55554	-3.88967
C	1.04143	-2.89269	-0.09306
C	0.19643	-4.00170	-0.12330
C	2.24526	-2.89688	0.63704
C	0.50828	-5.11174	0.67937
C	2.56013	-4.06686	1.34875
C	1.69499	-5.15780	1.40069
H	3.49839	-4.09723	1.89410
H	1.94708	-6.02817	2.00131
C	-2.03397	-5.00665	-3.09340
H	-2.60661	-5.92313	-2.89476
H	-1.88768	-4.95856	-4.17848
C	-0.69865	-4.99364	-2.31454
H	0.03629	-4.37545	-2.84266
H	-0.26410	-5.98902	-2.18062
C	-0.59435	-6.14424	0.62184
H	-0.30617	-7.00343	-0.00003
H	-0.84687	-6.54291	1.61097
C	-1.75141	-5.35016	-0.01501
H	-2.30115	-4.80865	0.76383
H	-2.46890	-5.97778	-0.55145
C	-4.15960	-0.14674	-0.69492
C	-4.59405	-0.17024	0.65695
C	-4.26827	1.05345	-1.44340
C	-5.09808	1.00144	1.22961
C	-4.79341	2.19130	-0.81640
C	-5.20504	2.19759	0.51581
H	-5.42866	0.97336	2.26452
H	-4.87950	3.11170	-1.38854
C	3.19760	-1.73783	0.70031
C	3.41295	-1.07222	1.93441
C	3.96438	-1.37765	-0.43557
C	4.39488	-0.07427	1.99821
C	4.93460	-0.37604	-0.30946
C	5.17769	0.28481	0.89757
H	4.57904	0.42152	2.94939

H	5.53629	-0.12653	-1.17838
C	-4.59985	-1.43887	1.50502
C	-3.78756	-1.29920	2.81331
C	-6.04233	-1.90782	1.81624
H	-4.13334	-2.24483	0.92999
C	-3.79907	-2.60293	3.62669
H	-2.75933	-1.00596	2.57449
H	-4.21220	-0.49328	3.42874
C	-6.05242	-3.20853	2.63416
H	-6.59560	-2.04420	0.87831
H	-6.56967	-1.12188	2.37546
C	-5.23063	-3.07344	3.92457
H	-3.23995	-2.46635	4.56166
H	-3.27091	-3.38613	3.06162
H	-7.08557	-3.49666	2.86845
H	-5.63379	-4.02244	2.02327
H	-5.21487	-4.02717	4.46812
H	-5.71868	-2.34390	4.58825
C	-5.73249	3.46863	1.16145
C	-4.76996	4.00462	2.24713
C	-7.15666	3.30626	1.74013
H	-5.78966	4.23520	0.37356
C	-5.28566	5.30584	2.88071
H	-3.77488	4.15890	1.81123
H	-4.65009	3.24058	3.02882
C	-7.66968	4.60960	2.37255
H	-7.83881	2.96958	0.94932
H	-7.15146	2.51465	2.50305
C	-6.70424	5.13621	3.44445
H	-5.29227	6.10068	2.11986
H	-4.59827	5.63729	3.66981
H	-7.78799	5.37115	1.58727
H	-8.66698	4.44999	2.80249
H	-7.06922	6.08805	3.85138
H	-6.67607	4.42706	4.28540
C	-3.85651	1.16579	-2.90947
C	-5.08769	1.26831	-3.84436
C	-2.90098	2.34967	-3.18904
H	-3.31098	0.25643	-3.18231
C	-4.67827	1.32333	-5.32449
H	-5.65701	2.17386	-3.58818
H	-5.76816	0.42451	-3.67243
C	-2.47854	2.39486	-4.66486
H	-3.39564	3.29762	-2.93313
H	-2.01429	2.27064	-2.55344
C	-3.69507	2.47106	-5.59804
H	-5.57102	1.42413	-5.95609
H	-4.20552	0.36930	-5.60158
H	-1.89054	1.49615	-4.89805
H	-1.80825	3.24620	-4.83198
H	-4.21143	3.43093	-5.44373
H	-3.37525	2.45474	-6.64814
C	3.84046	-2.10201	-1.77196
C	3.62110	-1.14990	-2.96938
C	5.06454	-3.01560	-2.02856
H	2.96663	-2.75962	-1.73008
C	3.47484	-1.93245	-4.28341
H	4.47377	-0.46273	-3.06172
H	2.73891	-0.52362	-2.79802
C	4.92838	-3.78953	-3.34912
H	5.97572	-2.40049	-2.05681
H	5.18723	-3.71332	-1.18994
C	4.68275	-2.84692	-4.53662
H	3.34181	-1.23342	-5.11835
H	2.55996	-2.54274	-4.24077
H	5.82651	-4.39710	-3.52169
H	4.08699	-4.49398	-3.26772
H	5.57743	-2.22620	-4.69595
H	4.53823	-3.42646	-5.45778
C	6.30655	1.29256	1.05097
C	7.68116	0.58093	1.10814
C	6.32675	2.39326	-0.03239
H	6.16596	1.79464	2.02122
C	8.83516	1.57181	1.32198
H	7.83568	0.03442	0.16659
H	7.67143	-0.17239	1.90581
C	7.47675	3.38804	0.19056
H	6.44005	1.93328	-1.02375
H	5.36816	2.92619	-0.04780
C	8.83645	2.67745	0.25585
H	8.73802	2.02986	2.31778
H	9.79339	1.03647	1.31885
H	7.30758	3.93139	1.13257
H	7.47586	4.14167	-0.60666
H	9.63574	3.40172	0.45878
H	9.05897	2.23313	-0.72570
C	2.65193	-1.42127	3.21308
C	3.57802	-2.06221	4.27616
C	1.90279	-0.21688	3.83014
H	1.88576	-2.16235	2.96461
C	2.80539	-2.46303	5.54244
H	4.37109	-1.34910	4.54370
H	4.08603	-2.93726	3.85166
C	1.12847	-0.61862	5.09590
H	2.61966	0.57651	4.08804
H	1.21249	0.19165	3.08553
C	2.04378	-1.27152	6.14087
H	3.49517	-2.88721	6.28373
H	2.08967	-3.25951	5.29022
H	0.33112	-1.32392	4.81945
H	0.62927	0.26099	5.52280
H	2.76735	-0.52667	6.50504
H	1.45991	-1.59145	7.01353
P	-0.34679	-0.65386	-0.33011
O	-0.71732	0.10676	-1.65541
O	0.13907	0.14355	0.83661
H	-0.03915	0.70618	-2.12750
H	0.20211	1.80700	1.44138
Cl	1.05614	2.20266	-2.87644
O	0.44523	2.77341	1.40414

