Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature

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1 Theoretical Components

Canonical transition state theory (TST).

According to traditional transition theory, the high-pressure limit rate constant is:

$$k_{\infty}(T) = \kappa(T) rpd \frac{k_B T}{h} \frac{Q_{TS}(T)}{Q_R(T)} \exp\left[-\frac{V^{\neq}}{RT}\right] \quad (1)$$

where $V^{\neq}$ denotes the electronic activation barrier height including zero point energy (ZPE). $Q_{TS}(T)$ and $Q_R(T)$ denote the canonical partition functions for the transition states and reactants, respectively; T is the temperature ranging; $\kappa(T)$, k_B, R, rpd and h are tunneling factor, Boltzmann's constant, gas constant, degeneracy of the reaction paths and Planck's constant, respectively. The rpd is the reaction path degeneracy and can be written as,

$$rpd = \frac{\sigma_R \times n_{TS}}{\sigma_{TS} \times n_R} \quad (2)$$

where n_{TS} and n_R are the number of optical isomers for transition states and reactants, respectively. σ_{TS} and σ_R correspond to the external symmetry number of the transition states and the reactants, respectively. In this study, the values of rpd for all the reactions are 1.

The microscopic rate constants are calculated by using RRKM theory in the following equation:

$$k(E) = l^{+}\left(\frac{G^{+}(E)}{hN(E+E_0)}\right) \quad (3)$$

where l^{+} is the reaction path degeneracy and $G^{+}(E)$ is the total number of states of the transition structure with energy less than or equal to E and h is Planck's constant and $N(E+E_0)$ is the density of states of the reactant at energy $E+E_0$. The direct count algorithm of Beyer and Swinehart is used to calculate the density and sum of states. A master-equation method is used to calculate pressure-dependent rate constants. A brief description about how the master equation is used in the ChemRate program is presented below. The time evolution of the population of the species in the system is described by the master equation:

$$\frac{d\rho_i^{\alpha}}{dt} = \omega \sum_j P_{ij}^{\alpha} \rho^{\alpha}{}_j - \omega \sum_j P^{\alpha} \rho_i^{\alpha} - {}_i k^{\alpha} \rho^{\alpha}{}_i + \sum_{\beta} k^{\beta} \rho^{\beta}{}_l + R_l \quad (4)$$

where ρ_i^{α} is the molecular population of the isomer α at energy level E_i, P_{ij}^{α} is the collision energy transfer probability from energy level j to energy level i of isomer α, ω is the collision frequency, which is proportional to the concentration of the third body M, hence, it is pressure dependent, k_i^{α} is the sum of rates for all the decomposition and isomerization channels from energy level E_i, k_l^{β} is the rate of isomerization from isomer β at energy level E_l to isomer α at energy level E_i, and R_i is the chemical activation flux, which is assumed to be constant. Index l for isomer β corresponds to the same energy as i for α, i.e., $E_l=E_i$.

2 The IRC-MAX calculations for R1, R9 and R18

It can been seen from Figure S1 that the geometries obtained by IRCMAX are very close to the

geometries of the TS at MP2 level. Therefore, the MP2 geometries are acceptable.

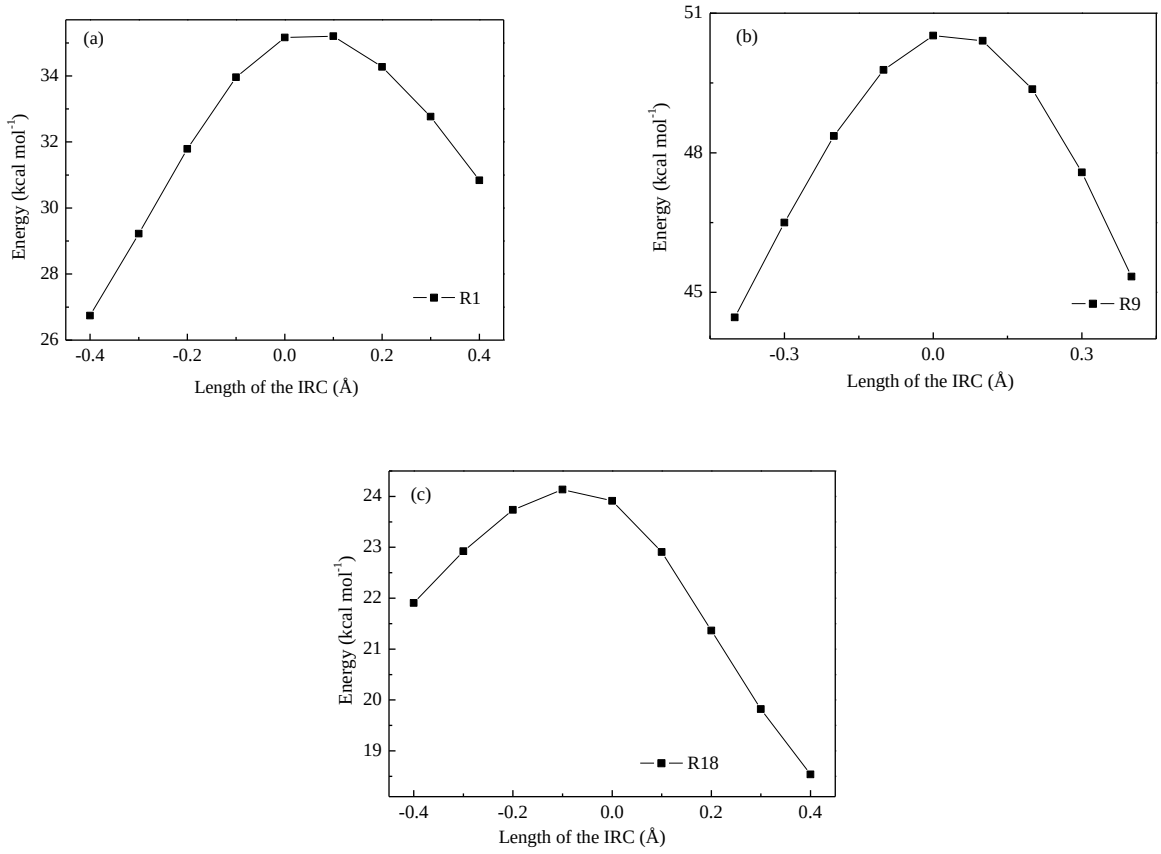

Figure S1. Results of the IRC-MAX calculations CBS-QB3//MP2/CBSB7 for representative reactions. Reaction energies are relative to •O2QOOH.

3 The difference of barrier heights for selected reactions between this work and literatures

In Sharma's work [ref 36], a standard CBS-QB3 method is used for the single-point electronic energy and ZPE. A standard CBS-QB3 method means that geometry optimization is done using the method involved in the composite scheme of CBS-QB3 method. In our work, geometric optimization for all species are done at MP2/CBSB7 level, hence the the single-point electronic energy and ZPE are done by CBS-QB3 method without geometric optimixation.

Reaction for $OOCH_2CH_2OOH$ is taken as an example to illustrate the difference of barrier heights by the two schemes. The geometries of the reactant and the transition state of 1,4-hydrogen shift in the •O2CH2CH2OOH are listed in Table S1 and Table S2. The barrier height without zero-point energy corrections for $OOCH_2CH_2OOH$ is 35.0 kcal mol^{-1} at CBS-QB3//B3LYP/CBSB7 level calculated by Sharma and 35.2 kcal mol^{-1} at CBS-QB3//MP2/CBSB7 level calculated in this study, which is 0.2 kcal mol^{-1} larger than Sharma's. We also calculated the barrier height of this reaction using CBS-QB3 method with the freezen Sharma's geometries obtained at B3LYP level and found that the barrier height is 0.2 kcal mol^{-1} larger than values using standard CBS-QB3 methode. In the

part 3.2.2 of ref 36, a comparison of the IRC-MAX calculation between by CBS-QB3//B3LYP/6-31G(d) and by CBS-QB3//MP2/CBSB7 method has been made by Sharma et al. and they concluded that the barrier heights without zero-point energy corrections along both trajectories are the same, however, our calculation showes that the ZPEs for these two cases have a difference of 0.6 kcal mol^{-1}.

Table S1 Comparison of geometry of reactant of R9 between this work and Sharma's

O2CCOO•											
Bond				Angle				dihedral angle			
atom numbers	Sharma's	this work	AD[a]	atom numbers	Sharma's	this work	AD[a]	atom numbers	Sharma's	this work	AD[a]
1 2	0.97	0.97	0.00								
1 3	1.45	1.45	0.00	3 1 2	99.3	98.6	0.64				
3 4	1.41	1.41	0.00	4 3 1	108.2	107.0	1.22	4 3 1 2	98.1	100.1	1.97
4 5	1.09	1.09	0.00	5 4 3	103.4	103.5	0.09	5 4 3 1	-179.2	-179.6	0.45
4 6	1.10	1.10	0.00	6 4 3	111.2	111.2	0.01	6 4 3 1	63.7	62.6	1.10
4 7	1.52	1.52	0.01	7 4 3	113.8	113.4	0.40	7 4 3 1	-58.8	-60.0	1.20
7 8	1.09	1.09	0.00	8 7 4	110.7	110.8	0.07	8 7 4 3	-171.2	-171.6	0.35
7 9	1.09	1.09	0.00	9 7 4	111.5	111.8	0.31	9 7 4 3	65.4	64.6	0.86
1 0	1.45	1.45	0.00	10 7 4	111.4	110.7	0.72	10 7 4 3	-55.0	-55.5	0.49
10 11	1.32	1.30	0.03	11 10 7	111.7	111.3	0.41	11 10 7 4	77.9	82.5	4.55

[a]Absolute difference.

Table S2 Comparison of geometry of transition state of R9 between this work and Sharma's

TS											
Bond				Angle				dihedral angle			
atom numbers	Sharma's	this work	AD[a]	atom numbers	Sharma's	this work	AD[a]	atom numbers	Sharma's	this work	AD[a]
1 2	1.42	1.39	0.03								
2 3	1.42	1.41	0.01	3 2 1	103.3	102.4	0.90				
3 4	1.09	1.09	0.00	4 3 2	107.3	108.1	0.72	4 3 2 1	-168.3	-170.4	2.08
3 5	1.10	1.10	0.00	5 3 2	111.8	111.8	0.01	5 3 2 1	70.1	66.6	3.47
3 6	1.53	1.53	0.00	6 3 2	102.8	101.1	1.69	6 3 2 1	-46.8	-49.2	2.43
1 7	1.26	1.27	0.01	7 1 2	93.1	89.1	3.96	7 1 2 3	35.8	34.6	1.19
6 8	1.09	1.09	0.00	8 6 3	117.8	116.6	1.23	8 6 3 2	-76.7	-74.8	1.88
6 9	1.37	1.37	0.00	9 6 3	111.6	111.6	0.07	9 6 3 2	149.8	152.6	2.81
9 10	1.45	1.45	0.00	10 9 6	108.2	107.6	0.58	10 9 6 3	164.1	168.4	4.34
10 11	0.97	0.97	0.00	11 10 9	99.2	99.2	0.06	11 10 9 6	157.2	115.2	41.94

[a]Absolute difference.

Some representative reactions are chosen to show the difference of ZPE between Sharma's and this work and the results are listed in Table S3. It can be seen that the differences are between 0.2 kcal mol^{-1} to 0.6 kcal mol^{-1}.

Table S3. Comparison of ZPEs between this work and Sharma's

Reactions	ZPE(kcal mol^{-1})		
	Sharma's	this work	AD[a]
R9(1,4)	-4.2	-3.6	0.6
R10(1,4)	-4.2	-3.6	0.6

R18(1,5)	-4.4	-4.0	0.4
R23(1,5)	-4.3	-4.0	0.3
R28(1,6)	-4.4	-4.0	0.4
R36(1,7)	-4.6	-4.3	0.2

[a]Absolute difference.

Table S4. Comparison of barrier heights between this work and Miyoshi's

Reactions	Barrier heights(kcal mol^{-1})		
	Miyoshi's	this work	AD[a]
R9(1,4)	29.1	31.5	2.4
R18(1,5)	20.3	20	0.3
R28(1,6)	19.1	21.3	2.2

[a]Absolute difference.

4 The effect of anharmonic correction on the rate constants

To show the effect of anharmonic correction for low-frequence vibration using 1D-hinderd internal rotor model on the rate constants, a comparison of the rate constants for reaction R9 is performed and the results are fiven in Table S5. It can be seen that the difference are with a factor of 3.

Table S5. A comparsion of the rate constants including the hinder rotor correction with those not including the hinder rotor corrections for raection R9

	500K	600K	700K	800K	900K	1000K	1100K	1200K
high-pressure limit[a]	5.02E+01	1.86E+03	3.30E+04	3.57E+05	2.70E+06	1.56E+07	7.37E+07	2.95E+08
high-pressure limit[b]	1.92E+01	9.93E+02	1.98E+04	2.12E+05	1.48E+06	7.62E+06	3.10E+07	1.06E+08
0.01atm[c]	2.64E+01	4.56E+02	2.71E+03	8.55E+03	1.80E+04	2.90E+04	3.90E+04	4.59E+04
0.01atm[d]	1.55E+01	3.06E+02	1.99E+03	6.66E+03	1.46E+04	2.44E+04	3.35E+04	4.03E+04

[a]The rate constants not including the hinder rotor corrections at high-pressure limit. [b]The rate constants including the hinder rotor corrections at high-pressure limit. [c]The rate constants not including the hinder rotor corrections at 0.01atm. [d]The rate constants including the hinder rotor corrections at 0.01atm.

5 The high pressure limit rate constants of the reverse rate constants for abstraction from a non–OOH substituted carbon atom

Table S6. The high pressure limit rate constants of the reverse rate constants for abstraction from a non–OOH substituted carbon atom.

	Modified Arrhenius parameters		
Reactions	A(s^{-1})	n	E(kcal mol^{-1})
1,4-H(p)			
R44	1.10E-11	6.46	4.2
R45	4.04E-12	6.44	3.5

R46	5.32E-11	6.20	3.7
1,4-H(s)			
R47	1.35E-11	6.25	4.0
R48	1.61E-11	6.17	4.2
R49	1.74E-10	6.05	4.7
1,4-H(t)			
R50	4.76E-11	6.03	4.0
R51	2.22E-10	5.96	5.2
R52	1.56E-09	5.69	5.1
1,5-H(p)			
R53	6.24E+05	1.38	1.0
R54	9.32E+04	1.67	2.1
R55	1.68E+05	1.58	1.7
1,5-H(s)			
R56	3.97E+03	1.86	2.5
R57	1.53E+04	1.86	3.0
R58	2.68E+04	1.81	2.9
1,5-H(t)			
R59	1.37E+03	2.13	3.1
R60	2.45E+03	1.84	2.1
R61	2.47E+04	1.70	1.8
1,6-H(p)			
R62	1.66E+03	2.01	2.0
R63	1.35E+03	2.03	2.0
R64	1.79E+03	2.00	2.0
1,6-H(s)			
R65	5.15E+01	2.42	2.6
R66	1.09E+02	2.22	2.1
R67	2.86E+02	2.16	2.4
1,6-H(t)			
R68	6.80E+03	1.86	1.9
R69	2.10E+03	2.01	1.6
1,7-H(p)			
R70	1.96E+03	1.93	1.9
R71	2.00E+02	2.14	2.5
1,7-H(s)			
R72	1.10E+02	2.25	2.3
R73	8.43E+02	1.93	1.9
1,7-H(t)			
R74	7.57E+02	1.92	1.2

6 Pressure dependent rate constants of studied reactions

Table S7. Calculated rate constants, rate rules and ratios of rate constants of reactions to the value of the smallest H-shift reaction in each class for abstraction from an –OOH substituted carbon atom at different pressures.