C	0.72045	2.90470	-0.40411
C	1.91695	2.89221	1.46673
C	2.15928	3.22595	-0.01803
H	0.42546	1.89284	-0.55946
H	0.01977	3.67678	-0.69465
H	2.35534	1.94822	1.79083
H	2.14896	3.68826	2.17386
H	2.82899	2.50273	-0.49381
C	2.63324	4.64105	-0.31790
C	2.21584	5.31396	-1.47458
C	3.54632	5.27761	0.53443
C	2.68188	6.59938	-1.75368
H	1.54662	4.81852	-2.17127
C	4.01648	6.56128	0.25211
H	3.90598	4.77176	1.42738
C	3.57960	7.23016	-0.89118
H	2.34429	7.10510	-2.65438
H	4.72212	7.03637	0.92850
H	3.94079	8.23110	-1.11142

1 imaginary frequency: -393.82 cm^{-1}.

SCF energy: -4055.660615 hartree
zero-point correction: +1.542810 hartree
enthalpy correction: +1.617964 hartree
free energy correction: +1.426107 hartree
quasiharmonic free energy correction: +1.452387 hartree

TS(*S*)_B3

C	-0.84683	-4.48206	-0.77106
O	0.71809	-1.82895	-0.94853
O	-1.52584	-1.65077	0.33877
C	-2.39866	-2.32476	-0.53544
C	-1.99350	-3.52926	-1.10269
C	-3.65901	-1.75726	-0.80297
C	-2.78914	-4.10132	-2.10923
C	-4.47311	-2.43197	-1.72751
C	-4.03366	-3.56381	-2.41521
H	-5.46030	-2.03070	-1.93148
H	-4.66411	-4.01820	-3.17545
C	1.25202	-2.91961	-0.24626
C	0.48977	-4.08331	-0.14524
C	2.55356	-2.83663	0.28477
C	0.99670	-5.16204	0.59888
C	3.05516	-3.97879	0.93205
C	2.28401	-5.12370	1.12017
H	4.06833	-3.94316	1.31993
H	2.68634	-5.97008	1.67120
C	-2.08916	-5.29190	-2.72937
H	-2.56113	-6.23868	-2.43264
H	-2.11166	-5.26091	-3.82466
C	-0.65669	-5.17290	-2.16217
H	-0.05346	-4.51904	-2.80236
H	-0.13933	-6.13408	-2.08492
C	-0.03215	-6.26304	0.71908
H	0.20771	-7.10954	0.06057
H	-0.09796	-6.66499	1.73652
C	-1.32403	-5.55133	0.27295
H	-1.77450	-5.03166	1.12678
H	-2.07718	-6.22977	-0.13819
C	-4.14952	-0.50212	-0.13975
C	-4.38982	-0.48366	1.25745
C	-4.44046	0.65326	-0.91501
C	-4.90071	0.68132	1.84244
C	-4.95222	1.78574	-0.27176
C	-5.18735	1.82912	1.10434
H	-5.08982	0.69241	2.91348
H	-5.17157	2.66524	-0.87010
C	3.42411	-1.61513	0.21244
C	3.79815	-0.94964	1.41087
C	3.96804	-1.19127	-1.02378
C	4.71870	0.10333	1.34008
C	4.88271	-0.12993	-1.03176
C	5.28686	0.52401	0.13261
H	5.02240	0.59082	2.26326
H	5.31655	0.18063	-1.97902
C	-4.16456	-1.69345	2.15982
C	-3.16073	-1.40631	3.30032
C	-5.49272	-2.23905	2.73838
H	-3.73775	-2.50281	1.55920
C	-2.92991	-2.64799	4.17538
H	-2.21378	-1.05735	2.87459
H	-3.54358	-0.59195	3.93196
C	-5.26058	-3.47773	3.61845
H	-6.18088	-2.47877	1.91772
H	-5.98187	-1.45603	3.33491
C	-4.24909	-3.19659	4.73925
H	-2.23629	-2.40824	4.99205
H	-2.44111	-3.42836	3.57232
H	-6.21359	-3.82086	4.04197
H	-4.88530	-4.30056	2.99133
H	-4.06621	-4.10753	5.32415
H	-4.67739	-2.45977	5.43543
C	-5.71749	3.08005	1.78545
C	-7.08134	3.54096	1.22292
C	-4.69701	4.24166	1.73512
H	-5.87312	2.83322	2.84686
C	-7.60202	4.79556	1.94199
H	-7.80840	2.72315	1.30460
H	-6.97794	3.75823	0.15031
C	-5.21935	5.49621	2.45192
H	-3.74730	3.91530	2.17748
H	-4.48268	4.48505	0.68439
C	-6.57928	5.94052	1.89376
H	-7.81761	4.54781	2.99223
H	-8.55331	5.11456	1.49687
H	-5.32186	5.28246	3.52645
H	-4.48732	6.30961	2.36565

H	-6.95399	6.80962	2.44964
H	-6.45199	6.26737	0.85093
C	-4.23907	0.71792	-2.42754
C	-5.58873	0.68829	-3.18899
C	-3.42304	1.94760	-2.88980
H	-3.66885	-0.16472	-2.73497
C	-5.38369	0.68148	-4.71182
H	-6.17934	1.57097	-2.90287
H	-6.18195	-0.18355	-2.88519
C	-3.20087	1.93327	-4.40949
H	-3.95283	2.87244	-2.61953
H	-2.45794	1.97246	-2.37585
C	-4.53064	1.87142	-5.17505
H	-6.35707	0.68665	-5.22042
H	-4.88501	-0.25541	-5.00187
H	-2.58419	1.06264	-4.67399
H	-2.62301	2.81638	-4.70672
H	-5.09112	2.80333	-5.00465
H	-4.34915	1.81064	-6.25611
C	3.66282	-1.89374	-2.34211
C	3.14970	-0.93026	-3.43633
C	4.88619	-2.69155	-2.85722
H	2.86876	-2.62631	-2.16778
C	2.82620	-1.68010	-4.73707
H	3.91271	-0.16858	-3.64865
H	2.26795	-0.38800	-3.07885
C	4.56780	-3.43274	-4.16531
H	5.72722	-2.00276	-3.02249
H	5.21377	-3.40265	-2.08758
C	4.03624	-2.47804	-5.24498
H	2.48833	-0.96853	-5.50051
H	1.98559	-2.36788	-4.55955
H	5.46242	-3.95777	-4.52527
H	3.81213	-4.20716	-3.96511
H	4.83499	-1.77757	-5.53146
H	3.77364	-3.03891	-6.15152
C	6.35512	1.60561	0.08295
C	5.89870	2.95027	0.69052
C	7.67032	1.13598	0.75063
H	6.58006	1.79253	-0.97772
C	7.00037	4.01915	0.61489
H	5.61719	2.79741	1.74296
H	5.00007	3.30284	0.16900
C	8.76923	2.20690	0.67632
H	7.46979	0.89160	1.80390
H	8.00862	0.20622	0.27659
C	8.30070	3.54033	1.27673
H	7.19745	4.25764	-0.44052
H	6.65252	4.94953	1.08209
H	9.05064	2.36391	-0.37550
H	9.67219	1.85289	1.19010
H	9.08373	4.30203	1.17141
H	8.13238	3.41223	2.35667
C	3.27326	-1.35748	2.78807
C	4.39238	-1.96510	3.67001
C	2.57633	-0.20270	3.54425
H	2.51357	-2.13332	2.64990
C	3.86542	-2.41554	5.04081
H	5.18586	-1.21764	3.81406
H	4.86218	-2.80959	3.15054
C	2.05133	-0.65440	4.91688
H	3.28097	0.62923	3.68924
H	1.74841	0.17105	2.93303
C	3.16444	-1.26710	5.77905
H	4.69048	-2.81207	5.64682
H	3.15464	-3.24354	4.90133
H	1.25468	-1.39841	4.77011
H	1.58946	0.19487	5.43712
H	3.90429	-0.48928	6.02126
H	2.75690	-1.61933	6.73535
P	-0.30373	-0.78266	-0.25302
O	-0.90587	-0.03404	-1.49765
O	0.29633	0.02864	0.84969
H	-0.35265	0.63079	-2.03797
H	0.29902	1.67922	1.49611
Cl	0.49994	2.23563	-2.89116
O	0.43618	2.66567	1.44846
C	0.43882	2.84992	-0.37638
C	1.88154	2.94041	1.30203
C	1.85360	3.37846	-0.17423
H	0.28639	1.80505	-0.51757
H	-0.40326	3.50714	-0.54914
H	2.45320	2.02935	1.48066
H	2.14622	3.70864	2.02776
H	2.54647	2.79387	-0.78763
C	2.04814	4.86369	-0.44847
C	1.40882	5.47442	-1.53712
C	2.91235	5.63598	0.33904
C	1.61140	6.82734	-1.81086
H	0.77121	4.88082	-2.18567
C	3.11810	6.98892	0.06206
H	3.44293	5.18715	1.17473
C	2.46250	7.59158	-1.01106
H	1.10441	7.28210	-2.65773
H	3.79059	7.56914	0.68844
H	2.61850	8.64526	-1.22622

1 imaginary frequency: -392.59 cm^{-1}.