Reactions	Pressure(atm)	Modified Arrhenius parameters			500K		1200K	
		A(s^{-1})	*n*	*E(kcal mol-1)*	k	k/k_{sma}	k	k/k_{sma}[a]
1,3-H(s) rate rule	**0.01**	**1.00E+65**	**-16.75**	**51.4**	**1.11E-04**	**37.9**	**8.48E+03**	**3.6**
	0.1	**1.00E+70**	**-17.80**	**56.9**	**1.13E-04**	**36.8**	**4.88E+04**	**4.0**
	1	**5.53E+60**	**-14.72**	**54.3**	**1.14E-04**	**36.5**	**2.38E+05**	**4.5**
	10	**5.47E+55**	**-12.84**	**55.4**	**1.14E-04**	**36.4**	**9.09E+05**	**5.4**
	100	**2.97E+47**	**-9.95**	**56.4**	**1.14E-04**	**36.4**	**2.46E+06**	**6.7**
R1	0.01	7.84E+61	-15.54	58.4	2.93E-06	1.0	2.33E+03	1.0
	0.1	2.44E+52	-12.32	56.5	3.08E-06	1.0	1.23E+04	1.0
	1	3.97E+37	-7.57	52.0	3.11E-06	1.0	5.28E+04	1.0
	10	3.56E+20	-2.23	46.0	3.12E-06	1.0	1.69E+05	1.0
	100	3.65E+06	2.10	40.7	3.12E-06	1.0	3.69E+05	1.0
R2	0.01	3.35E+69	-17.92	57.4	1.31E-04	44.8	7.19E+03	3.1
	0.1	4.32E+57	-13.98	54.6	1.34E-04	43.7	3.91E+04	3.2
	1	3.75E+39	-8.24	48.7	1.35E-04	43.3	1.73E+05	3.3
	10	1.03E+20	-2.15	41.5	1.35E-04	43.3	5.67E+05	3.4
	100	2.62E+05	2.36	35.9	1.35E-04	43.3	1.22E+06	3.3
R3	0.01	3.35E+69	-17.92	57.4	2.83E-05	9.7	8.64E+03	3.7
	0.1	4.32E+57	-13.98	54.6	2.87E-05	9.3	4.84E+04	3.9
	1	3.75E+39	-8.24	48.7	2.87E-05	9.2	2.25E+05	4.3
	10	1.03E+20	-2.15	41.5	2.87E-05	9.2	7.95E+05	4.7
	100	2.62E+05	2.36	35.9	2.87E-05	9.2	1.90E+06	5.2
R4	0.01	3.08E+90	-24.09	66.5	2.82E-04	96.3	1.58E+04	6.8
	0.1	4.93E+79	-20.43	64.4	2.87E-04	93.1	9.56E+04	7.8
	1	1.42E+61	-14.51	58.6	2.88E-04	92.3	5.01E+05	9.5
	10	2.11E+38	-7.37	50.5	2.88E-04	92.2	2.11E+06	12.5
	100	2.65E+17	-0.90	42.5	2.88E-04	92.2	6.36E+06	17.2
1,3-H(t) rate rule	**0.01**	**1.00E+80**	**-21.13**	**58.2**	**1.00E-03**	**42.8**	**1.59E+04**	**3.0**
	0.1	**1.00E+80**	**-20.74**	**60.3**	**1.02E-03**	**42.7**	**9.57E+04**	**3.3**
	1	**1.00E+65**	**-16.01**	**53.9**	**1.03E-03**	**42.7**	**4.97E+05**	**4.0**
	10	**9.48E+46**	**-10.38**	**46.6**	**1.03E-03**	**42.7**	**2.08E+06**	**5.2**
	100	**5.17E+46**	**-9.80**	**52.2**	**1.03E-03**	**42.7**	**6.39E+06**	**7.4**
R5	0.01	6.47E+71	-18.51	60.7	2.34E-05	1.0	5.35E+03	1.0
	0.1	1.44E+59	-14.34	57.6	2.39E-05	1.0	2.88E+04	1.0
	1	6.41E+40	-8.52	51.5	2.40E-05	1.0	1.25E+05	1.0
	10	2.45E+21	-2.47	44.4	2.40E-05	1.0	4.03E+05	1.0
	100	1.02E+07	1.97	38.8	2.40E-05	1.0	8.59E+05	1.0
R6	0.01	1.07E+77	-20.17	59.2	5.94E-04	25.4	1.32E+04	2.5
	0.1	2.31E+64	-15.98	56.1	6.02E-04	25.2	7.39E+04	2.6

	1	6.51E+44	-9.79	49.6	6.04E-04	25.1	3.41E+05	2.7
	10	4.09E+23	-3.19	41.8	6.04E-04	25.1	1.17E+06	2.9
	100	6.47E+07	1.68	35.7	6.04E-04	25.1	2.64E+06	3.1
R7	0.01	3.87E+88	-23.66	62.8	2.10E-03	89.8	2.11E+04	3.9
	0.1	2.35E+80	-20.77	61.9	2.16E-03	90.1	1.30E+05	4.5
	1	4.57E+63	-15.38	57.0	2.16E-03	90.1	7.00E+05	5.6
	10	2.71E+41	-8.41	49.2	2.17E-03	90.1	3.05E+06	7.6
	100	1.09E+20	-1.78	41.1	2.17E-03	90.1	9.63E+06	11.2
R8	0.01	1.98E+96	-25.89	67.2	1.29E-03	54.9	2.40E+04	4.5
	0.1	1.65E+87	-22.73	65.9	1.31E-03	54.6	1.50E+05	5.2
	1	3.17E+69	-17.03	60.6	1.31E-03	54.5	8.23E+05	6.6
	10	1.58E+46	-9.73	52.4	1.31E-03	54.5	3.72E+06	9.2
	100	3.07E+23	-2.70	43.8	1.31E-03	54.5	1.24E+07	14.5
1,4-H(s) rate rule	**0.01**	**1.00E+50**	**-12.69**	**34.1**	**1.08E+01**	**0.7**	**2.14E+05**	**4.9**
	0.1	**1.88E+47**	**-11.55**	**34.1**	**1.23E+01**	**0.6**	**1.29E+06**	**4.9**
	1	**2.77E+45**	**-10.65**	**35.1**	**1.28E+01**	**0.6**	**6.89E+06**	**4.7**
	10	**3.13E+45**	**-10.25**	**38.6**	**1.29E+01**	**0.6**	**3.06E+07**	**4.4**
	100	**3.24E+45**	**-9.85**	**42.8**	**1.29E+01**	**0.6**	**1.00E+08**	**4.0**
R9	0.01	2.93E+43	-10.87	29.6	1.55E+01	1.0	4.34E+04	1.0
	0.1	9.91E+45	-11.23	33.0	1.92E+01	1.0	2.64E+05	1.0
	1	3.82E+42	-9.82	33.9	2.07E+01	1.0	1.47E+06	1.0
	10	1.83E+31	-6.07	31.1	2.11E+01	1.0	6.96E+06	1.0
	100	1.53E+14	-0.68	25.4	2.11E+01	1.0	2.53E+07	1.0
R10	0.01	1.78E+50	-12.81	34.0	6.31E+00	0.4	4.28E+04	1.0
	0.1	3.62E+50	-12.50	36.6	6.97E+00	0.4	2.55E+05	1.0
	1	3.12E+42	-9.70	35.5	7.14E+00	0.3	1.35E+06	0.9
	10	1.64E+26	-4.49	30.4	7.17E+00	0.3	5.84E+06	0.8
	100	2.27E+07	1.39	23.6	7.17E+00	0.3	1.83E+07	0.7
R11	0.01	1.30E+53	-13.64	34.9	1.05E+01	0.7	6.08E+04	1.4
	0.1	1.00E+54	-13.49	37.9	1.13E+01	0.6	3.65E+05	1.4
	1	4.83E+45	-10.61	36.7	1.15E+01	0.6	1.95E+06	1.3
	10	4.06E+28	-5.16	31.3	1.15E+01	0.5	8.56E+06	1.2
	100	7.20E+08	0.99	24.1	1.15E+01	0.5	2.75E+07	1.1
R12	0.01	3.12E+55	-14.34	36.0	1.10E+01	0.7	6.73E+04	1.6
	0.1	9.95E+55	-14.07	38.8	1.17E+01	0.6	4.02E+05	1.5
	1	3.61E+46	-10.85	37.2	1.18E+01	0.6	2.13E+06	1.5
	10	6.69E+03	2.19	19.7	1.18E+01	0.6	9.27E+06	1.3
	100	1.32E+08	1.22	23.8	1.18E+01	0.6	2.92E+07	1.2
1,4-H(t) rate rule	**0.01**	**9.57E+45**	**-11.55**	**30.4**	**5.23E+01**	**0.9**	**8.13E+04**	**1.1**
	0.1	**1.00E+50**	**-12.36**	**34.5**	**6.31E+01**	**0.8**	**4.98E+05**	**1.1**
	1	**1.71E+46**	**-10.91**	**34.2**	**6.66E+01**	**0.8**	**2.74E+06**	**1.1**
	10	**1.57E+45**	**-10.22**	**36.6**	**6.72E+01**	**0.8**	**1.27E+07**	**1.0**
	100	**1.92E+45**	**-9.83**	**40.7**	**6.73E+01**	**0.8**	**4.45E+07**	**1.0**
R13	0.01	1.74E+44	-11.12	28.4	5.91E+01	1.0	7.09E+04	1.0

	0.1	1.81E+49	-12.22	32.9	7.47E+01	1.0	4.42E+05	1.0
	1	5.59E+47	-11.37	34.7	8.06E+01	1.0	2.51E+06	1.0
	10	9.55E+36	-7.78	32.3	8.18E+01	1.0	1.22E+07	1.0
	100	1.80E+19	-2.19	26.3	8.19E+01	1.0	4.59E+07	1.0
R14	0.01	3.81E+45	-11.51	28.4	1.15E+02	1.9	1.00E+05	1.4
	0.1	9.26E+51	-13.02	33.5	1.44E+02	1.9	6.31E+05	1.4
	1	2.31E+51	-12.44	35.7	1.54E+02	1.9	3.61E+06	1.4
	10	4.96E+40	-8.87	33.4	1.56E+02	1.9	1.77E+07	1.5
	100	2.96E+22	-3.12	27.2	1.56E+02	1.9	6.76E+07	1.5
R15	0.01	9.84E+49	-12.76	32.4	2.43E+01	0.4	7.09E+04	1.0
	0.1	8.95E+51	-12.93	35.7	2.69E+01	0.4	4.23E+05	1.0
	1	3.42E+44	-10.32	34.9	2.74E+01	0.3	2.22E+06	0.9
	10	1.03E+28	-5.05	29.8	2.75E+01	0.3	9.49E+06	0.8
	100	1.08E+09	0.86	22.8	2.75E+01	0.3	2.90E+07	0.6
R16	0.01	3.31E+52	-13.51	33.2	3.28E+01	0.6	8.40E+04	1.2
	0.1	2.68E+56	-14.26	37.5	3.64E+01	0.5	5.17E+05	1.2
	1	1.35E+51	-12.27	37.7	3.72E+01	0.5	2.86E+06	1.1
	10	6.43E+35	-7.33	33.2	3.73E+01	0.5	1.33E+07	1.1
	100	3.75E+15	-1.00	26.0	3.73E+01	0.5	4.69E+07	1.0
R17	0.01	3.51E+51	-13.21	32.9	3.04E+01	0.5	8.06E+04	1.1
	0.1	5.57E+53	-13.46	36.4	3.29E+01	0.4	4.79E+05	1.1
	1	8.80E+45	-10.74	35.4	3.34E+01	0.4	2.52E+06	1.0
	10	6.04E+28	-5.27	30.0	3.34E+01	0.4	1.08E+07	0.9
	100	2.08E+09	0.79	22.8	3.34E+01	0.4	3.31E+07	0.7
1,5-H(s) rate rule	**0.01**	**1.13E+16**	**-2.89**	**8.8**	**2.60E+04**	**1.5**	**3.85E+05**	**1.3**
	0.1	**6.18E+18**	**-3.40**	**10.6**	**8.66E+04**	**1.6**	**2.63E+06**	**1.3**
	1	**6.17E+22**	**-4.28**	**13.4**	**2.01E+05**	**1.8**	**1.66E+07**	**1.2**
	10	**5.33E+36**	**-8.02**	**22.5**	**3.10E+05**	**1.9**	**9.50E+07**	**1.2**
	100	**2.28E+37**	**-7.87**	**24.6**	**3.53E+05**	**1.9**	**4.66E+08**	**1.2**
R18	0.01	9.91E+19	-4.07	10.9	1.69E+04	1.0	3.04E+05	1.0
	0.1	4.81E+25	-5.45	14.2	5.32E+04	1.0	2.09E+06	1.0
	1	5.07E+32	-7.21	18.7	1.15E+05	1.0	1.34E+07	1.0
	10	4.49E+38	-8.63	23.2	1.66E+05	1.0	7.80E+07	1.0
	100	7.45E+37	-8.03	25.0	1.85E+05	1.0	3.87E+08	1.0
R19	0.01	2.93E+20	-4.19	11.0	2.16E+04	1.3	3.78E+05	1.2
	0.1	2.77E+26	-5.66	14.5	6.93E+04	1.3	2.63E+06	1.3
	1	1.17E+34	-7.59	19.2	1.49E+05	1.3	1.70E+07	1.3
	10	6.78E+40	-9.25	24.1	2.12E+05	1.3	9.91E+07	1.3
	100	4.20E+40	-8.82	26.2	2.33E+05	1.3	4.98E+08	1.3
R20	0.01	1.99E+20	-4.14	10.9	2.18E+04	1.3	3.77E+05	1.2
	0.1	2.86E+26	-5.66	14.5	6.53E+04	1.2	2.56E+06	1.2
	1	1.28E+34	-7.60	19.3	1.30E+05	1.1	1.61E+07	1.2
	10	1.18E+40	-9.02	24.0	1.74E+05	1.0	9.10E+07	1.2
	100	9.23E+37	-8.03	25.3	1.86E+05	1.0	4.37E+08	1.1

R21	0.01	2.08E+25	-5.61	14.2	8.72E+03	0.5	2.96E+05	1.0
	0.1	1.99E+33	-7.66	19.1	1.89E+04	0.4	1.91E+06	0.9
	1	4.55E+40	-9.49	24.2	2.65E+04	0.2	1.11E+07	0.8
	10	7.92E+40	-9.20	26.6	2.88E+04	0.2	5.59E+07	0.7
	100	1.38E+30	-5.66	23.9	2.92E+04	0.2	2.22E+08	0.6
R22	0.01	5.65E+16	-3.08	8.3	6.10E+04	3.6	5.73E+05	1.9
	0.1	3.39E+21	-4.20	11.0	2.26E+05	4.3	3.95E+06	1.9
	1	2.73E+28	-5.94	15.1	5.85E+05	5.1	2.55E+07	1.9
	10	1.90E+36	-7.94	20.2	9.70E+05	5.8	1.51E+08	1.9
	100	8.18E+39	-8.66	24.0	1.13E+06	6.1	7.86E+08	2.0
1,5-H(t) rate rule	**0.01**	**7.88E+15**	**-2.83**	**8.2**	**4.66E+04**	**1.3**	**5.13E+05**	**1.1**
	0.1	**4.09E+21**	**-4.22**	**11.6**	**1.64E+05**	**1.3**	**3.53E+06**	**1.1**
	1	**6.85E+21**	**-4.00**	**12.2**	**3.92E+05**	**1.3**	**2.25E+07**	**1.1**
	10	**2.52E+27**	**-5.31**	**16.2**	**5.99E+05**	**1.3**	**1.29E+08**	**1.1**
	100	**8.98E+31**	**-6.32**	**20.4**	**6.72E+05**	**1.3**	**6.39E+08**	**1.1**
R23	0.01	1.48E+18	-3.51	9.4	3.71E+04	1.0	4.56E+05	1.0
	0.1	2.48E+23	-4.76	12.4	1.30E+05	1.0	3.16E+06	1.0
	1	2.55E+30	-6.52	16.7	3.09E+05	1.0	2.03E+07	1.0
	10	2.47E+37	-8.26	21.5	4.73E+05	1.0	1.18E+08	1.0
	100	2.89E+38	-8.22	24.2	5.33E+05	1.0	5.88E+08	1.0
R24	0.01	3.22E+17	-3.31	8.8	5.11E+04	1.4	5.36E+05	1.2
	0.1	2.83E+22	-4.48	11.6	1.92E+05	1.5	3.76E+06	1.2
	1	2.49E+29	-6.22	15.7	4.98E+05	1.6	2.45E+07	1.2
	10	1.14E+37	-8.16	20.8	8.18E+05	1.7	1.46E+08	1.2
	100	2.72E+40	-8.81	24.4	9.48E+05	1.8	7.52E+08	1.3
R25	0.01	6.45E+19	-3.99	10.4	2.88E+04	0.8	4.34E+05	1.0
	0.1	7.52E+25	-5.48	13.9	9.04E+04	0.7	2.96E+06	0.9
	1	5.46E+33	-7.49	18.8	1.84E+05	0.6	1.85E+07	0.9
	10	1.31E+40	-9.04	23.6	2.44E+05	0.5	1.03E+08	0.9
	100	1.24E+38	-8.08	24.9	2.60E+05	0.5	4.86E+08	0.8
R26	0.01	1.58E+18	-3.51	9.3	4.18E+04	1.1	4.94E+05	1.1
	0.1	4.16E+23	-4.82	12.4	1.43E+05	1.1	3.39E+06	1.1
	1	1.00E+31	-6.69	16.9	3.27E+05	1.1	2.15E+07	1.1
	10	1.40E+38	-8.47	21.9	4.75E+05	1.0	1.23E+08	1.0
	100	3.10E+38	-8.22	24.2	5.20E+05	1.0	5.96E+08	1.0
R27	0.01	2.85E+16	-2.98	8.1	7.45E+04	2.0	6.48E+05	1.4
	0.1	2.71E+21	-4.17	10.9	2.66E+05	2.0	4.37E+06	1.4
	1	3.37E+28	-5.96	15.1	6.43E+05	2.1	2.75E+07	1.4
	10	1.89E+36	-7.93	20.3	9.84E+05	2.1	1.57E+08	1.3
	100	2.66E+38	-8.21	23.4	1.10E+06	2.1	7.74E+08	1.3
1,6-H(s) rate rule	**0.01**	**2.57E+17**	**-3.28**	**9.9**	**9.20E+03**	**1.1**	**3.01E+05**	**1.1**
	0.1	**4.15E+20**	**-3.92**	**12.1**	**2.24E+04**	**1.1**	**1.98E+06**	**1.1**
	1	**8.27E+24**	**-4.88**	**15.3**	**3.61E+04**	**1.1**	**1.19E+07**	**1.0**
	10	**1.51E+31**	**-6.38**	**20.2**	**4.22E+04**	**1.1**	**6.35E+07**	**1.0**