SCF energy: -4055.660045 hartree
zero-point correction: +1.543002 hartree
enthalpy correction: +1.618051 hartree
free energy correction: +1.427309 hartree
quasiharmonic free energy correction: +1.452559 hartree

TS(*S*)_B4

C	-0.86381	-4.35991	-1.05292
O	0.76326	-1.75015	-0.89713

O	-1.59097	-1.59399	0.18634	C	-4.98111	-3.62234	4.02493
C	-2.38614	-2.18272	-0.81579	H	-3.01450	-2.94605	4.66725
C	-1.94818	-3.35230	-1.42964	H	-3.02267	-3.78344	3.11945
C	-3.60542	-1.56914	-1.16040	H	-6.82719	-4.08843	2.97156
C	-2.64612	-3.82622	-2.55293	H	-5.36312	-4.48602	2.07912
C	-4.32819	-2.14500	-2.21775	H	-4.90613	-4.60185	4.51507
C	-3.83891	-3.23067	-2.94552	H	-5.49623	-2.95706	4.73414
H	-5.28178	-1.70331	-2.48817	C	-5.91807	3.00079	1.68417
H	-4.39313	-3.60724	-3.80162	C	-7.23209	3.49922	1.03945
C	1.20572	-2.89827	-0.22418	C	-4.92203	4.17312	1.84600
C	0.41003	-4.04212	-0.27130	H	-6.16926	2.65000	2.69697
C	2.45480	-2.88945	0.42572	C	-7.84600	4.66964	1.82312
C	0.81598	-5.18022	0.44489	H	-7.94565	2.66845	0.97072
C	2.86236	-4.08322	1.04534	H	-7.03075	3.82134	0.00782
C	2.04720	-5.21268	1.08828	C	-5.53798	5.34317	2.62826
H	3.83515	-4.10354	1.52676	H	-4.01247	3.81585	2.34514
H	2.37366	-6.10297	1.61993	H	-4.61274	4.52324	0.85065
C	-1.91258	-4.99087	-3.18364	C	-6.84768	5.82538	1.98691
H	-2.43673	-5.94067	-3.00831	H	-8.15596	4.31604	2.81792
H	-1.81803	-4.88158	-4.27001	H	-8.75675	5.02037	1.32075
C	-0.54586	-4.95800	-2.46333	H	-5.73886	5.02145	3.66115
H	0.13696	-4.28014	-2.98831	H	-4.81895	6.16990	2.69491
H	-0.06281	-5.93807	-2.40261	H	-7.29153	6.63062	2.58637
C	-0.24443	-6.25659	0.38907	H	-6.62832	6.25575	0.99831
H	0.04429	-7.06772	-0.29402	C	-3.97031	1.08049	-2.56448
H	-0.42451	-6.71826	1.36661	C	-5.22405	1.16987	-3.47008
C	-1.46822	-5.48301	-0.14054	C	-3.08719	2.33030	-2.78979
H	-1.99788	-5.01069	0.69515	H	-3.38165	0.22074	-2.90142
H	-2.18597	-6.11228	-0.67475	C	-4.84810	1.33256	-4.95131
C	-4.15518	-0.37821	-0.42900	H	-5.83499	2.02721	-3.15145
C	-4.55998	-0.50823	0.92348	H	-5.85523	0.28207	-3.33696
C	-4.34393	0.85940	-1.10011	C	-2.69575	2.48263	-4.26691
C	-5.12018	0.59799	1.57301	H	-3.62880	3.23338	-2.47334
C	-4.91786	1.92609	-0.39871	H	-2.18629	2.26675	-2.17295
C	-5.30851	1.82542	0.93835	C	-3.93235	2.54548	-5.17397
H	-5.43437	0.49595	2.60924	H	-5.75747	1.42122	-5.56065
H	-5.06240	2.86890	-0.91852	H	-4.33125	0.42286	-5.29161
C	3.35973	-1.69353	0.49278	H	-2.06498	1.63222	-4.56121
C	3.64766	-1.09929	1.74844	H	-2.07515	3.37721	-4.39473
C	4.00985	-1.21853	-0.67412	H	-4.49583	3.46584	-4.95660
C	4.58196	-0.05566	1.80143	H	-3.63262	2.60583	-6.22839
C	4.93235	-0.17218	-0.55839	C	3.80625	-1.85316	-2.04576
C	5.24503	0.42077	0.66777	C	3.36682	-0.83774	-3.12485
H	4.82361	0.38468	2.76676	C	5.06881	-2.61935	-2.51159
H	5.44023	0.17208	-1.45488	H	3.00749	-2.59737	-1.96752
C	-4.47985	-1.82351	1.69334	C	3.13835	-1.52471	-4.47929
C	-3.65064	-1.71585	2.99374	H	4.13911	-0.06505	-3.24577
C	-5.88922	-2.38870	1.99694	H	2.46001	-0.31460	-2.80431
H	-3.98171	-2.56772	1.06390	C	4.84766	-3.29842	-3.87230
C	-3.58121	-3.06091	3.73400	H	5.91364	-1.91959	-2.58611
H	-2.64265	-1.35930	2.75385	H	5.34867	-3.36461	-1.75563
H	-4.10133	-0.96649	3.65971	C	4.38398	-2.29593	-4.93998
C	-5.81515	-3.73128	2.74013	H	2.85080	-0.77818	-5.22987
H	-6.44853	-2.50316	1.05964	H	2.29074	-2.22165	-4.39346
H	-6.45034	-1.66608	2.60629	H	5.76920	-3.80123	-4.19402

H	4.08662	-4.08551	-3.76148
H	5.19627	-1.58117	-5.14098
H	4.18553	-2.81516	-5.88676
C	6.31530	1.49468	0.78776
C	7.72866	0.91372	0.53737
C	6.07388	2.71580	-0.12755
H	6.29716	1.85890	1.82697
C	8.82566	1.97745	0.69521
H	7.76695	0.49744	-0.47954
H	7.90664	0.07499	1.22210
C	7.17071	3.77930	0.03614
H	6.04326	2.38836	-1.17598
H	5.09209	3.15621	0.08544
C	8.56876	3.19293	-0.20754
H	8.86158	2.30725	1.74443
H	9.80696	1.53783	0.47470
H	7.12520	4.19203	1.05534
H	6.98157	4.61683	-0.64671
H	9.33743	3.95903	-0.04350
H	8.65313	2.88587	-1.26065
C	3.01707	-1.57064	3.05888
C	4.06325	-2.22980	3.99220
C	2.26980	-0.45002	3.81790
H	2.26708	-2.33268	2.82531
C	3.42664	-2.75030	5.28975
H	4.84232	-1.49417	4.23863
H	4.57247	-3.04748	3.46665
C	1.63365	-0.96986	5.11748
H	2.96695	0.36450	4.06318
H	1.49592	-0.03605	3.16327
C	2.67004	-1.63974	6.03171
H	4.19869	-3.18531	5.93772
H	2.72754	-3.56419	5.04693
H	0.84815	-1.69733	4.86596
H	1.13532	-0.14607	5.64497
H	3.38899	-0.88324	6.38073
H	2.18284	-2.04345	6.92861
P	-0.29775	-0.72445	-0.22869
O	-0.76249	0.12000	-1.47068
O	0.21498	-0.00312	0.97583
H	-0.14443	0.80136	-1.91250
H	0.21498	1.59892	1.72370
Cl	0.82483	2.42574	-2.57576
O	0.38254	2.58173	1.75779
C	0.55872	2.88182	-0.03905
C	1.84160	2.81958	1.76856
C	1.97601	3.31356	0.31517
H	0.36530	1.85939	-0.26692
H	-0.22955	3.59586	-0.23863
H	2.37061	1.88887	1.97451
H	2.04624	3.55850	2.54290
H	2.68664	2.70957	-0.25756
C	2.29324	4.79083	0.13356
C	1.75555	5.51748	-0.93779
C	3.18037	5.43855	1.00440
C	2.07943	6.86326	-1.11440
H	1.10418	5.02010	-1.64986
C	3.50826	6.78341	0.82439
H	3.63136	4.89450	1.83098
C	2.95246	7.50300	-0.23326
H	1.65032	7.41009	-1.94975
H	4.19664	7.26599	1.51314
H	3.20285	8.55108	-0.37354

1 imaginary frequency: -390.68 cm^{-1}.

SCF energy: -4055.660128 hartree
zero-point correction: +1.542637 hartree
enthalpy correction: +1.617816 hartree
free energy correction: +1.426033 hartree
quasiharmonic free energy correction: +1.452143 hartree

PC(*R*)

C	-0.49536	-4.50360	-0.04763
O	-1.42507	-1.61564	0.50546
O	0.93787	-1.79229	-0.53983
C	1.47189	-2.74517	0.34256
C	0.75328	-3.90947	0.60250
C	2.74450	-2.51280	0.89950
C	1.24490	-4.80153	1.57038
C	3.23805	-3.48163	1.78827
C	2.48739	-4.59735	2.15822
H	4.22796	-3.33609	2.20888
H	2.87732	-5.29946	2.89094
C	-2.15773	-2.44895	-0.35719
C	-1.63733	-3.70247	-0.66664
C	-3.40146	-2.01396	-0.85247
C	-2.28342	-4.48403	-1.63734
C	-4.06443	-2.87588	-1.74233
C	-3.50051	-4.07744	-2.17227
H	-5.03616	-2.57505	-2.11978
H	-4.01722	-4.68926	-2.90755
C	0.25345	-5.91551	1.82428
H	0.58965	-6.86129	1.37687
H	0.10734	-6.10878	2.89313
C	-1.02182	-5.38745	1.13485
H	-1.58181	-4.74937	1.82847
H	-1.69475	-6.18057	0.79555
C	-1.47601	-5.72682	-1.94413
H	-1.94879	-6.62671	-1.52676
H	-1.37079	-5.89978	-3.02129
C	-0.12518	-5.42795	-1.25672
H	0.52592	-4.87150	-1.94097
H	0.41223	-6.32858	-0.94470
C	3.58866	-1.32005	0.55451
C	4.11615	-1.18290	-0.75587