	100	**3.89E+37**	**-8.18**	**26.8**	**4.33E+04**	**1.1**	**2.79E+08**	**1.0**
R28	0.01	6.88E+24	-5.48	14.0	8.16E+03	1.0	2.78E+05	1.0
	0.1	1.81E+32	-7.36	18.5	1.98E+04	1.0	1.86E+06	1.0
	1	9.37E+39	-9.30	23.7	3.16E+04	1.0	1.14E+07	1.0
	10	9.87E+42	-9.83	27.2	3.68E+04	1.0	6.23E+07	1.0
	100	6.71E+35	-7.33	26.3	3.79E+04	1.0	2.81E+08	1.0
R29	0.01	3.82E+22	-4.81	12.3	1.55E+04	1.9	3.53E+05	1.3
	0.1	4.92E+29	-6.60	16.5	4.16E+04	2.1	2.37E+06	1.3
	1	7.82E+25	-5.15	16.1	7.21E+04	2.3	1.47E+07	1.3
	10	7.45E+42	-9.82	26.2	8.69E+04	2.4	8.08E+07	1.3
	100	7.37E+37	-7.96	26.2	8.99E+04	2.4	3.73E+08	1.3
R30	0.01	8.58E+24	-5.49	13.8	1.13E+04	1.4	3.40E+05	1.2
	0.1	1.71E+33	-7.63	18.7	2.56E+04	1.3	2.23E+06	1.2
	1	8.31E+41	-9.86	24.5	3.78E+04	1.2	1.36E+07	1.2
	10	1.34E+45	-10.44	28.2	4.21E+04	1.1	7.31E+07	1.2
	100	1.92E+37	-7.74	27.0	4.28E+04	1.1	3.30E+08	1.2
R31	0.01	2.98E+36	-8.86	21.2	1.78E+03	0.2	2.33E+05	0.8
	0.1	8.29E+45	-11.31	27.4	2.55E+03	0.1	1.45E+06	0.8
	1	3.31E+49	-11.99	31.3	2.80E+03	0.1	8.05E+06	0.7
	10	6.95E+41	-9.33	30.3	2.84E+03	0.1	3.78E+07	0.6
	100	1.57E+25	-4.07	24.7	2.84E+03	0.1	1.34E+08	0.5
1,6-H(t) rate rule	**0.01**	**8.45E+14**	**-2.53**	**7.7**	**4.04E+04**	**1.2**	**5.12E+05**	**1.1**
	0.1	**1.02E+18**	**-3.15**	**9.6**	**1.26E+05**	**1.2**	**3.43E+06**	**1.1**
	1	**9.43E+21**	**-4.02**	**12.3**	**2.53E+05**	**1.1**	**2.11E+07**	**1.1**
	10	**6.29E+26**	**-5.13**	**16.1**	**3.31E+05**	**1.1**	**1.16E+08**	**1.1**
	100	**1.09E+33**	**-6.61**	**21.5**	**3.49E+05**	**1.0**	**5.35E+08**	**1.0**
R32	0.01	1.37E+19	-3.79	10.0	3.35E+04	1.0	4.56E+05	1.0
	0.1	8.53E+24	-5.21	13.3	1.09E+05	1.0	3.12E+06	1.0
	1	3.94E+32	-7.16	18.0	2.30E+05	1.0	1.96E+07	1.0
	10	1.57E+39	-8.77	22.9	3.14E+05	1.0	1.09E+08	1.0
	100	7.06E+37	-8.01	24.5	3.36E+05	1.0	5.17E+08	1.0
R33	0.01	2.55E+19	-3.86	10.1	3.66E+04	1.1	4.97E+05	1.1
	0.1	3.09E+25	-5.36	13.6	1.16E+05	1.1	3.37E+06	1.1
	1	3.65E+33	-7.44	18.5	2.34E+05	1.0	2.10E+07	1.1
	10	1.80E+40	-9.08	23.5	3.08E+05	1.0	1.16E+08	1.1
	100	2.23E+38	-8.15	24.8	3.25E+05	1.0	5.43E+08	1.0
R34	0.01	3.32E+21	-4.49	11.5	2.34E+04	0.7	4.28E+05	0.9
	0.1	2.52E+28	-6.22	15.5	6.68E+04	0.6	2.89E+06	0.9
	1	8.10E+36	-8.41	20.8	1.20E+05	0.5	1.78E+07	0.9
	10	2.86E+42	-9.70	25.4	1.47E+05	0.5	9.72E+07	0.9
	100	1.11E+38	-8.03	25.6	1.52E+05	0.5	4.40E+08	0.8
R35	0.01	2.03E+17	-3.22	8.6	6.80E+04	2.0	6.67E+05	1.5
	0.1	1.06E+23	-4.63	11.9	2.12E+05	1.9	4.34E+06	1.4
	1	7.35E+30	-6.64	16.7	4.26E+05	1.9	2.61E+07	1.3

	10	3.77E+37	-8.29	21.6	5.55E+05	1.8	1.41E+08	1.3
	100	5.39E+35	-7.38	23.0	5.84E+05	1.7	6.41E+08	1.2
1,7-H(s) rate rule	**0.01**	**1.42E+16**	**-2.90**	**8.7**	**2.46E+04**	**1.1**	**4.24E+05**	**1.1**
	0.1	**2.45E+19**	**-3.56**	**10.8**	**7.13E+04**	**1.1**	**2.86E+06**	**1.1**
	1	**1.69E+23**	**-4.39**	**13.6**	**1.34E+05**	**1.1**	**1.79E+07**	**1.1**
	10	**9.06E+28**	**-5.75**	**17.9**	**1.69E+05**	**1.0**	**1.00E+08**	**1.0**
	100	**4.13E+35**	**-7.35**	**23.7**	**1.77E+05**	**1.0**	**4.79E+08**	**1.0**
R36	0.01	3.94E+19	-4.98	-1.2	2.25E+04	1.0	3.96E+05	1.0
	0.1	1.45E+26	-6.62	2.7	6.54E+04	1.0	2.68E+06	1.0
	1	1.59E-16	6.81	-11.2	1.25E+05	1.0	1.69E+07	1.0
	10	1.31E-33	12.33	-16.4	1.62E+05	1.0	9.60E+07	1.0
	100	6.12E+08	-0.04	2.8	1.71E+05	1.0	4.70E+08	1.0
R37	0.01	1.96E+20	-4.12	10.7	2.97E+04	1.3	4.61E+05	1.2
	0.1	6.58E+26	-5.75	14.5	8.80E+04	1.3	3.10E+06	1.2
	1	1.51E+35	-7.91	19.6	1.67E+05	1.3	1.92E+07	1.1
	10	2.88E+41	-9.42	24.5	2.10E+05	1.3	1.06E+08	1.1
	100	3.55E+38	-8.19	25.4	2.19E+05	1.3	4.96E+08	1.1
R38	0.01	7.12E+21	-4.58	11.7	2.16E+04	1.0	4.16E+05	1.1
	0.1	8.36E+28	-6.37	15.8	6.05E+04	0.9	2.81E+06	1.1
	1	4.65E+37	-8.63	21.3	1.09E+05	0.9	1.76E+07	1.0
	10	7.07E+43	-10.11	26.1	1.34E+05	0.8	9.87E+07	1.0
	100	3.70E+40	-8.76	27.0	1.39E+05	0.8	4.71E+08	1.0
1,7-H(t) rate rule	**0.01**	**6.60E+14**	**-2.49**	**7.5**	**5.43E+04**	**0.8**	**6.00E+05**	**1.0**
	0.1	**6.03E+17**	**-3.08**	**9.3**	**1.81E+05**	**0.7**	**4.04E+06**	**0.9**
	1	**3.41E+21**	**-3.89**	**11.9**	**3.95E+05**	**0.6**	**2.50E+07**	**0.9**
	10	**1.13E+26**	**-4.90**	**15.4**	**5.55E+05**	**0.6**	**1.39E+08**	**0.9**
	100	**1.05E+32**	**-6.32**	**20.6**	**6.01E+05**	**0.6**	**6.55E+08**	**0.9**
R39	0.01	5.73E+16	-3.07	8.3	6.92E+04	1.0	6.29E+05	1.0
	0.1	5.08E+21	-4.25	11.0	2.51E+05	1.0	4.29E+06	1.0
	1	5.77E+28	-6.03	15.3	6.10E+05	1.0	2.70E+07	1.0
	10	1.96E+36	-7.93	20.3	9.23E+05	1.0	1.53E+08	1.0
	100	6.22E+37	-8.03	23.1	1.02E+06	1.0	7.40E+08	1.0
R40	0.01	5.92E+18	-3.66	9.6	4.85E+04	0.7	5.89E+05	0.9
	0.1	9.95E+24	-5.21	13.2	1.44E+05	0.6	3.86E+06	0.9
	1	1.53E+33	-7.31	18.3	2.71E+05	0.4	2.33E+07	0.9
	10	1.59E+39	-8.75	23.0	3.37E+05	0.4	1.24E+08	0.8
	100	4.56E+35	-7.35	23.6	3.50E+05	0.3	5.53E+08	0.7
R41	0.01	2.04E+19	-3.82	9.9	4.53E+04	0.7	5.81E+05	0.9
	0.1	2.56E+25	-5.32	13.4	1.46E+05	0.6	3.96E+06	0.9
	1	5.31E+33	-7.47	18.4	3.03E+05	0.5	2.49E+07	0.9
	10	1.63E+41	-9.35	23.7	4.04E+05	0.4	1.40E+08	0.9
	100	3.37E+40	-8.78	25.6	4.29E+05	0.4	6.71E+08	0.9
1,8-H (s)								
R42	0.01	1.31E+27	-6.13	15.3				

	0.1	1.18E+36	-8.46	20.8
	1	5.28E+43	-10.37	26.3
	10	3.89E+43	-9.95	28.6
	100	1.65E+32	-6.21	25.8
1,9-H (s)				
R43	0.01	1.31E+27	-6.13	15.3
	0.1	5.10E+32	-7.46	19.4
	1	1.42E+34	-7.53	22.2
	10	3.37E+24	-4.33	20.0
	100	2.40E+09	0.42	14.7

[a]k_{sma} is the rate constant for the smallest H-shift reaction in each class.

Table S8. Calculated rate constants, rate rules for abstraction from a non–OOH substituted carbon atom at different pressures.

Reactions	Pressure(atm)	Modified Arrhenius parameters		
		A(s^{-1})	n	E(kcal mol^{-1})
1,4-H (p) rate rule	**0.01**	**1.00E+66**	**-17.30**	**45.2**
	0.1	**1.00E+60**	**-15.12**	**44.6**
	1	**2.84E+43**	**-9.84**	**38.9**
	10	**3.83E+24**	**-3.87**	**32.5**
	100	**8.60E+08**	**1.11**	**27.9**
R44	0.01	2.34E+61	-15.78	47.2
	0.1	1.41E+52	-12.63	45.7
	1	4.09E+35	-7.33	40.6
	10	4.36E+15	-1.08	33.4
	100	1.42E-01	4.02	27.2
R45	0.01	1.49E+65	-17.02	45.3
	0.1	4.39E+60	-15.25	46.0
	1	1.91E+47	-10.86	42.5
	10	1.96E+27	-4.56	35.7
	100	1.40E+07	1.69	28.2
R46	0.01	2.13E+66	-17.43	43.9
	0.1	1.18E+65	-16.63	46.0
	1	2.21E+54	-13.02	43.8
	10	1.92E+35	-6.97	37.6
	100	5.01E+13	-0.25	29.7
1,4-H (s) rate rule	**0.01**	**1.00E+56**	**-14.50**	**36.5**
	0.1	**1.00E+60**	**-15.28**	**40.8**
	1	**1.00E+55**	**-13.39**	**40.9**
	10	**1.99E+43**	**-9.24**	**44.5**
	100	**4.05E+23**	**-3.31**	**31.2**
R47	0.01	3.48E+56	-14.61	38.5
	0.1	1.42E+57	-14.38	41.3
	1	1.57E+50	-11.90	40.7

	10	9.95E+34	-7.00	36.3
	100	3.46E+15	-0.90	29.4
R48	0.01	4.31E+61	-16.09	40.7
	0.1	1.40E+63	-16.12	44.0
	1	2.88E+56	-13.71	43.6
	10	7.46E+40	-8.68	39.1
	100	1.72E+20	-2.22	31.8
R49	0.01	2.60E+58	-15.22	36.7
	0.1	3.27E+64	-16.63	41.9
	1	2.81E+63	-15.89	44.1
	10	4.78E+52	-12.26	41.9
	100	2.23E+33	-6.14	35.5
1,4-H (t) rate rule	**0.01**	**1.00E+50**	**-12.99**	**28.8**
	0.1	**1.00E+50**	**-12.59**	**30.8**
	1	**1.00E+50**	**-12.06**	**34.6**
	10	**5.27E+32**	**-6.57**	**28.3**
	100	**2.39E+12**	**-0.16**	**21.2**
R50	0.01	2.59E+49	-12.60	31.5
	0.1	7.08E+53	-13.52	35.9
	1	1.94E+50	-12.05	36.9
	10	8.89E+36	-7.69	33.3
	100	3.56E+17	-1.60	26.6
R51	0.01	1.44E+50	-13.85	19.7
	0.1	8.84E+56	-15.47	25.2
	1	3.49E+09	-0.40	9.6
	10	1.16E-01	3.13	7.5
	100	5.77E-27	11.03	-1.6
R52	0.01	1.85E+52	-13.46	31.9
	0.1	5.95E+60	-15.59	38.0
	1	4.15E+62	-15.72	41.5
	10	2.03E+54	-12.83	40.4
	100	2.85E+36	-7.13	34.7
1,5-H (p) rate rule	**0.01**	**1.15E+36**	**-8.74**	**21.8**
	0.1	**1.00E+50**	**-12.52**	**29.9**
	1	**1.00E+50**	**-12.19**	**31.0**
	10	**2.73E+49**	**-11.63**	**33.0**
	100	**1.96E+44**	**-9.67**	**34.0**
R53	0.01	5.66E+39	-9.84	23.8
	0.1	1.66E+48	-11.99	29.3
	1	7.18E+53	-13.29	34.0
	10	1.42E+51	-12.09	35.2
	100	8.81E+37	-7.80	31.5
R54	0.01	7.82E+24	-5.44	16.1
	0.1	2.14E+51	-12.91	30.7