C	3.93507	-0.37242	1.55124
C	4.95956	-0.10355	-1.03895
C	4.79164	0.68252	1.20824
C	5.31417	0.84405	-0.07591
H	5.36345	-0.00977	-2.04337
H	5.06974	1.40298	1.97431
C	-4.03811	-0.71786	-0.44175
C	-4.45760	-0.53131	0.89949
C	-4.28732	0.29830	-1.40248
C	-5.09361	0.66549	1.25003
C	-4.93538	1.46890	-0.99208
C	-5.34285	1.68103	0.32751
H	-5.41769	0.80749	2.27850
H	-5.12613	2.24127	-1.73183
C	3.85648	-2.19826	-1.86483
C	3.20194	-1.57095	-3.11754
C	5.14785	-2.95763	-2.25650
H	3.15940	-2.95413	-1.49032
C	2.93518	-2.62702	-4.20149
H	2.26856	-1.07290	-2.83329
H	3.86211	-0.79520	-3.53046
C	4.87938	-4.00983	-3.34370
H	5.57989	-3.43234	-1.36614
H	5.89774	-2.24127	-2.62089
C	4.21380	-3.38886	-4.58069
H	2.49745	-2.15048	-5.08797
H	2.18433	-3.34191	-3.83153
H	4.22224	-4.79175	-2.93437
H	5.81712	-4.50757	-3.62337
H	3.98995	-4.16584	-5.32324
H	4.91976	-2.69377	-5.05947
C	6.25095	1.99684	-0.39827
C	5.72424	2.89290	-1.54241
C	7.68564	1.51139	-0.71420
H	6.31530	2.62719	0.50190
C	6.67530	4.06358	-1.83594
H	4.72755	3.27093	-1.28435
H	5.60502	2.28771	-2.45237
C	8.63455	2.68392	-1.00847
H	8.06461	0.91320	0.12415
H	7.65447	0.84061	-1.58493
C	8.09931	3.57489	-2.13887
H	6.69916	4.73541	-0.96512
H	6.28887	4.65726	-2.67417
H	8.75384	3.28901	-0.09721
H	9.63269	2.30354	-1.26139
H	8.76958	4.42910	-2.29952
H	8.09296	3.00167	-3.07803
C	3.43753	-0.45847	2.99269
C	4.57206	-0.84978	3.97250
C	2.76396	0.84252	3.48898
H	2.67562	-1.24331	3.04543
C	4.05595	-1.00101	5.41215
H	5.35360	-0.07665	3.94226
H	5.05184	-1.78048	3.64501
C	2.22825	0.68566	4.92064
H	3.48776	1.66924	3.47292
H	1.95466	1.12206	2.80790
C	3.33932	0.26870	5.89505
H	4.88773	-1.24895	6.08452
H	3.35672	-1.84926	5.45493
H	1.43366	-0.07495	4.92758
H	1.76492	1.62412	5.25103
H	4.07106	1.08622	5.97854
H	2.92840	0.11436	6.90115
C	-3.89970	0.16647	-2.87372
C	-5.13539	-0.06631	-3.77901
C	-3.09828	1.37512	-3.40690
H	-3.24872	-0.70821	-2.97871
C	-4.73301	-0.26719	-5.24874
H	-5.80684	0.80120	-3.69853
H	-5.71359	-0.92985	-3.42652
C	-2.67908	1.16886	-4.86976
H	-3.71037	2.28643	-3.34356
H	-2.21517	1.54445	-2.78801
C	-3.89196	0.90590	-5.77395
H	-5.63001	-0.40217	-5.86777
H	-4.15058	-1.19660	-5.33637
H	-2.11801	2.04441	-5.21844
H	-1.98768	0.31534	-4.92943
H	-4.51886	1.80986	-5.80950
H	-3.56956	0.70980	-6.80507
C	-6.04316	2.96131	0.75138
C	-5.14720	4.21005	0.57960
C	-7.39198	3.16370	0.02316
H	-6.26653	2.87110	1.82540
C	-5.86053	5.49336	1.03363
H	-4.86369	4.30719	-0.47841
H	-4.21479	4.07048	1.14113
C	-8.10232	4.44785	0.47856
H	-8.03502	2.29060	0.19133
H	-7.21380	3.21365	-1.06056
C	-7.20271	5.68135	0.31112
H	-6.03816	5.44331	2.11829
H	-5.21175	6.36275	0.86554
H	-8.38582	4.34876	1.53712
H	-9.03697	4.57828	-0.08210
H	-7.71328	6.57876	0.68363
H	-7.01610	5.84962	-0.76013
C	-4.30673	-1.60258	1.97525
C	-3.46662	-1.13050	3.18487
C	-5.67982	-2.13358	2.45461
H	-3.78226	-2.45970	1.54070
C	-3.31120	-2.24289	4.23339
H	-3.95122	-0.26248	3.65389
H	-2.48277	-0.79457	2.83946
C	-5.52340	-3.24406	3.50526
H	-6.26345	-1.30697	2.88407
H	-6.25262	-2.50239	1.59419
C	-4.67279	-2.78081	4.69727

H	-2.73572	-1.87127	5.09121
H	-2.72424	-3.06745	3.80057
H	-5.04474	-4.11787	3.03804
H	-6.51145	-3.57789	3.84818
H	-5.20951	-1.98534	5.23582
H	-4.53642	-3.60344	5.41134
P	-0.20112	-0.74299	-0.10066
O	0.36166	-0.07441	1.23509
O	-0.53036	0.16644	-1.22263
H	-0.09982	0.76419	1.46104
H	0.07663	1.67974	-2.26016
Cl	-0.94924	2.89231	1.74484
O	-0.00021	2.56887	-2.65883
C	-0.73567	3.43100	-0.00154
C	0.83519	3.47520	-1.97332
C	0.73234	3.39057	-0.42505
H	-1.33666	2.74446	-0.59357
H	-1.16583	4.43234	-0.04346
H	1.89624	3.33819	-2.23819
H	0.54616	4.47619	-2.31422
H	1.12570	2.40731	-0.13972
C	1.59514	4.45773	0.22736
C	1.28083	5.81998	0.11121
C	2.75237	4.10120	0.93117
C	2.09325	6.79522	0.68927
H	0.39228	6.12875	-0.43498
C	3.56879	5.07494	1.51056
H	3.01662	3.05109	1.02653
C	3.24145	6.42577	1.39268
H	1.82920	7.84484	0.58936
H	4.45880	4.77493	2.05793
H	3.87389	7.18511	1.84479

There are no imaginary frequencies.