	1	6.56E+58	-14.74	36.2
	10	9.40E+58	-14.39	38.8
	100	1.69E+48	-10.80	36.4
R55	0.01	2.62E+42	-10.61	24.9
	0.1	4.72E+52	-13.30	31.1
	1	1.29E+61	-15.42	37.1
	10	1.65E+62	-15.34	40.1
	100	1.42E+52	-11.95	38.1
1,5-H (s) rate rule	**0.01**	**6.05E+23**	**-5.17**	**13.2**
	0.1	**2.13E+30**	**-6.79**	**16.9**
	1	**1.07E+38**	**-8.75**	**21.5**
	10	**1.00E+50**	**-11.93**	**29.1**
	100	**1.00E+50**	**-11.58**	**30.8**
R56	0.01	5.31E+34	-8.37	20.5
	0.1	1.36E+43	-10.52	25.6
	1	1.14E+51	-12.51	31.1
	10	8.66E+53	-12.97	34.7
	100	6.76E+46	-10.47	33.9
R57	0.01	9.60E+24	-5.51	13.9
	0.1	1.16E+32	-7.30	17.9
	1	7.84E+40	-9.58	23.2
	10	1.51E+49	-11.68	28.9
	100	1.96E+51	-11.92	32.2
R58	0.01	2.01E+21	-4.42	11.3
	0.1	1.86E+27	-5.88	14.6
	1	2.45E+35	-7.97	19.3
	10	8.11E+44	-10.45	25.2
	100	4.48E+51	-12.08	30.4
1,5-H (t) rate rule	**0.01**	**2.22E+18**	**-3.55**	**9.4**
	0.1	**2.67E+23**	**-4.76**	**12.2**
	1	**9.95E+29**	**-6.40**	**16.0**
	10	**1.43E+46**	**-10.82**	**25.7**
	100	**4.76E+46**	**-10.64**	**27.4**
R59	0.01	9.79E+25	-5.81	14.6
	0.1	6.25E+33	-7.80	19.1
	1	5.72E+42	-10.12	24.8
	10	6.98E+48	-11.55	29.7
	100	6.20E+45	-10.26	30.7
R60	0.01	5.97E+19	-3.97	10.3
	0.1	3.83E+25	-5.39	13.5
	1	3.84E+33	-7.44	18.3
	10	3.02E+42	-9.74	24.0
	100	6.28E+46	-10.65	28.1
R61	0.01	2.61E+16	-2.96	7.9

	0.1	4.99E+20	-3.93	10.2
	1	8.18E+26	-5.47	13.7
	10	2.54E+35	-7.67	18.8
	100	4.12E+43	-9.76	24.4
1,6-H (p) rate rule	**0.01**	**6.35E+38**	**-9.56**	**22.8**
	0.1	**1.00E+50**	**-12.52**	**29.6**
	1	**1.00E+55**	**-13.64**	**33.8**
	10	**1.00E+50**	**-11.80**	**33.2**
	100	**1.14E+42**	**-9.04**	**32.2**
R62	0.01	1.87E+51	-13.18	31.3
	0.1	6.77E+58	-15.04	36.9
	1	1.77E+59	-14.75	39.6
	10	7.66E+48	-11.28	37.4
	100	3.07E+30	-5.47	31.2
R63	0.01	5.23E+41	-10.40	24.6
	0.1	6.71E+51	-13.04	30.9
	1	4.27E+58	-14.68	36.3
	10	2.45E+56	-13.60	37.8
	100	9.88E+42	-9.24	34.1
R64	0.01	8.62E+34	-8.41	20.0
	0.1	1.67E+45	-11.12	26.1
	1	6.32E+54	-13.59	32.5
	10	6.01E+57	-14.08	36.3
	100	2.78E+49	-11.21	35.0
1,6-H (s) rate rule	**0.01**	**1.03E+19**	**-3.76**	**9.9**
	0.1	**5.16E+24**	**-5.15**	**13.1**
	1	**7.93E+31**	**-6.96**	**17.5**
	10	**6.53E+38**	**-8.68**	**22.2**
	100	**1.44E+40**	**-8.72**	**24.8**
R65	0.01	1.75E+33	-7.94	19.3
	0.1	2.43E+42	-10.31	24.9
	1	4.62E+50	-12.40	30.6
	10	4.71E+52	-12.60	33.9
	100	7.25E+43	-9.59	32.4
R66	0.01	1.76E+24	-5.29	13.3
	0.1	6.34E+31	-7.21	17.6
	1	1.47E+41	-9.66	23.3
	10	1.15E+49	-11.63	29.0
	100	1.18E+49	-11.25	31.4
R67	0.01	2.58E+16	-2.96	7.9
	0.1	1.84E+21	-4.10	10.6
	1	2.03E+28	-5.88	14.7
	10	1.14E+37	-8.15	20.2
	100	5.95E+42	-9.49	24.9

1,6-H (t) rate rule	**0.01**	**8.65E+17**	**-3.42**	**9.0**
	0.1	**8.76E+22**	**-4.61**	**11.8**
	1	**3.51E+29**	**-6.26**	**15.6**
	10	**4.97E+44**	**-10.39**	**24.8**
	100	**1.87E+42**	**-9.37**	**24.5**
R68	0.01	4.60E+22	-4.82	12.3
	0.1	8.33E+29	-6.66	16.5
	1	8.44E+38	-9.00	22.0
	10	6.56E+45	-10.68	27.2
	100	5.83E+43	-9.70	28.6
R69	0.01	4.10E+16	-3.01	8.0
	0.1	1.05E+21	-4.03	10.4
	1	2.63E+27	-5.62	14.0
	10	1.18E+36	-7.87	19.2
	100	1.68E+44	-9.93	24.8
1,7-H (p) rate rule	**0.01**	**7.49E+42**	**-10.73**	**25.3**
	0.1	**1.00E+50**	**-12.50**	**30.0**
	1	**1.00E+58**	**-14.47**	**36.2**
	10	**1.00E+49**	**-11.44**	**33.8**
	100	**3.93E+37**	**-7.66**	**31.5**
R70	0.01	3.98E+46	-11.82	27.9
	0.1	3.74E+55	-14.11	34.0
	1	9.10E+57	-14.42	37.5
	10	1.95E+49	-11.45	36.1
	100	3.89E+31	-5.84	30.3
R71	0.01	2.19E+40	-9.99	23.5
	0.1	9.71E+50	-12.79	30.1
	1	2.39E+58	-14.60	35.7
	10	3.33E+56	-13.64	37.4
	100	1.81E+43	-9.32	33.9
1,7-H (s) rate rule	**0.01**	**1.82E+18**	**-3.52**	**9.4**
	0.1	**9.70E+23**	**-4.92**	**12.6**
	1	**4.14E+31**	**-6.87**	**17.2**
	10	**5.61E+38**	**-8.65**	**22.1**
	100	**1.77E+39**	**-8.44**	**24.4**
R72	0.01	1.75E+28	-6.46	15.9
	0.1	9.01E+36	-8.72	21.0
	1	3.48E+46	-11.21	27.1
	10	1.73E+52	-12.52	31.9
	100	9.17E+47	-10.86	32.4
R73	0.01	2.90E+16	-2.97	8.0
	0.1	2.88E+21	-4.16	10.8
	1	4.78E+28	-5.99	15.1
	10	9.73E+36	-8.13	20.4

		100	2.47E+40	-8.78	24.1
1,7-H (t)					
	R74	0.01	6.57E+17	-3.37	8.9
		0.1	1.68E+23	-4.68	11.9
		1	1.85E+17	-2.54	10.6
		10	2.69E+39	-8.84	22.0
		100	2.73E+42	-9.37	25.6

Table S9. Calculated rate constants at different pressures in Table 6-9 which are not listed. (The substituent groups in the same ring-size transition state are connected to the same carbon with unbranched chain.)

Reactions	Pressure(atm)	Modified Arrhenius parameters		
		A(s^{-1})	*n*	*E(kcal mol-1)*
1,3-H				
R1(C2)	—	—	—	—
R2(C3)	—	—	—	—
R3(C4)	—	—	—	—
R4(C5)	—	—	—	—
C6	0.01	1.50E+96	-25.70	70.2
	0.1	7.09E+84	-21.88	67.9
	1	7.28E+65	-15.80	62.1
	10	1.03E+42	-8.33	53.6
	100	3.62E+18	-1.06	44.8
	∞	2.60E-10	7.56	33.7
C7	0.01	3.27E+99	-26.74	70.1
	0.1	1.25E+88	-22.89	67.9
	1	2.86E+68	-16.61	61.8
	10	6.22E+43	-8.90	53.0
	100	7.73E+19	-1.50	43.9
	∞	1.51E-07	6.66	33.4
1,4-H				
R9(C2)	—	—	—	—
R10(C3)	—	—	—	—
R11(C4)	—	—	—	—
R12(C5)	—	—	—	—
C6	0.01	7.52E+57	-15.04	36.9
	0.1	6.24E+58	-14.89	40.0
	1	2.10E+49	-11.66	38.3
	10	5.59E+30	-5.76	32.3
	100	3.27E+24	-3.60	32.0
	∞	6.20E-10	6.57	17.1
C7	0.01	7.77E+76	-20.89	44.5
	0.1	1.51E+79	-21.10	48.6

	1	7.14E+50	-12.15	39.1
	10	1.99E+39	-8.38	36.0
	100	4.79E+13	-0.44	26.3
	∞	3.23E-09	6.36	17.6
1,5-H				
R18(C3)	—	—	—	—
R20(C4)	—	—	—	—
C5	0.01	1.22E+19	-3.96	9.0
	0.1	1.18E+26	-5.74	12.6
	1	1.77E+36	-8.45	18.2
	10	4.77E+47	-11.50	25.1
	100	1.42E+53	-12.75	30.0
	∞	7.19E+03	2.87	13.8
C6	0.01	1.61E+18	-3.69	8.3
	0.1	5.28E+24	-5.34	11.7
	1	5.11E+34	-8.00	17.1
	10	1.05E+47	-11.33	24.3
	100	7.77E+54	-13.29	30.1
	∞	2.97E+04	2.75	14.0
C7	0.01	1.06E+29	-7.01	12.7
	0.1	4.22E+25	-5.62	12.1
	1	9.10E+36	-8.68	18.3
	10	8.33E+49	-12.18	25.9
	100	1.41E+56	-13.65	31.2
	∞	4.50E+04	2.65	14.1
1,6-H				
R28(C4)	—	—	—	—
C5	0.01	1.08E+28	-6.62	14.4
	0.1	6.24E+38	-9.50	20.3
	1	4.46E+50	-12.66	27.5
	10	1.66E+57	-14.22	32.8
	100	1.35E+51	-12.00	32.7
	∞	2.29E+02	3.22	15.1
C6	0.01	3.25E+31	-7.42	18.1
	0.1	7.24E+40	-9.85	23.9
	1	3.35E+47	-11.46	29.1
	10	1.17E+45	-10.35	30.4
	100	4.03E+31	-5.99	26.5
	∞	8.79E+01	3.24	15.4
C7	0.01	2.91E+32	-7.93	16.7
	0.1	3.78E+45	-11.50	24.0
	1	4.05E+58	-15.00	31.9
	10	5.28E+63	-16.11	36.8
	100	3.96E+54	-12.97	35.4

	∞	2.93E+02	3.21	16.3
1,7-H				
R36(C5)	—	—	—	—
R38(C6)	—	—	—	—
C7	0.01	2.01E+22	-4.91	10.6
	0.1	4.48E+30	-7.10	15.0
	1	7.27E+42	-10.41	21.7
	10	1.05E+56	-13.96	29.5
	100	5.46E+61	-15.27	34.5
	∞	2.86E+05	2.46	15.1

7 Calculated Barrier width *L* and used Lennard-Jones parameters

Table S10. Calculated Barrier width *L* (Å).

Reactions	Barrier width *L*	Reactions	Barrier width *L*	Reactions	Barrier width *L*
R1	1.35	R26	0.63	R51	0.84
R2	1.27	R27	0.65	R52	0.84
R3	1.31	R28	0.64	R53	0.71
R4	1.3	R29	0.61	R54	0.78
R5	1.32	R30	0.65	R55	0.76
R6	1.26	R31	0.63	R56	0.79
R7	1.29	R32	0.59	R57	0.8
R8	1.3	R33	0.58	R58	0.79
R9	0.8	R34	0.57	R59	0.8
R10	0.81	R35	0.63	R60	0.75
R11	0.8	R36	0.64	R61	0.72
R12	0.8	R37	0.59	R62	0.77
R13	0.8	R38	0.61	R63	0.76
R14	0.77	R39	0.57	R64	0.76
R15	0.79	R40	0.59	R65	0.77
R16	0.82	R41	0.56	R66	0.75
R17	0.79	R42	0.89	R67	0.73
R18	0.68	R43	0.67	R68	0.71
R19	0.66	R44	0.86	R69	0.7
R20	0.66	R45	0.83	R70	0.76
R21	0.62	R46	0.83	R71	0.79
R22	0.65	R47	0.83	R72	0.76
R23	0.65	R48	0.84	R73	0.71
R24	0.64	R49	0.84	R74	0.69
R25	0.62	R50	0.8		

Table S11 Lennard-Jones parameters σ (Å) and ε (K) used in this study.

	Ar	C2[a]	C3[a]	C4[a]	C5[a]	C6[a]	C7[a]
σ	3.33	4.16	4.76	5.18	5.18	5.29	5.68
ε	136.5	224.7	252.0	357.0	357.0	464.8	495.3

[a]In Cn, n represents the number of carbon atoms in the •O_2QOOH radicals.

8 Cartesian coordinates, absolute energies, ZPEs, and a list of vibrational frequencies of reactants, products, and transition states

The Optimized Geometries of all the reactions at MP2/CBSB7 Level (TS_n is the transition state of the reaction R_n)

O_2CCOO•

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.54888200	-0.87135600	0.50048000
H	0.79744400	-1.48062900	0.45237000
O	1.24895300	-0.06561400	-0.66106400
C	0.63951300	1.11797400	-0.19492100
H	0.43242400	1.67688700	-1.11179100
H	1.32391200	1.69201000	0.44301500
C	-0.64573000	0.87109300	0.57597500
H	-1.15759200	1.81185800	0.78727500
H	-0.46615900	0.31792900	1.49654500
O	-1.58318000	0.10544100	-0.22148100
O	-1.32624500	-1.16252900	-0.16215300

Absolute energies (Hartree): -379.462939 ZPE (Hartree): 0.082737

Harmonic Vibrational Frequencies (cm^{-1}):

130.5390 139.7353 222.1342 279.8630 415.2115 509.4272 516.8840 602.1138 857.4901 876.6199 926.1490 1021.9920 1123.2141 1164.6583 1272.8493 1305.9964 1334.8905 1411.0553 1417.6344 1426.9945 1485.3797 1503.2603 3075.1890 3139.2765 3161.4281 3218.4966 3778.9596

TS_1

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.79050800	-0.25210200	0.52212900
H	-1.20680400	0.96417000	0.45018300
H	-0.78928600	-0.53813200	1.57501400
C	0.47970200	-0.41163400	-0.26904300
H	0.76778900	-1.46918100	-0.30563300
H	0.32346200	-0.04150400	-1.28827900

O	1.46063100	0.33998900	0.42239600
O	2.72467200	0.00882500	-0.19517000
H	2.93360100	0.86213200	-0.59350100
O	-1.93650200	-0.60672200	-0.17082200
O	-2.26929200	0.78352400	-0.22594200

Absolute energies (Hartree): -379.382436 ZPE (Hartree): 0.077296

Harmonic Vibrational Frequencies (cm^{-1}):

-2178.8765 72.5612 92.9723 184.9346 204.2956 220.1573 420.2320 479.2604 758.1487 828.5123 930.0040 1073.0844 1123.0448 1135.0125 1156.7153 1199.6617 1249.1733 1329.0522 1380.0994 1433.0583 1533.5523 1717.8070 2190.4761 3072.1230 3133.5186 3171.3649 3840.3161

$O_2CC•OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.76504500	0.27502300	0.05592100
H	-2.79004600	1.09795100	0.55767000
O	-1.41064300	0.34936600	-0.45037200
C	-0.69407500	-0.69505600	0.21498000
H	-1.12955100	-1.66610700	-0.03966700
H	-0.75749100	-0.54283100	1.30028000
C	0.71209000	-0.62762200	-0.25094600
H	1.25067200	-1.44064700	-0.71826700
O	1.45874600	0.26960500	0.45669400
O	2.79131100	0.28420300	-0.09045700
H	2.72338200	1.06212000	-0.65849700

Absolute energies (Hartree): -379.440397 ZPE (Hartree): 0.078731

Harmonic Vibrational Frequencies (cm^{-1}):

57.4003 66.0680 107.4142 223.1720 235.7385 301.4816 324.4284 389.5748 457.5809 626.4161 892.2356 949.6273 993.1031 1059.9545 1136.3952 1223.1157 1290.0475 1361.2805 1372.3754 1391.3021 1438.3211 1520.4744 3061.7422 3136.8492 3274.1752 3825.5800 3843.1152

$O_2CCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.04921900	-1.10704700	0.63702100
C	-1.44838400	-0.91303600	0.05431200
C	1.03538200	-0.93187100	-0.42695400
O	2.03879400	0.05318600	-0.02410200
O	1.53482900	1.23227700	0.08947000
O	-1.56651700	0.29988300	-0.66668500
O	-1.41294700	1.36870000	0.29445800
H	-2.20269600	-0.95766100	0.84739600

H	-1.67384100	-1.67487600	-0.69992400
H	0.61950000	-0.57005300	-1.36874400
H	1.63058200	-1.82976800	-0.59385300
H	-0.47410500	1.57220900	0.15772400
H	0.10448800	-0.36564800	1.42322900
H	0.01612900	-2.09484000	1.10277500

Absolute energies (Hartree): -418.717765 ZPE (Hartree): 0.11216

Harmonic Vibrational Frequencies (cm^{-1}):

88.8138 135.1685 144.5730 239.8810 270.0081 363.4063 423.1505 526.8698 563.3394 609.2432 764.5317 866.8122 896.5683 948.0209 1029.6235 1094.5904 1109.6224 1138.6491 1266.6564 1298.1712 1308.0575 1344.8576 1377.6207 1418.0103 1440.4211 1448.4853 1496.2588 1501.5860 1515.6038 3083.7639 3113.4490 3131.4507 3147.5210 3177.6041 3207.5841 3742.7370

TS_2

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.16748400	0.54604900	-0.64138200
H	-0.91378500	-0.69405200	-0.86574600
H	-1.60965200	0.94148900	-1.55825600
O	1.38732800	-0.76874500	0.22458600
O	2.42533900	-0.19414500	-0.61400700
H	3.19014600	-0.62916200	-0.21950500
O	-2.11497500	0.11097300	0.27973000
O	-1.77011100	-1.23006200	-0.07587100
C	0.78933300	0.32095800	0.90991300
H	1.55381000	0.88028100	1.45995600
H	0.10211400	-0.16054000	1.61024900
C	0.02619700	1.23681900	-0.03938200
H	0.69708400	1.57903600	-0.83143900
H	-0.32864100	2.11582100	0.51434000

Absolute energies (Hartree): -418.644619 ZPE (Hartree): 0.106638

Harmonic Vibrational Frequencies (cm^{-1}):

-2177.7198 77.3253 110.0059 130.3599 160.2953 215.4114 259.7750 401.9663 483.3052 584.2740 693.1464 828.7341 877.3726 907.2085 964.2427 1016.3365 1087.4092 1145.1861 1147.8563 1208.3584 1255.8921 1305.7873 1360.5207 1362.9945 1395.2860 1433.1389 1483.6019 1496.3906 1721.3443 2188.1826 3078.2257 3091.5943 3152.5557 3162.3516 3176.1792 3846.2349

$O_2CCC•OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.49561600	0.36359000	-0.02177700
H	-3.84086100	0.05919300	-0.86901800

O	-2.33208600	-0.49125600	0.07849700
C	1.26176000	0.28959400	0.14297800
H	1.43106700	1.07341900	0.87699900
O	2.36092400	-0.46107200	-0.16845500
O	3.51090000	0.42167900	-0.13111600
H	4.10149900	-0.14024000	0.38446800
C	-1.20544300	0.36210700	-0.04131200
H	-1.24228500	1.13529500	0.73498100
H	-1.19305600	0.84645500	-1.02457200
C	0.01446900	-0.53234900	0.13887000
H	0.06601900	-1.25747400	-0.67877900
H	-0.10006800	-1.09628100	1.07551200

Absolute energies (Hartree): -418.695638 ZPE (Hartree): 0.107974

Harmonic Vibrational Frequencies (cm^{-1}):

53.6999 87.9918 94.5540 129.3103 166.3807 190.3939 206.6860 297.3258 324.3070 478.6281 555.6894 693.5193 834.4070 918.1225 919.2242 1062.8066 1090.6670 1114.2083 1157.8492 1202.2451 1243.8932 1288.4684 1307.2663 1371.8118 1398.8476 1416.6599 1449.2298 1506.3160 1551.1290 3052.8524 3069.6965 3122.0283 3145.3168 3203.0599 3842.9677 3847.6788

$O_2CCCCOO$•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.76453900	0.70955900	-0.05057100
H	-2.03837400	1.49335600	0.66573900
H	-2.60950500	0.52934600	-0.72418900
C	-0.52720900	1.11891100	-0.84273000
H	-0.81665700	1.95150900	-1.49505100
H	-0.22922600	0.29873000	-1.50205500
C	0.65220300	1.57458200	0.02308600
H	1.39767500	2.08143400	-0.60001100
H	0.30229200	2.30872800	0.76065000
C	1.36358800	0.47336700	0.79587200
H	0.68561300	-0.14172300	1.38459800
H	2.16250500	0.88053400	1.41927700
O	-1.57407400	-0.43313200	0.77258600
O	-1.47422400	-1.56675400	-0.11945100
H	-0.50997900	-1.67874400	-0.14042900
O	2.06686800	-0.40798000	-0.13343900
O	1.39535500	-1.46484500	-0.43500500

Absolute energies (Hartree): -457.975776 ZPE (Hartree): 0.141173

Harmonic Vibrational Frequencies (cm^{-1}):

79.9096 95.5909 150.5263 164.5137 230.0609 278.2993 298.5287 432.1632 459.2746 515.4297 555.6292 576.5443 819.7060 824.9843 838.1476 892.6507 937.3317 989.6862 1053.9185 1093.9666 1130.2913 1158.8982

1232.2414 1264.8545 1318.9637 1331.6490 1369.2683 1400.6952 1416.8663 1427.2340 1429.7556 1466.2655 1482.1177 1493.0812 1504.8222 1515.5771 3071.9664 3075.6339 3090.3611 3127.0693 3133.5235 3138.7941 3155.1029 3222.2906 3723.6012

TS_3

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.25033900	0.67624800	-0.17182800
H	-2.42068400	-0.24013100	-1.06021100
H	-3.03146500	1.41980800	-0.35016800
O	2.43970000	-0.66087700	-0.06911400
O	3.78428200	-0.19409600	0.20579500
H	4.18945000	-0.38602300	-0.64764200
O	-2.61710200	-0.28139000	0.76650100
O	-2.77330200	-1.20991100	-0.30989600
C	0.18154200	-0.02220100	-0.16692400
H	-0.06778700	-0.75764400	0.60161100
H	0.11344600	-0.52122500	-1.13929000
C	1.60148200	0.47579900	0.04495400
H	1.87570300	1.22383600	-0.71154200
H	1.71497100	0.92295000	1.04000900
C	-0.81765200	1.13384400	-0.10582700
H	-0.64016000	1.84537900	-0.92043400
H	-0.69229700	1.68111200	0.83913100

Absolute energies (Hartree): -457.896285 ZPE (Hartree): 0.135158

Harmonic Vibrational Frequencies (cm^{-1}):

-2184.6086 51.6304 75.7171 90.1624 138.8128 150.2584 166.2395 179.9333 293.2748 375.8881 446.2336 555.1830 711.4557 783.3347 870.2650 890.1389 922.7275 983.5757 1077.8274 1095.3067 1134.1866 1141.3297 1167.2869 1211.6780 1239.0511 1283.2662 1308.8957 1333.0009 1368.3278 1370.7658 1399.6450 1445.9661 1491.0269 1519.5461 1552.9701 1713.5148 2183.2224 3050.2392 3059.0276 3100.0709 3110.2323 3122.9308 3143.6458 3172.7529 3846.9432

$O_2CCCC•OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.77030000	-0.69158400	-0.06058000
H	3.64295800	-1.53198600	0.39473100
O	2.39732600	-0.41308200	-0.42548900
C	-1.79463400	0.30636400	-0.17871300
H	-2.01427100	0.69962200	-1.16888500
O	-2.72433600	-0.56644400	0.31773600
O	-4.02891500	-0.10700100	-0.12011500
H	-4.36847400	-0.94637900	-0.45227600

C	2.00431600	0.71898100	0.33639000
H	2.68375900	1.55385600	0.13191700
H	2.04366500	0.48182600	1.40834300
C	-0.40740000	-0.07273000	0.22334900
H	-0.39699200	-0.28133900	1.30024000
H	-0.08784900	-0.99391300	-0.28367600
C	0.58461500	1.04992300	-0.09357100
H	0.58259000	1.26093100	-1.16870700
H	0.27823200	1.96704300	0.42117300

Absolute energies (Hartree): -457.950841 ZPE (Hartree): 0.136864

Harmonic Vibrational Frequencies (cm^{-1}):

49.6242 60.0184 81.5533 121.4947 133.3166 175.7457 188.6533 204.2915 275.1103 326.8428 378.2464 491.2484 573.6235 686.4439 773.1073 903.8397 909.7844 947.7367 973.0015 1080.3035 1113.1227 1119.1255 1166.0924 1193.8572 1229.5725 1264.8907 1295.0170 1332.4076 1373.8976 1382.7198 1407.6706 1425.5931 1438.7273 1492.6947 1506.5791 1546.7151 3052.0428 3054.9994 3086.3985 3107.2243 3120.8841 3147.1882 3195.2032 3841.7652 3847.8400

$O_2CCCCCOO$•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.39718400	0.83719000	0.53002000
H	0.89090400	0.19940600	1.25357300
H	1.82531700	1.70925300	1.02900200
C	0.50823000	1.21138500	-0.64316300
H	1.02723600	1.95772700	-1.25455700
H	0.34981600	0.32388700	-1.25644300
C	-0.84586100	1.77265600	-0.18402000
H	-1.40326900	2.09153200	-1.07350700
H	-0.67529500	2.67847500	0.41268100
C	-1.71908500	0.80633300	0.62825800
H	-2.60750700	1.35110300	0.97281200
H	-1.20314100	0.46598800	1.53018100
C	-2.22746900	-0.41248600	-0.13537900
H	-2.76571900	-0.10372300	-1.03914900
H	-2.90802600	-0.99423400	0.49906400
O	-1.22431100	-1.27115700	-0.65361900
O	-0.54652800	-1.84377100	0.49943900
H	0.37080600	-1.74000100	0.19765200
O	2.56464600	0.09029600	0.06615800
O	2.25880400	-1.12910200	-0.21767900

Absolute energies (Hartree): -497.22894 ZPE (Hartree): 0.170361

Harmonic Vibrational Frequencies (cm^{-1}):

74.3636 101.1275 135.0638 145.4195 154.1401 249.9842 256.2476 291.5590 328.9931 407.8996 445.7879

538.2757 567.2926 601.9225 762.6665 823.1974 844.8217 869.0539 905.9301 954.1297 974.6096 1029.6975 1075.3122 1133.4429 1142.4245 1156.9279 1239.1010 1253.4048 1301.9404 1319.8802 1331.2237 1360.5499 1373.1187 1397.1773 1412.5690 1427.9437 1437.4708 1460.6962 1487.4253 1501.0599 1505.4168 1516.5271 1526.8112 3060.6532 3065.7753 3083.8241 3097.9551 3112.5520 3130.0562 3132.2124 3152.4539 3184.3263 3211.6581 3725.7976

TS_4

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.89171000	0.56975500	-0.15183700
H	-2.97855100	-0.33713600	-1.06134800
H	-3.74286400	1.23728500	-0.31003900
O	3.30607600	0.34112600	0.11944700
O	4.33562700	-0.67800000	0.11392100
H	4.78592600	-0.43921900	-0.70446400
O	-3.15986900	-0.44110000	0.76495100
O	-3.22946500	-1.35550400	-0.33240900
C	-0.40121800	0.10709000	-0.16391600
H	-0.58409700	-0.65322400	0.60184400
H	-0.45619900	-0.39888900	-1.13566300
C	0.98653400	0.71935200	0.02392100
H	1.16701000	1.48412900	-0.74042600
H	1.04998100	1.20891700	1.00201400
C	2.07451800	-0.33823200	-0.06542900
H	1.94634500	-1.09648200	0.71590700
H	2.05975500	-0.83437800	-1.04531100
C	-1.50811100	1.15871800	-0.08199600
H	-1.39904600	1.89653200	-0.88548300
H	-1.42727600	1.70018700	0.87122700

Absolute energies (Hartree): -497.151222 ZPE (Hartree): 0.163995

Harmonic Vibrational Frequencies (cm^{-1}):

-2172.1892 45.6240 57.0861 73.0946 122.0591 124.9901 140.1899 160.2877 197.3355 269.3115 291.9270 395.3386 486.4055 554.3273 711.7055 761.4432 819.7595 876.4518 916.2086 929.6926 991.8671 1068.8997 1078.2501 1096.9736 1133.8421 1149.8627 1171.1654 1211.0710 1228.8305 1261.4221 1290.4922 1326.0066 1342.2286 1351.7907 1368.5811 1371.6729 1418.2842 1442.3686 1489.4348 1510.1942 1522.7343 1552.7465 1712.8011 2181.6587 3053.8402 3057.6422 3076.3695 3084.3376 3112.1842 3119.3408 3134.8744 3142.3492 3154.5533 3843.7002

$O_2CCCCC•OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-4.76811400	0.36231500	0.01646300
H	-5.12269100	0.12269400	-0.84747500

O	-3.59086000	-0.48211100	0.02721400
C	2.54174800	0.30883300	0.07631000
H	2.67299100	1.14826600	0.75558900
O	3.66303100	-0.44535700	-0.13676000
O	4.79864200	0.45799000	-0.14071400
H	5.38082000	-0.04815600	0.43815700
C	-2.47470200	0.39207000	-0.02693100
H	-2.51350800	1.09542800	0.81356900
H	-2.48666700	0.96236100	-0.96554400
C	1.30291300	-0.52477000	0.08869400
H	1.32935000	-1.21037900	-0.76641100
H	1.25986700	-1.15012600	0.99493700
C	-1.23755300	-0.48656000	0.05788600
H	-1.27866900	-1.06668600	0.98631700
H	-1.24445200	-1.19758900	-0.77600900
C	0.04462600	0.34510100	0.01788100
H	0.04598800	1.05315600	0.85637600
H	0.07318900	0.94030100	-0.90216500

Absolute energies (Hartree): -497.204679 ZPE (Hartree): 0.165504

Harmonic Vibrational Frequencies (cm^{-1}):

39.1130 55.9473 64.7711 87.3361 111.7503 140.7183 150.9082 182.3014 194.8105 201.1327 249.2024 330.4335 466.9756 476.0944 553.4018 682.7452 759.5918 826.3966 910.8505 919.5978 951.6436 1054.1626 1063.4392 1093.7948 1105.8094 1135.0696 1168.9364 1192.3354 1225.3004 1253.4508 1283.5187 1318.3675 1323.2776 1340.6068 1368.5984 1388.9754 1410.0906 1433.2165 1441.2858 1501.0123 1510.2525 1523.1610 1552.7798 3023.8335 3053.1238 3068.1160 3084.3953 3106.1942 3109.2137 3123.4807 3148.8914 3195.6521 3843.6198 3848.2853

$O_2CC(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.01656600	-0.27526700	0.70655800
H	-1.81149700	0.67064200	0.75220200
O	-1.48186900	-0.54794400	-0.60890100
C	-0.20128000	-1.10725900	-0.42195100
H	0.14930500	-1.29852400	-1.44133100
H	-0.26279000	-2.05219700	0.13347400
C	0.77459500	-0.18543200	0.29640400
H	0.42514000	0.02214800	1.30832700
O	0.80981300	1.10034400	-0.39442300
O	-0.15385800	1.87907800	-0.02080500
C	2.19369700	-0.71446100	0.28315400
H	2.86151700	-0.03127100	0.81139200
H	2.22812800	-1.68957100	0.77569000

H	2.54797300	-0.82800700	-0.74483100

Absolute energies (Hartree): -418.724144 ZPE (Hartree): 0.11082

Harmonic Vibrational Frequencies (cm^{-1}):

115.8228 136.1392 183.8631 199.0380 238.5252 315.9330 361.8710 438.8992 525.6535 532.0453 606.8243 848.0653 869.4086 936.1185 947.4280 1090.8701 1129.0803 1187.6299 1195.8557 1305.2680 1323.0866 1344.6331 1398.9502 1417.8132 1429.9724 1433.7766 1481.1928 1507.5467 1520.3000 3070.1915 3088.4494 3149.3099 3166.7182 3185.1575 3191.0049 3772.1129

TS_5

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.71008600	0.21714400	0.03533400
H	-1.05709100	-0.38538700	-1.04137800
C	0.62138600	-0.34148800	0.47825400
H	0.85359700	0.02460400	1.48705900
H	0.57629100	-1.43572200	0.48677800
O	1.58092800	0.13674000	-0.44827600
O	2.87211000	-0.24373200	0.07834600
H	3.11712500	-0.91361100	-0.57125400
O	-1.77224800	-0.44174800	0.65221000
O	-2.04582000	-1.07410100	-0.60063200
C	-0.87873000	1.70471000	-0.09381400
H	-0.81270400	2.15503200	0.90347500
H	-0.09209900	2.12501100	-0.72225700
H	-1.86030300	1.93059400	-0.51425200