SCF energy: -4055.718850 hartree
zero-point correction: +1.544641 hartree
enthalpy correction: +1.620409 hartree
free energy correction: +1.427429 hartree
quasiharmonic free energy correction: +1.453728 hartree

PC(*S*)

C	-0.18959	-4.38266	1.31330
O	-1.21459	-1.48307	0.94337
O	1.06878	-1.96694	-0.16082
C	1.75096	-2.60989	0.88849
C	1.09660	-3.61272	1.59721
C	3.07365	-2.22900	1.18338
C	1.70747	-4.14168	2.74543
C	3.69148	-2.87588	2.26723
C	3.01077	-3.78813	3.07444
H	4.72128	-2.62192	2.49696
H	3.50051	-4.21533	3.94600
C	-1.90049	-2.56558	0.36964
C	-1.37793	-3.85052	0.51381
C	-3.12556	-2.33195	-0.28596
C	-2.03894	-4.92404	-0.10712
C	-3.79846	-3.45197	-0.80249
C	-3.25640	-4.73433	-0.74818
H	-4.75971	-3.29485	-1.28055
H	-3.78077	-5.56996	-1.20494
C	0.75669	-5.06765	3.47420
H	1.05434	-6.11970	3.36645
H	0.72111	-4.86122	4.54999
C	-0.59096	-4.78634	2.77090
H	-1.09203	-3.93642	3.24827
H	-1.27934	-5.63660	2.79506
C	-1.24288	-6.20147	0.03433
H	-1.68801	-6.87080	0.78382
H	-1.19154	-6.76843	-0.90215
C	0.13282	-5.67923	0.49150
H	0.73267	-5.40158	-0.38304
H	0.70712	-6.40836	1.07046
C	3.82470	-1.19008	0.40268
C	4.26951	-0.00197	1.04274
C	4.15130	-1.41406	-0.95822
C	5.02252	0.92047	0.30798
C	4.90242	-0.45016	-1.64148
C	5.34964	0.72354	-1.03577
H	5.36379	1.82428	0.80546
H	5.15585	-0.62509	-2.68452
C	-3.75320	-0.97737	-0.45872
C	-4.28979	-0.29084	0.66162
C	-3.92524	-0.43958	-1.76098
C	-4.99146	0.90166	0.45239
C	-4.63725	0.75833	-1.90526
C	-5.18739	1.44280	-0.82182
H	-5.42107	1.40855	1.31172
H	-4.77948	1.16816	-2.90215
C	3.97811	0.31748	2.50782
C	5.25458	0.22622	3.38008
C	3.30921	1.69717	2.70779
H	3.26807	-0.42396	2.88758
C	4.95373	0.49456	4.86272
H	5.72572	-0.75799	3.26274
H	5.98993	0.95938	3.01800
C	3.00065	1.96329	4.19006
H	2.39169	1.73337	2.11316
H	3.96813	2.49334	2.33381
C	4.26004	1.84962	5.06143
H	5.88192	0.45124	5.44772
H	4.30374	-0.30471	5.24880
H	2.55062	2.95797	4.30594
H	2.24788	1.24122	4.53805
H	4.00779	1.99722	6.11953
H	4.95963	2.65506	4.79142
C	6.16222	1.74120	-1.81868
C	7.58144	1.94060	-1.23840