Absolute energies (Hartree): -418.647923 ZPE (Hartree): 0.105715

Harmonic Vibrational Frequencies (cm^{-1}):

-2128.2416 74.1284 89.8514 165.7818 185.6251 214.6875 222.9449 334.4628 358.7392 467.4674 477.1417 719.8291 919.2601 931.3822 940.3725 1006.1330 1090.4749 1127.4785 1145.0214 1227.3604 1273.5376 1303.8761 1376.6968 1407.5582 1421.5293 1495.9703 1505.9486 1530.2751 1711.6318 2190.6302 3064.3893 3076.0630 3134.1149 3169.7131 3206.0172 3837.2875

$O_2CC•(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.98372800	-0.20685200	-0.04832200
H	3.08870600	-1.13130200	0.20519700
O	1.61832500	-0.24851700	-0.53002700
C	0.84366800	0.46681100	0.43346700
H	1.16557100	1.51265800	0.47045900
H	0.98106800	0.00975000	1.42295400
C	-0.57819000	0.36852800	-0.00300000

O	-1.11681200	-0.79713300	0.49191500
O	-2.36491300	-1.08874300	-0.17753400
H	-2.03385500	-1.67277800	-0.87200200
C	-1.45439400	1.56331500	-0.17584500
H	-2.34877700	1.31527600	-0.74746500
H	-1.77813700	1.95454600	0.80047700
H	-0.90370500	2.34988800	-0.69560700

Absolute energies (Hartree): -418.701327 ZPE (Hartree): 0.10765

Harmonic Vibrational Frequencies (cm^{-1}):

41.3475 86.0021 102.6039 130.2579 231.5706 240.9420 256.9699 291.9366 359.6320 382.5371 424.5753 597.0094 839.4547 940.0687 956.9353 995.6039 1012.7707 1034.3294 1089.5782 1239.4901 1297.9063 1343.8567 1363.6867 1382.3701 1423.1958 1436.1242 1487.3734 1510.8808 1522.9005 3035.5180 3052.9074 3129.4281 3150.6737 3202.9461 3819.2077 3840.3324

$O_2CCC(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.04072100	-0.75551200	0.82387100
C	-1.22150000	-1.31383100	0.16946000
C	1.03349800	-0.23617100	-0.21829700
O	1.44009300	1.14293600	0.10621200
O	0.45603200	1.96995300	0.04131600
O	-1.81570900	-0.38854500	-0.72439800
O	-2.25397600	0.73538600	0.07214500
H	-1.94513600	-1.62213400	0.93212600
H	-0.99044600	-2.16946000	-0.47507000
H	0.54750700	-0.15602300	-1.19355300
H	-1.49558800	1.32808100	-0.05352500
H	-0.24859000	0.06288600	1.48539800
H	0.50410300	-1.53030400	1.44445600
C	2.32787400	-1.01659800	-0.29978800
H	2.99089000	-0.60169000	-1.06239800
H	2.83982200	-1.00145900	0.66634100
H	2.10236600	-2.05507000	-0.55744000

Absolute energies (Hartree): -457.979247 ZPE (Hartree): 0.140267

Harmonic Vibrational Frequencies (cm^{-1}):

66.8841 125.3308 133.5451 212.3740 215.1214 250.3337 317.3864 366.7225 412.9071 468.0158 536.7417 568.3458 602.0346 805.0943 847.2522 880.7784 910.7215 999.0638 1024.1232 1096.6346 1142.7850 1161.4109 1191.7792 1266.2285 1292.6488 1345.6757 1355.9460 1397.2272 1415.6745 1422.5467 1436.3716 1450.5764 1495.4937 1499.3709 1508.4716 1522.4046 3080.3290 3083.3887 3101.6102 3139.9036 3144.5567 3174.9406 3179.2037 3185.5655 3736.5751

TS_6

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.05339900	0.32637300	0.02745900
H	-0.66023200	-0.37060800	-0.97079000
O	1.79717000	-0.57000500	-0.38853800
O	2.55735700	0.64342400	-0.63146200
H	3.44438700	0.26500200	-0.63157400
O	-1.71126800	-0.82500000	0.47517800
O	-1.25825100	-1.48606600	-0.70824900
C	1.19374100	-0.41006300	0.88724600
H	1.96315300	-0.20843900	1.64096700
H	0.72921700	-1.38102900	1.07674900
C	0.13978500	0.68841300	0.87977300
H	0.58841800	1.61776900	0.51945700
H	-0.21987500	0.85475100	1.90440800
C	-1.98812800	1.41032200	-0.44061600
H	-2.75374800	0.98325600	-1.09101900
H	-2.48085900	1.85952200	0.42984200
H	-1.44251900	2.19069200	-0.97663800

Absolute energies (Hartree): -457.908778 ZPE (Hartree): 0.13494

Harmonic Vibrational Frequencies (cm^{-1}):

-2120.8777 70.5724 77.3952 137.1730 166.5644 196.5188 220.8874 227.8261 305.6073 408.6075 417.4874 480.3650 576.2984 663.8495 837.8859 885.7657 891.0452 958.8944 999.4710 1025.4746 1095.5787 1124.9623 1127.7348 1223.6340 1258.6580 1276.9331 1314.0399 1358.4228 1400.8598 1417.4023 1429.0855 1480.7919 1496.3794 1502.2856 1504.7361 1720.4546 2189.9680 3069.8931 3072.3520 3087.4520 3157.4230 3161.7236 3175.8280 3194.3238 3843.3132

$O_2CCC•(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.67200800	0.10153200	-0.40312500
H	-4.00297400	-0.76994500	-0.64965100
O	-2.55054000	-0.29664300	0.42083400
C	1.09082700	0.14017500	-0.00952400
O	2.02218200	-0.85916100	0.18359100
O	3.22422500	-0.54699200	-0.55992100
H	3.84266400	-0.47710200	0.17700600
C	-1.38258400	0.05836000	-0.30292800
H	-1.40256700	1.12951600	-0.53221300
H	-1.32470400	-0.50513200	-1.24169700
C	-0.20819000	-0.28972100	0.60552600
H	-0.18605700	-1.37036800	0.77225300
H	-0.36073600	0.20076700	1.57764800

C	1.54585600	1.56100700	0.09902800
H	0.69631100	2.23109100	-0.04954700
H	1.95877500	1.75647600	1.10187200
H	2.31295900	1.79588600	-0.63931900

Absolute energies (Hartree): -457.956858 ZPE (Hartree): 0.136871

Harmonic Vibrational Frequencies (cm^{-1}):

42.0985 82.7868 98.7752 133.0030 154.4120 192.2815 208.5292 212.4439 288.8172 314.2013 350.2264 385.3369 503.8296 580.4299 810.7220 843.8131 922.3581 983.7974 1001.6376 1048.6811 1081.1930 1110.0515 1127.0384 1231.5310 1259.3599 1298.5327 1326.3147 1354.3292 1371.8399 1399.2994 1425.7016 1432.8831 1490.7446 1499.2991 1512.8486 1547.9542 3022.4443 3052.4121 3071.2531 3125.5488 3146.7810 3152.6586 3197.7130 3841.5290 3842.0568

$O_2CCCC(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.88894300	-1.02510300	-0.04180900
H	-1.83624000	-1.93940500	-0.64497000
H	-2.87853300	-0.95984200	0.42395800
C	-0.79629800	-1.02471000	1.02218700
H	-1.04456400	-1.81007400	1.74642100
H	-0.82112900	-0.07869600	1.57046500
C	0.60965600	-1.29785000	0.47782700
H	1.29072400	-1.53717700	1.30402100
H	0.58223400	-2.17820200	-0.17767500
C	1.24441100	-0.16399100	-0.31888000
H	0.56969600	0.21642000	-1.08514200
O	-1.75989000	0.01026500	-1.00646700
O	-2.08348600	1.24487700	-0.32649600
H	-1.18887400	1.57933100	-0.14928000
O	1.48480200	0.95518500	0.60755000
O	0.58927600	1.87796500	0.54492300
C	2.60669800	-0.51685500	-0.88358600
H	2.50114600	-1.33223900	-1.60385500
H	3.04751800	0.34453700	-1.39036200
H	3.27926000	-0.83993200	-0.08410100

Absolute energies (Hartree): -497.232603 ZPE (Hartree): 0.16914

Harmonic Vibrational Frequencies (cm^{-1}):

71.0966 91.6702 119.4205 157.9498 181.4451 215.1306 252.5145 293.0285 342.9924 384.7336 428.5965 463.0213 523.7361 560.7490 583.3589 807.2965 818.5184 872.2211 894.4709 926.6508 939.1153 1029.3514 1047.2499 1120.0125 1140.7676 1170.8019 1174.0159 1238.9607 1285.7711 1330.2063 1340.1784 1389.2662 1400.4926 1406.9867 1418.1602 1429.0950 1431.8978 1470.4228 1480.3224 1491.5803 1504.8793 1508.3676 1516.7621 3065.3440 3074.4942 3084.2122 3088.9504 3120.6387 3137.8015 3155.0357 3172.9054 3185.5257 3190.9712 3714.5142

TS_7

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.93210500	-0.27062000	-0.07088800
H	1.97560200	0.58356400	-1.02615800
O	-2.89323600	0.52118500	-0.14056300
O	-4.17889700	-0.07368800	0.16769100
H	-4.58539800	-0.01760300	-0.70462000
O	2.12336600	0.81384600	0.79087300
O	2.17886800	1.66262600	-0.35818400
C	-0.57334900	0.14750600	-0.16104400
H	-0.42185900	0.97514000	0.53579400
H	-0.54802200	0.55709800	-1.17632600
C	-1.92918100	-0.49167800	0.08955900
H	-2.10079800	-1.33651700	-0.59165100
H	-2.00734600	-0.85094000	1.12294600
C	0.54940700	-0.87419300	0.01557600
H	0.46765000	-1.67349100	-0.73015800
H	0.47031700	-1.34435100	1.00713000
C	3.12738800	-1.18552900	-0.14866800
H	4.03640600	-0.59711800	-0.28651200
H	3.21183200	-1.74071700	0.79290200
H	3.02257900	-1.89973800	-0.96909200

Absolute energies (Hartree): -497.160292 ZPE (Hartree): 0.163346

Harmonic Vibrational Frequencies (cm^{-1}):

-219.3787 75.5551 96.2838 129.1662 159.4837 182.2916 254.5618 294.2708 360.8577 390.3596 429.3552 464.1394 527.1008 571.8498 585.6627 809.6732 818.2902 875.7437 903.6390 927.9460 953.7739 1049.5635 1054.6750 1117.0867 1128.7787 1151.4489 1176.6530 1239.4569 1276.5472 1329.4290 1340.0916 1385.4988 1401.4287 1407.4002 1416.4452 1429.9325 1439.9770 1471.6694 1478.2836 1491.4272 1504.1322 1511.3292 1517.9561 3063.0977 3074.6203 3088.4552 3089.1441 3118.6179 3138.1004 3155.9895 3178.5526 3180.8995 3194.9294 3714.5965

$O_2CCCC•(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.03974800	-0.23718200	-0.58535800
H	3.93679500	-0.96482400	-1.20970100
O	2.65974200	0.19071700	-0.49471400
C	-1.57502700	0.12864800	0.10628300
O	-2.41142900	-0.92795000	-0.20021600
O	-3.78307500	-0.56307700	0.08553600
H	-4.13730700	-0.59284900	-0.81108700

C	2.22579500	-0.13394500	0.81807100
H	2.87778700	0.35312900	1.55173700
H	2.26820300	-1.22129300	0.96919900
C	-0.15693700	-0.33865800	-0.03489900
H	-0.13159300	-1.41637000	0.16366300
H	0.19495300	-0.18826000	-1.06629800
C	0.79729000	0.37407600	0.93050600
H	0.79692400	1.45303200	0.74516200
H	0.45837900	0.21706000	1.96031100
C	-1.97419900	1.49196200	-0.36411700
H	-1.22370300	2.22445400	-0.06056400
H	-2.04169600	1.51357700	-1.46413500
H	-2.94015900	1.78977500	0.04466700

Absolute energies (Hartree): -497.211671 ZPE (Hartree): 0.165746

Harmonic Vibrational Frequencies (cm^{-1}):

26.1846 55.5094 84.0498 123.4072 124.9126 155.1322 204.4395 216.6104 227.9586 269.4340 305.3049 338.8793 351.5585 428.7326 510.9437 594.8150 758.5491 840.9093 895.2331 925.1223 955.5919 985.3076 1029.8200 1045.7944 1109.2955 1117.5654 1135.0796 1219.7107 1250.6918 1273.9849 1307.6207 1340.7270 1347.5809 1373.6140 1394.4854 1410.1067 1422.7004 1429.5632 1485.9973 1494.7221 1497.7800 1513.5832 1546.6553 3019.5995 3043.6824 3054.4338 3090.2952 3117.3994 3120.4052 3147.8196 3153.5519 3198.7582 3840.9727 3841.4358

O_2CCCCC(C)OO•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.37421300	-0.25270700	-0.22028700
H	0.75661100	0.12411200	-1.03653500
C	0.51894200	-0.73493700	0.94236800
H	1.18196900	-1.18442600	1.69230300
H	0.03394800	0.12955700	1.39775200
C	-0.54977500	-1.75603600	0.52319500
H	-1.09540800	-2.06397700	1.42428300
H	-0.06125800	-2.66057900	0.14045400
C	-1.56025300	-1.25909600	-0.51949800
H	-2.18528400	-2.10725000	-0.82796600
H	-1.05803600	-0.90605900	-1.42475000
C	-2.51602200	-0.17570700	-0.02918200
H	-3.05622400	-0.51761000	0.86147200
H	-3.24502000	0.06508300	-0.81322700
O	-1.90411200	1.02079300	0.42269600
O	-1.29666500	1.63071200	-0.75011500
H	-0.43555800	1.86518200	-0.36514700
O	2.15813400	0.91136900	0.23214300

O	1.44538800	1.98213600	0.29148200
C	2.39825100	-1.25247900	-0.71445000
H	3.00137800	-0.82450800	-1.51876400
H	3.05858300	-1.55255300	0.10409600
H	1.89019500	-2.14128000	-1.09648800

Absolute energies (Hartree): -536.490497 ZPE (Hartree): 0.198433

Harmonic Vibrational Frequencies (cm^{-1}):

69.0952 73.6788 121.0799 137.4733 153.4412 194.7561 215.7849 244.3198 285.8530 321.3260 356.8347 400.0359 431.9014 489.9758 540.4812 565.8140 612.7490 773.4964 822.2901 840.6886 865.1332 897.9560 932.9562 964.7700 987.3683 1046.6635 1083.3254 1135.7425 1142.5440 1164.6220 1189.0801 1240.5873 1255.6024 1311.3434 1325.5669 1359.5584 1370.1851 1388.9120 1398.1288 1411.0384 1419.9376 1429.0061 1439.8397 1465.2500 1486.8308 1500.9121 1502.6971 1504.5289 1514.3424 1525.3182 3063.7338 3066.2330 3080.5764 3083.5283 3085.1216 3113.6243 3130.1482 3147.2064 3162.0974 3178.8453 3183.8756 3185.1033 3710.9613

TS_8

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.51841900	-0.22403500	-0.07339200
H	2.50785700	0.62939500	-1.02950000
O	-3.69132000	-0.46960400	0.13000000
O	-4.79964700	0.45976900	0.04932100
H	-5.21495200	0.13642400	-0.75845500
O	2.64762400	0.87182300	0.78699100
O	2.64625300	1.72136600	-0.36279500
C	-0.01095800	0.04495800	-0.14328600
H	0.10229900	0.86538500	0.57212600
H	0.01465600	0.48887400	-1.14609900
C	-1.34749400	-0.66425200	0.07491600
H	-1.45673100	-1.48978500	-0.63812700
H	-1.38333700	-1.09218000	1.08294000
C	-2.51588500	0.29344500	-0.09164300
H	-2.45822500	1.10935100	0.63828800
H	-2.52937900	0.72348800	-1.10233400
C	1.17350700	-0.90704200	0.01598800
H	1.13064500	-1.70311800	-0.73679000
H	1.12473600	-1.39030700	1.00328400
C	3.76729300	-1.06407800	-0.15446400
H	4.63844700	-0.42210100	-0.29814800
H	3.88936100	-1.61026200	0.78824100
H	3.70205500	-1.78597500	-0.97227000

Absolute energies (Hartree): -536.415197 ZPE (Hartree): 0.19217

Harmonic Vibrational Frequencies (cm^{-1}):