C	5.43942	3.10293	-1.94434
H	6.28294	1.34591	-2.83887
C	8.39866	2.94951	-2.05997
H	8.09927	0.97425	-1.19350
H	7.50124	2.29843	-0.20174
C	6.25831	4.11146	-2.76491
H	4.45107	2.95359	-2.39703
H	5.26370	3.51152	-0.93834
C	7.67004	4.29558	-2.18897
H	8.57774	2.53757	-3.06442
H	9.38623	3.09295	-1.60278
H	6.33507	3.75477	-3.80288
H	5.73416	5.07526	-2.80706
H	8.25056	4.98445	-2.81600
H	7.59727	4.76298	-1.19549
C	3.75758	-2.67927	-1.71390
C	2.88428	-2.37729	-2.95466
C	4.98948	-3.52487	-2.11886
H	3.15823	-3.31027	-1.04991
C	2.47088	-3.66588	-3.68111
H	3.44608	-1.73955	-3.65203
H	1.99894	-1.80970	-2.65016
C	4.57550	-4.81143	-2.85115
H	5.64435	-2.93032	-2.77143
H	5.57967	-3.76824	-1.22599
C	3.69161	-4.51197	-4.07133
H	1.87650	-3.42054	-4.57093
H	1.81509	-4.25667	-3.02365
H	4.02165	-5.45972	-2.15550
H	5.46821	-5.37363	-3.15499
H	4.28416	-3.96583	-4.82070
H	3.37284	-5.44790	-4.54856
C	-3.40906	-1.12597	-3.02673
C	-4.56895	-1.71426	-3.86947
C	-2.54691	-0.20358	-3.92092
H	-2.76568	-1.96022	-2.72738
C	-4.05747	-2.45271	-5.11631
H	-5.23726	-0.89696	-4.17687
H	-5.17791	-2.38985	-3.25678
C	-2.02495	-0.94325	-5.16310
H	-3.13837	0.66319	-4.24592
H	-1.70582	0.18959	-3.34303
C	-3.17126	-1.54910	-5.98498
H	-4.90606	-2.83143	-5.70110
H	-3.47806	-3.33306	-4.80082
H	-1.43355	-0.25679	-5.78276
H	-1.34057	-1.74390	-4.84616
H	-3.78473	-0.73670	-6.40249
H	-2.77447	-2.11178	-6.83991
C	-6.00468	2.70676	-1.03705
C	-7.48377	2.51507	-0.62631
C	-5.40714	3.94197	-0.32591
H	-5.99449	2.92119	-2.11648
C	-8.31771	3.78156	-0.87328
H	-7.52993	2.25247	0.44032
H	-7.90887	1.66417	-1.17334
C	-6.24474	5.20703	-0.57128
H	-5.35040	3.74739	0.75472
H	-4.37713	4.09651	-0.67129
C	-7.71206	5.00315	-0.16677
H	-9.35094	3.62079	-0.53946
H	-8.36702	3.97739	-1.95491
H	-6.19782	5.46903	-1.63876
H	-5.81224	6.05486	-0.02435
H	-8.29760	5.90358	-0.39285
H	-7.77088	4.85736	0.92228
C	-4.22063	-0.85951	2.07579
C	-3.78450	0.16750	3.14383
C	-5.56501	-1.51218	2.48271
H	-3.47220	-1.65719	2.09048
C	-3.68348	-0.48700	4.53024
H	-4.51846	0.98412	3.20012
H	-2.82991	0.62752	2.86727
C	-5.48294	-2.15304	3.87733
H	-6.35431	-0.74615	2.47337
H	-5.85295	-2.26431	1.73696
C	-5.00704	-1.15045	4.93949
H	-3.38522	0.26196	5.27462
H	-2.88526	-1.24443	4.51552
H	-4.78078	-2.99951	3.84061
H	-6.45902	-2.57133	4.15654
H	-5.77398	-0.37211	5.07030
H	-4.90197	-1.64956	5.91182
P	0.05317	-0.77484	0.23145
O	-0.37861	-0.35907	-1.24522
O	0.56815	0.30077	1.11372
H	-0.59908	0.59528	-1.32448
H	-0.25699	1.50674	2.32037
Cl	-1.08228	2.84740	-1.66855
O	-0.81421	2.21096	2.70958
C	-1.35873	3.32931	0.08314
C	-0.27748	3.46465	2.34024
C	-0.04293	3.60057	0.81092
H	-2.00857	4.20418	0.03862
H	-1.89431	2.49830	0.53995
H	-0.99003	4.22128	2.68937
H	0.68052	3.66469	2.84387
H	0.65275	2.79936	0.53854
C	0.59347	4.93220	0.45590
C	-0.06872	6.14522	0.69794
C	1.87784	4.97704	-0.10115
C	0.53310	7.36503	0.38883
H	-1.06612	6.14217	1.13262
C	2.48346	6.19541	-0.41282
H	2.40589	4.04678	-0.29682
C	1.81276	7.39426	-0.16894
H	0.00203	8.29314	0.58410
H	3.47910	6.20580	-0.84904
H	2.28177	8.34405	-0.41181

There are no imaginary frequencies.

SCF energy: -4055.718714 hartree
zero-point correction: +1.544360 hartree
enthalpy correction: +1.620266 hartree
free energy correction: +1.426125 hartree
quasiharmonic free energy correction: +1.453330 hartree

(*R*)-3a

C	1.57642	-0.49294	-0.74155
H	1.20357	-1.37928	-1.25593
H	1.61468	0.34853	-1.43376
C	0.73080	-0.16292	0.49504
H	0.93711	-0.92697	1.25515
C	1.12725	1.20122	1.10888
H	2.19846	1.20139	1.32799
H	0.58672	1.33704	2.05742
O	0.90843	2.29492	0.22957
H	-0.05180	2.40562	0.14057
Cl	3.30756	-0.85562	-0.30151
C	-0.75643	-0.21355	0.17166
C	-1.29786	0.43783	-0.94997
C	-1.63408	-0.89492	1.02774
C	-2.67165	0.40596	-1.20246
H	-0.64516	0.96314	-1.64146
C	-3.00602	-0.92515	0.77903
H	-1.23471	-1.40934	1.89903
C	-3.53069	-0.27316	-0.33862
H	-3.06778	0.91212	-2.07893
H	-3.66472	-1.46189	1.45670
H	-4.59882	-0.29838	-0.53616

There are no imaginary frequencies.

SCF energy: -885.195575 hartree
zero-point correction: +0.182567 hartree
enthalpy correction: +0.193987 hartree
free energy correction: +0.145384 hartree
quasiharmonic free energy correction: +0.146323 hartree

(*S*)-3a

C	-1.57642	-0.49294	-0.74155
H	-1.20357	-1.37928	-1.25593
H	-1.61468	0.34853	-1.43376
C	-0.73080	-0.16292	0.49504
H	-0.93711	-0.92697	1.25515
C	-1.12725	1.20122	1.10888
H	-2.19846	1.20139	1.32799
H	-0.58672	1.33704	2.05742
O	-0.90843	2.29492	0.22957
H	0.05180	2.40562	0.14057
Cl	-3.30756	-0.85562	-0.30151
C	0.75643	-0.21355	0.17166
C	1.63408	-0.89492	1.02774
C	1.29787	0.43783	-0.94997
C	3.00602	-0.92515	0.77903
H	1.23471	-1.40934	1.89903
C	2.67165	0.40596	-1.20246
H	0.64517	0.96314	-1.64146
C	3.53069	-0.27316	-0.33862
H	3.66472	-1.46189	1.45670
H	3.06778	0.91212	-2.07893
H	4.59882	-0.29838	-0.53616

SCF energy: -885.195575 hartree
zero-point correction: +0.182567 hartree
enthalpy correction: +0.193987 hartree
free energy correction: +0.145384 hartree
quasiharmonic free energy correction: +0.146323 hartree

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