-2118.2483 41.9584 47.7173 67.6138 106.4626 120.0917 139.7742 152.1268 198.5968 209.5609 218.1661 257.6668 330.5212 401.0864 421.7613 491.5069 530.1573 695.3385 754.0516 816.8938 911.3539 913.1439 928.7958 979.1005 1008.9039 1059.2964 1080.9942 1096.3499 1110.3130 1130.8355 1168.9112 1202.7708 1230.3798 1272.5735 1277.1093 1292.7605 1325.7023 1340.6526 1358.7987 1370.5066 1416.0660 1417.6267 1441.2224 1486.1515 1502.4233 1504.9024 1509.4060 1522.1073 1552.8001 1708.3537 2181.4054 3048.9147 3053.6855 3071.7895 3075.8612 3083.7914 3112.1110 3115.9620 3134.5037 3154.6302 3161.9376 3193.4534 3843.4664

O_2CCCCC•(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-4.50257100	-0.33087300	-0.39231300
H	-4.62852300	-1.09233600	-0.97031400
O	-3.26895500	-0.74173300	0.25182600
C	2.80458200	0.24960900	-0.06826300
H	2.93178800	1.29116600	0.21864000
O	3.93378300	-0.51775500	0.01906000
O	5.05676900	0.31840700	-0.36254200
H	5.65199700	0.09037900	0.36127600
C	-2.23499300	0.12280700	-0.22257900
H	-2.22784100	0.08333500	-1.32190000
C	1.57729400	-0.52004700	0.29343500
H	1.60541300	-1.49119500	-0.21444600
H	1.54946300	-0.72952300	1.37512100
C	-0.95787900	-0.51087900	0.31817100
H	-1.02488100	-0.54918400	1.41263000
H	-0.90678900	-1.54524900	-0.04195800
C	0.30677500	0.23815800	-0.10306500
H	0.32428800	1.23189200	0.35866800
H	0.30427700	0.38933200	-1.18940700
C	-2.45857400	1.55131600	0.24715600
H	-2.38156900	1.59803700	1.33798200
H	-1.71947700	2.22709300	-0.19210700
H	-3.45358800	1.88611600	-0.05155700

Absolute energies (Hartree): -536.465445 ZPE (Hartree): 0.194368

Harmonic Vibrational Frequencies (cm^{-1}):

37.5829 52.6948 66.0737 92.2527 115.1886 142.7940 150.1621 183.6662 197.7780 206.0934 237.0295 256.0597 320.0470 348.9084 458.5498 486.9794 499.2221 570.8221 681.9295 760.8936 856.5364 888.5256 904.3081 922.8380 966.3186 1004.3033 1061.4366 1079.8082 1108.9396 1145.2002 1163.8849 1175.2615 1195.9564 1231.6536 1258.9771 1301.6347 1320.5635 1342.0144 1357.7012 1373.0219 1402.4594 1405.7517 1413.8796 1431.8905 1433.5600 1499.8657 1501.1513 1506.7115 1519.9367 1526.6772 3021.7929 3049.6667 3068.7378 3076.9020 3080.0794 3106.4552 3120.8094 3141.4997 3170.8254 3189.2409 3195.3435 3841.3439 3848.2374

TS_9

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-1.63331500	-1.10665900	-0.23288200
O	-1.98304800	0.14221100	0.27012200
C	-0.89371100	0.94885400	-0.13390100
H	-0.98827600	1.91757200	0.36084800
H	-0.84990200	1.05789200	-1.22285500
C	0.29190000	0.09803600	0.32986300
H	-0.37258300	-0.94326600	0.05217900
H	0.49512800	0.08558000	1.40368200
O	1.40740800	0.32772600	-0.43561800
O	2.53090800	-0.29276800	0.23069800
H	2.75086900	-0.96319200	-0.42818700

Absolute energies (Hartree): -379.406898 ZPE (Hartree): 0.076769

Harmonic Vibrational Frequencies (cm^{-1}):

-2825.5600 95.7631 168.5834 192.0772 253.9766 402.0242 445.0630 605.8449 703.3135 898.1353 928.9096 993.8997 1082.7942 1139.9828 1182.2167 1197.9725 1274.9358 1296.6854 1351.6020 1393.3337 1418.5174 1517.3167 1891.1905 3094.9897 3150.3958 3183.8078 3834.5090

TS_{10}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-1.37908400	-1.23831000	-0.73520300
O	-1.75551900	-0.63177800	0.46045100
C	-0.82110800	0.43611600	0.59592800
H	-0.91721300	0.78597700	1.62870100
C	0.48252900	-0.34351300	0.35784800
H	-0.10916800	-1.05440100	-0.50771200
H	0.77539400	-1.02409300	1.16200300
O	1.50803100	0.45757200	-0.07805500
O	2.73062900	-0.31206500	0.00446600
H	2.93183300	-0.38478600	-0.93705400
C	-1.03464900	1.56516800	-0.39587400
H	-2.02672300	1.99495700	-0.23944400
H	-0.27995600	2.34195800	-0.24925800
H	-0.96726200	1.19042000	-1.41792000

Absolute energies (Hartree): -418.667465 ZPE (Hartree): 0.104994

Harmonic Vibrational Frequencies (cm^{-1}):

-2820.5608 93.2169 162.8009 180.1068 212.8502 234.8085 300.0062 351.2986 469.4945 496.0979 649.3784 724.3017 867.9373 919.6964 944.7615 972.0174 1087.5381 1140.1228 1160.3326 1195.5493 1203.7540 1293.2393 1313.0725 1387.9129 1391.1795 1397.1141 1431.6880 1506.3137 1519.8201 1898.3751 3092.8383 3122.6338 3146.6432 3185.2717 3202.7361 3832.2498

$O_2C•C(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.36945100	-1.08934200	0.08591800
H	2.12907800	-1.93313600	0.48624500
O	1.09267900	-0.74813400	-0.50988400
C	0.57297200	0.35654900	0.25005500
H	0.61456800	0.07713700	1.31263300
C	-0.84262300	0.49925500	-0.18459100
H	-1.28370400	1.43442800	-0.50837500
O	-1.67803600	-0.38460700	0.43309500
O	-3.00733600	-0.19729300	-0.09461800
H	-3.01413000	-0.89407600	-0.76328700
C	1.37356700	1.62362000	-0.00445600
H	1.00840800	2.44132500	0.62330600
H	2.42504800	1.44282800	0.22296000
H	1.28316800	1.90995900	-1.05560600

Absolute energies (Hartree): -418.700866 ZPE (Hartree): 0.107299

Harmonic Vibrational Frequencies (cm^{-1}):

62.2348 75.1666 116.4641 205.8331 234.1837 243.8024 258.8489 307.4093 372.3443 393.1838 499.1402 526.5303 616.9825 885.0021 929.1143 972.6990 977.6485 1102.8132 1148.2814 1180.3797 1233.0170 1305.6390 1356.5481 1383.9339 1390.4926 1418.6689 1443.2816 1507.4959 1522.5734 3054.5275 3085.5624 3176.9148 3197.4325 3251.3268 3823.6480 3839.6102

$O_2CC(CC)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.29915100	-0.17938600	0.95785400
H	-2.04382200	0.75524600	0.94280000
O	-2.00701900	-0.50661000	-0.42027500
C	-0.73977800	-1.12585200	-0.43186500
H	-0.57618300	-1.36407800	-1.48784900
H	-0.75023600	-2.04928300	0.16143400
C	0.38202300	-0.23308500	0.07978500
H	0.22546400	0.01258000	1.13206600
O	0.34230500	1.03472200	-0.64432900
O	-0.48712000	1.87533200	-0.11496400
C	1.76211000	-0.81752000	-0.15717500
H	1.76194000	-1.84393300	0.22654900
H	1.92851900	-0.87728500	-1.23898200
C	2.86710700	0.00111900	0.50951000
H	3.85047800	-0.42677500	0.29959600

H	2.85471200	1.02991700	0.14199400
H	2.72823100	0.02318200	1.59455900

Absolute energies (Hartree): -457.978603 ZPE (Hartree): 0.139723

Harmonic Vibrational Frequencies (cm^{-1}):

82.3448 108.5905 122.7102 156.6531 208.8669 240.2102 273.5128 345.3822 381.7239 460.7063 523.6986 530.1761 607.6513 769.5561 865.9872 882.3407 963.0736 994.8044 1041.0105 1101.8949 1133.3775 1171.0619 1199.0054 1285.7382 1311.2703 1320.9095 1330.2030 1394.4352 1413.0074 1418.7671 1430.4057 1434.3379 1479.9124 1494.2737 1521.0774 1528.2991 3070.8495 3081.8289 3084.3220 3134.3632 3146.7426 3160.8880 3172.1171 3181.6738 3771.4150

TS_{11}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	0.52519300	1.75772600	-0.75771400
O	1.04828000	1.34701400	0.46560300
C	0.51068800	0.03535000	0.62833100
H	0.69780300	-0.23341500	1.67437800
C	-0.96934400	0.34014700	0.34665300
H	-0.62186100	1.17527900	-0.53959200
H	-1.48437100	0.91656800	1.12031300
O	-1.67166600	-0.76349700	-0.06780700
O	-3.07870800	-0.42577300	-0.03018900
H	-3.27005300	-0.45532100	-0.97611700
C	1.11103500	-0.99568100	-0.31472200
H	0.59775200	-1.94829500	-0.14446300
H	0.90593000	-0.69005600	-1.34417200
C	2.61530400	-1.14031900	-0.08957900
H	3.04374200	-1.87197800	-0.77945700
H	3.11459400	-0.18157000	-0.24661100
H	2.82558100	-1.47196700	0.93247900

Absolute energies (Hartree): -457.922296 ZPE (Hartree): 0.133861

Harmonic Vibrational Frequencies (cm^{-1}):

-2813.8315 75.5298 98.7047 139.0629 170.6705 200.7682 226.6954 268.1758 312.3821 359.1972 476.7570 537.8708 671.6195 711.9514 807.5339 866.6280 921.9627 954.8627 1001.4767 1048.6514 1110.5742 1128.1866 1158.4947 1199.4663 1205.9328 1282.4214 1293.2643 1314.2908 1364.6287 1389.1412 1396.7065 1426.9238 1429.7643 1496.5995 1519.4535 1528.6795 1898.8476 3077.8893 3098.4443 3107.4504 3143.8055 3152.8600 3168.7322 3182.8784 3832.0598

$O_2C•C(CC)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.89615100	-1.88769900	0.22798400

H	1.50293000	-2.55197500	0.80622900
O	0.69185800	-1.40663800	-0.41918200
C	0.45198700	-0.08447600	0.09665200
H	0.49583600	-0.14206000	1.19488400
C	-0.92522800	0.26115300	-0.34059800
H	-1.18186500	1.12204100	-0.94496600
O	-1.88967000	-0.20125000	0.50518700
O	-3.17964900	0.10429600	-0.06502800
H	-3.36360700	-0.73567100	-0.50493000
C	1.48580500	0.91139000	-0.41553400
H	2.47243800	0.46863600	-0.25652900
H	1.34725700	1.02470500	-1.49674300
C	1.39563500	2.26421200	0.29075900
H	2.16663700	2.94576700	-0.07823600
H	0.42342500	2.73928800	0.13132800
H	1.53823600	2.14591600	1.36960600

Absolute energies (Hartree): -457.95496 ZPE (Hartree): 0.136193

Harmonic Vibrational Frequencies (cm^{-1}):

54.8885 69.7308 105.8492 115.4498 180.9659 221.2504 232.1725 253.2626 259.1475 314.8590 393.9569 426.8995 497.0298 516.8786 606.6089 803.2664 897.7808 935.5611 997.3990 1024.2998 1049.9796 1096.7753 1164.5721 1173.0513 1231.4026 1277.9356 1328.6976 1342.2912 1364.7393 1384.1645 1400.9324 1431.4776 1451.7548 1510.6590 1521.1768 1526.0005 3043.9765 3075.4151 3092.8863 3150.1497 3166.3114 3170.9128 3259.7850 3821.7908 3837.5636

$O_2CC(CCC)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.74664700	-0.33637800	0.99049500
H	-2.56444300	0.61534700	0.98317400
O	-2.46063100	-0.62312100	-0.39791800
C	-1.14831700	-1.13817300	-0.44503900
H	-0.98935400	-1.34925000	-1.50753400
H	-1.07152400	-2.06673400	0.13530500
C	-0.09036800	-0.16521900	0.05629600
H	-0.24171400	0.05270200	1.11547100
O	-0.24726200	1.10562800	-0.64721500
O	-1.12909300	1.86961300	-0.08771000
C	1.32539900	-0.63290200	-0.22150100
H	1.41619800	-1.67236800	0.11777000
H	1.48252300	-0.63336600	-1.30775200
C	2.38557500	0.23255600	0.45992000
H	2.24141700	1.27435800	0.15484000
H	2.23137800	0.19313300	1.54507900

C	3.80510100	-0.21854100	0.11909900
H	4.54977300	0.40639300	0.61944900
H	3.96889300	-1.25545000	0.42962900
H	3.98157800	-0.15702600	-0.95929100

Absolute energies (Hartree): -497.232728 ZPE (Hartree): 0.168494

Harmonic Vibrational Frequencies (cm^{-1}):

69.3068 75.0427 96.8561 131.5471 145.9097 206.4041 248.5966 252.6840 314.1141 340.1544 386.0442 453.7043 528.9119 539.5792 645.9184 743.7254 837.7192 871.2019 897.7253 924.2675 1013.1814 1055.1499 1076.9411 1111.1548 1133.5736 1174.6587 1197.2484 1267.3402 1288.8522 1311.2668 1325.3740 1348.4628 1356.5603 1404.5660 1418.4802 1419.4915 1431.9453 1433.2294 1478.8414 1490.6424 1512.8179 1521.5806 1527.1475 3066.2366 3071.9221 3072.5291 3080.2506 3117.5399 3136.7354 3146.4923 3160.3730 3162.4860 3167.1086 3770.6204

TS_{12}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-0.33746900	1.86211900	-0.94896100
O	0.13810400	1.80317200	0.35832900
C	-0.02484400	0.42837600	0.70496100
H	0.10944600	0.37836000	1.79162500
C	-1.48940000	0.23942700	0.27688300
H	-1.29295400	1.00539700	-0.71251300
H	-2.22986300	0.74147400	0.90608500
O	-1.80172600	-1.06955200	0.00839400
O	-3.24194500	-1.16071500	-0.10559400
H	-3.30892300	-1.38074200	-1.04334300
C	0.94202900	-0.50296900	-0.00802100
H	0.69421200	-1.53417400	0.27152400
H	0.79121400	-0.40896500	-1.08811000
C	2.39577800	-0.19205300	0.34615100
H	2.60099500	0.85414300	0.09800100
H	2.53219300	-0.29581200	1.43020900
C	3.37395300	-1.10798600	-0.38887600
H	4.41010100	-0.87435000	-0.12804000
H	3.18861900	-2.15724600	-0.13712500
H	3.26415100	-0.99704300	-1.47224200

Absolute energies (Hartree): -497.176374 ZPE (Hartree): 0.162599

Harmonic Vibrational Frequencies (cm^{-1}):

-2814.1696 66.4604 75.0703 88.8009 119.1540 171.1318 203.5663 222.9425 248.2609 296.6375 347.9191 359.1900 481.8122 552.4325 667.5004 711.3139 772.1711 862.6963 905.5207 923.4243 948.3740 963.1546 1053.4029 1087.3888 1124.4295 1132.4481 1161.3766 1198.9521 1205.2772 1265.2060 1283.7058 1292.5200 1329.0260 1345.7380 1388.5866 1390.7664 1401.0729 1428.2109 1430.8653 1492.9131 1513.6125 1521.3561 1527.3035 1898.4792 3069.9096 3072.2750 3085.0321 3107.6105 3128.8806 3142.8813 3149.1132 3161.5731

3163.3012 3832.0613

$O_2C•C(CCC)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-0.16688300	2.76681100	0.20241400
H	0.52810700	3.12964600	0.76432700
O	0.58672100	1.70787400	-0.43887800
C	0.10424700	0.46989500	0.11656200
H	0.12446800	0.56725000	1.21270700
C	1.07831700	-0.56167200	-0.32359400
H	0.82259100	-1.44592900	-0.89359600
O	2.16986900	-0.65230900	0.48865300
O	3.08499000	-1.60995900	-0.08406800
H	3.66958000	-1.00738000	-0.56161600
C	-1.31168400	0.16072300	-0.35354700
H	-1.91274700	1.06333800	-0.20586400
H	-1.28424300	-0.04224600	-1.43155500
C	-1.95093000	-1.00981300	0.39380900
H	-1.35155000	-1.91669500	0.25232200
H	-1.94126600	-0.79328300	1.46937800
C	-3.38613700	-1.26896000	-0.06554700
H	-3.83379200	-2.10557100	0.47855700
H	-4.00879800	-0.38390000	0.09822200
H	-3.41280600	-1.50561500	-1.13394100

Absolute energies (Hartree): -497.208967 ZPE (Hartree): 0.164954

Harmonic Vibrational Frequencies (cm^{-1}):

49.9804 67.5231 68.4873 100.4644 107.6872 179.8716 214.1221 239.9145 242.6221 251.4564 297.0671 319.9657 393.5503 451.0930 504.0003 522.2338 610.3390 757.0374 879.1725 918.9917 933.1550 982.0540 1013.3161 1048.2864 1084.9098 1120.7107 1162.8052 1171.8340 1228.4196 1263.9226 1307.4406 1316.2759 1342.8062 1356.8330 1381.4296 1386.0224 1415.0172 1428.9135 1450.0306 1505.2867 1513.0931 1520.8481 1528.3564 3043.3734 3068.9675 3070.7790 3080.8952 3115.0626 3147.6083 3160.7970 3163.3292 3259.9309 3821.8025 3836.3300

$O_2C(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	0.46284400	1.64925100	-0.49886600
H	-0.50235600	1.70015500	-0.56798900
O	0.54328400	0.92281000	0.75132400
C	0.76141400	-0.44608400	0.44340500
H	0.71301000	-0.90819500	1.43611900
C	-0.35538000	-1.02114100	-0.41750600

H	-0.26008700	-2.10553600	-0.49830300
H	-0.37585800	-0.56369900	-1.40668800
O	-1.65215700	-0.81264800	0.19661500
O	-2.11549000	0.36955800	-0.05354300
C	2.11906000	-0.68764800	-0.20186500
H	2.90291800	-0.29026900	0.44579300
H	2.29335400	-1.75741700	-0.35168400
H	2.17060800	-0.17757300	-1.16569300

Absolute energies (Hartree): -418.723383 ZPE (Hartree): 0.110934

Harmonic Vibrational Frequencies (cm^{-1}):

114.8693 150.2750 193.1598 214.3153 236.2770 298.4251 373.7318 466.3371 530.0322 588.0108 600.8635 836.8454 893.5085 931.3430 965.7283 998.0124 1133.9495 1167.0541 1189.9370 1274.3368 1317.8846 1336.6369 1401.5217 1414.1160 1420.9267 1424.5021 1499.0082 1506.4263 1524.0877 3086.9782 3112.3177 3134.5016 3179.5313 3196.4652 3212.3279 3769.9547

TS_{13}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.68050400	-0.72607400	-0.98570100
O	2.06470200	0.08550300	0.07788200
C	0.99358400	-0.07879200	0.98668000
H	1.10836000	0.66463300	1.77993200
H	0.95532800	-1.09669500	1.38853900
C	-0.22338200	0.14738500	0.07508600
H	0.41457200	-0.40041200	-0.86462800
O	-1.26805900	-0.62230300	0.55582600
O	-2.42824000	-0.42626900	-0.28954300
H	-2.45665000	-1.29780400	-0.70412700
C	-0.53573800	1.57533600	-0.28920200
H	-0.97392300	2.07865300	0.58050000
H	0.39577400	2.07344100	-0.56613100
H	-1.24150200	1.62775800	-1.11717900

Absolute energies (Hartree): -418.670735 ZPE (Hartree): 0.105083

Harmonic Vibrational Frequencies (cm^{-1}):

-2711.8807 86.8474 155.2898 207.9144 233.1006 248.8990 313.4422 359.1994 419.3130 476.3714 631.6170 703.4593 868.4854 906.2588 967.7174 982.8023 1030.0741 1143.8195 1157.6000 1229.3618 1257.3965 1282.9862 1328.3007 1367.4442 1390.0528 1416.9276 1495.9755 1510.6316 1515.1548 1878.4117 3077.2420 3092.2896 3174.0701 3174.9881 3212.7224 3829.9589

$O_2C(C)C(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z

O	2.07712900	-0.05994300	0.86824300
H	1.98594600	-0.94100400	0.47515600
O	1.42763500	0.70712100	-0.17148700
C	0.09287100	0.96300900	0.23702200
H	0.10293700	1.52184900	1.18411300
C	-0.67793300	-0.33322500	0.49505500
H	-0.18350800	-0.89459300	1.28846300
O	-0.61658600	-1.17867300	-0.69547700
O	0.46338700	-1.89098600	-0.73509400
C	-0.48377600	1.80905600	-0.88711400
H	-1.45831000	2.21329800	-0.60511800
H	0.19239100	2.64191600	-1.09029400
H	-0.59022600	1.21055800	-1.79461200
C	-2.14988700	-0.12898100	0.79031500
H	-2.61070100	-1.07201800	1.09154300
H	-2.26693000	0.59420500	1.60210200
H	-2.67176900	0.24648200	-0.09250100

Absolute energies (Hartree): -457.984447 ZPE (Hartree): 0.13925

Harmonic Vibrational Frequencies (cm^{-1}):

95.8432 135.6699 182.2909 199.8958 223.4846 247.9012 263.6251 299.6402 350.8832 413.5126 514.6529 540.3427 577.5852 640.5213 806.3629 878.5847 906.7292 969.6781 1022.7744 1031.6947 1119.0079 1174.2705 1192.8591 1227.5325 1321.9588 1338.8541 1369.9908 1385.1946 1408.7794 1416.1482 1432.4771 1434.3625 1502.9191 1509.2250 1522.9044 1527.3262 3061.6437 3089.2926 3094.1082 3164.6209 3183.7130 3188.9998 3192.4810 3194.5617 3768.7832

TS_{14}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-1.12947900	-1.85052900	-0.06581900
O	-1.81306600	-0.65099500	0.11081800
C	-0.96000500	0.29462700	-0.51553500
C	0.39867000	-0.07876200	0.11672900
H	0.04525100	-1.28640100	0.10841200
O	1.38431700	0.22468500	-0.80710900
O	2.68219100	-0.10031100	-0.24942500
H	2.88979500	-0.86731600	-0.79800700
C	0.64229700	0.35287100	1.53935500
H	0.83336900	1.43138000	1.56902800
H	-0.24639500	0.12240600	2.13074200
H	1.50444000	-0.16451900	1.95871800
H	-0.88412300	0.07686100	-1.58849200
C	-1.47167500	1.69409400	-0.25611900
H	-2.43238400	1.84078100	-0.75536800

H	-1.60116700	1.86763200	0.81424200
H	-0.75622300	2.41938400	-0.65356800

Absolute energies (Hartree): -457.932995 ZPE (Hartree): 0.133272

Harmonic Vibrational Frequencies (cm^{-1}):

-2699.5850 78.3494 139.8977 199.2410 214.8790 233.4264 257.9828 264.1064 278.8379 329.7474 366.7231 479.5679 577.6532 627.0558 680.6273 823.8648 897.5751 912.6835 952.4392 1047.7698 1083.4808 1145.3974 1156.0039 1199.2495 1229.2348 1264.9097 1308.3992 1365.8161 1385.9622 1391.6454 1418.0291 1434.2029 1495.3119 1501.0544 1514.4979 1523.9543 1879.9872 3079.9500 3086.1821 3087.8596 3176.3402 3180.9696 3189.7911 3210.2103 3828.9247

O_2C•(C)C(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.60312400	-1.05953900	-0.01492000
H	2.40194600	-1.92667500	0.35667900
O	1.29893500	-0.73780400	-0.56056600
C	0.73235200	0.26837100	0.29437500
H	0.84480500	-0.07849000	1.33326200
C	-0.72359900	0.28219600	-0.05876600
O	-1.31164500	-0.81715000	0.52714600
O	-2.59162200	-1.08244600	-0.09040200
H	-2.30734100	-1.71143400	-0.76614400
C	1.44217800	1.59814700	0.10605600
H	1.02418600	2.36305300	0.76666700
H	2.50025000	1.46967000	0.34009100
H	1.35069700	1.92745600	-0.93185500
C	-1.54111200	1.52081600	-0.21515400
H	-1.76117300	1.96998600	0.76545300
H	-1.01031000	2.25755800	-0.81919800
H	-2.49230300	1.28722100	-0.69408600

Absolute energies (Hartree): -457.961253 ZPE (Hartree): 0.136398

Harmonic Vibrational Frequencies (cm^{-1}):

50.2867 86.8402 111.0776 149.7680 234.8630 246.4250 261.5543 269.9161 292.1441 322.7453 352.4687 395.1042 441.5368 505.9149 598.2664 818.2902 890.1903 954.8178 969.6406 1019.5578 1024.6919 1071.7924 1130.6210 1152.1139 1239.2515 1329.2670 1354.0163 1381.8748 1385.7822 1400.1852 1425.0106 1426.6232 1485.9462 1509.5001 1511.0125 1527.0245 3033.7138 3035.5720 3086.1313 3156.7592 3179.2378 3193.9223 3206.9995 3817.8627 3835.6242

$O_2C(CC)COO$•

Cartesian Coordinates (Å)

At.	X	Y	Z
O	0.06511000	1.67481400	0.56914400

H	1.03393900	1.69074000	0.54514100
O	-0.16107400	0.93359400	-0.65520600
C	-0.38833600	-0.42341800	-0.30239500
H	-0.46771000	-0.89867900	-1.28853700
C	0.79634900	-1.02313200	0.44261300
H	0.68169800	-2.10415100	0.54114600
H	0.93190600	-0.56072300	1.42043900
O	2.02843900	-0.85243900	-0.30398300
O	2.54693200	0.31718000	-0.11104100
C	-1.68082400	-0.61846300	0.48510000
H	-1.79425300	-1.68685500	0.70678100
H	-1.58295700	-0.09185800	1.43934500
C	-2.89849000	-0.10365300	-0.28041500
H	-3.81019600	-0.22864200	0.30964400
H	-2.77614400	0.95588800	-0.51331000
H	-3.02374100	-0.64891100	-1.22138900

Absolute energies (Hartree): -457.978176 ZPE (Hartree): 0.139783

Harmonic Vibrational Frequencies (cm^{-1}):

64.8802 103.0304 147.5026 177.0483 195.3294 232.9587 298.1079 307.9454 378.6459 507.3551 530.5020 587.8793 592.0067 797.8982 848.5074 906.0725 938.2088 988.7723 1015.1953 1070.6788 1128.7418 1166.0098 1188.8493 1271.4628 1278.7630 1319.7113 1334.8148 1389.8129 1412.3968 1414.8898 1419.4066 1430.9469 1494.6402 1504.0874 1518.2765 1528.8908 3079.8520 3081.1479 3096.5489 3134.2790 3142.8920 3166.7286 3187.5406 3212.0702 3766.2806

TS_{15}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.17556300	-0.63963300	-0.73469800
O	2.18416400	0.50654500	0.05441000
C	1.12104400	0.26451300	0.95506800
H	0.92886200	1.19082000	1.50189700
H	1.34578300	-0.56440600	1.63464800
C	-0.00512000	-0.16462900	-0.00140000
H	0.86352700	-0.71003700	-0.73472900
O	-0.80937300	-1.07258100	0.66710400
O	-1.88226600	-1.48752000	-0.21450600
H	-1.58794500	-2.38967000	-0.39413600
C	-0.70561700	0.92950100	-0.77321400
H	0.07681700	1.60079400	-1.14103200
H	-1.20978900	0.49452700	-1.63851200
C	-1.71759900	1.68540500	0.09624600
H	-2.17001100	2.49933500	-0.47637900
H	-2.51054400	1.01443200	0.43221300

H	-1.23765400	2.12098300	0.97734600

Absolute energies (Hartree): -457.925694 ZPE (Hartree): 0.134313

Harmonic Vibrational Frequencies (cm^{-1}):

-2711.2483 94.9416 102.2092 151.0041 202.4846 224.0016 233.2670 282.6119 328.9891 374.4775 428.7962 517.6224 674.8746 713.8759 812.8045 847.2643 906.2286 988.8187 1008.9409 1025.5249 1063.2891 1129.9972 1143.9445 1220.9962 1229.3984 1277.3549 1323.5261 1330.7597 1368.5999 1379.6081 1393.0791 1426.2054 1499.3624 1512.1130 1519.2138 1526.0385 1876.5848 3083.9920 3093.0153 3109.7818 3162.8166 3174.0952 3177.3973 3190.1587 3826.6087

O_2C•(CC)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.28497400	-0.25228200	-0.07808400
H	3.56733400	0.55150500	-0.52983900
O	2.01826600	0.20878400	0.45303400
C	1.01100900	-0.47588000	-0.29443700
H	1.09897900	-1.55583800	-0.13415700
H	1.13774400	-0.25600800	-1.36300000
C	-0.30302900	0.02437700	0.20101300
O	-0.66952700	1.12451600	-0.54239500
O	-1.79205800	1.78840900	0.08418300
H	-1.31295200	2.43987200	0.61290100
C	-1.36781800	-0.88055900	0.72988000
H	-2.03573200	-0.32154200	1.38927900
H	-0.87961000	-1.65390200	1.33046400
C	-2.19246500	-1.52154400	-0.40111600
H	-2.96598300	-2.17749900	0.00849200
H	-2.67551200	-0.74475500	-0.99832600
H	-1.55368900	-2.11560700	-1.06176300

Absolute energies (Hartree): -457.956066 ZPE (Hartree): 0.137002

Harmonic Vibrational Frequencies (cm^{-1}):

31.1235 55.6673 81.2025 110.3844 199.1236 224.1486 230.9756 262.4608 276.3334 307.4212 367.9864 388.3971 542.1719 621.0955 804.1280 817.2618 917.8388 961.8262 978.9860 1005.0275 1057.4969 1072.1812 1093.9271 1237.3642 1255.5732 1319.5535 1350.3819 1363.7906 1375.1557 1386.0295 1420.6272 1436.3324 1496.5724 1517.5118 1521.9083 1523.1404 3054.1232 3076.2295 3105.9550 3126.4336 3155.8051 3168.3711 3182.3872 3816.2504 3840.3756

O_2C(C)C(CC)OO•

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.95407200	-0.51133800	-1.35926400
H	2.18441300	0.39853300	-1.11782900

O	1.56223300	-0.98803800	-0.05118700
C	0.14438800	-0.93890600	0.02680900
H	-0.27671300	-1.56255600	-0.77269400
C	-0.37674000	0.48555300	-0.17627900
H	-0.09314200	0.83660100	-1.17062700
O	0.29021200	1.37559900	0.77225500
O	1.42749200	1.80494500	0.32791900
C	-0.17322900	-1.51712600	1.39656800
H	-1.24812600	-1.67651800	1.50872800
H	0.33477300	-2.47741200	1.50690500
H	0.17317300	-0.84157800	2.18200100
C	-1.86651700	0.67086900	0.05809200
H	-2.09849700	1.72697200	-0.11469000
H	-2.09618700	0.46367800	1.10814700
C	-2.71716900	-0.20667000	-0.86330000
H	-2.60913000	-1.26822500	-0.62673200
H	-3.77427100	0.05130400	-0.76206600
H	-2.43277800	-0.06246700	-1.91027100

Absolute energies (Hartree): -497.237955 ZPE (Hartree): 0.16839

Harmonic Vibrational Frequencies (cm^{-1}):

90.6227 101.4950 138.3138 179.4217 191.2351 214.9840 238.4518 257.9172 278.0448 328.1593 407.8632 414.4120 513.7896 541.2354 573.0859 640.2169 774.2126 856.6706 902.0656 947.0567 968.9818 976.7688 1057.8694 1074.0026 1110.3758 1177.8490 1202.2408 1224.5281 1289.8158 1321.2601 1345.1551 1358.5007 1385.6811 1393.2535 1416.1805 1420.3193 1433.6088 1436.2568 1503.1669 1515.6040 1523.0707 1526.2669 1531.2815 3077.4508 3082.5282 3091.5939 3094.7053 3138.8226 3155.1095 3169.4830 3175.9778 3188.9869 3191.4596 3767.3693

TS_{16}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	0.15135600	2.24689800	0.25974900
O	1.19721300	1.34236700	0.10872300
C	0.61169100	0.31016400	-0.66724900
C	-0.69603100	0.05621900	0.11942100
H	-0.75070400	1.28891100	0.35962800
O	-1.63512900	-0.38033500	-0.80185800
O	-2.89965200	-0.61518600	-0.13313100
H	-3.39821400	0.12591000	-0.49990100
C	-0.64579900	-0.68493100	1.42987300
H	-0.46397500	-1.74984700	1.24772200
H	0.15943600	-0.27137500	2.03907900
H	-1.59279000	-0.58163700	1.95922600
H	0.29185200	0.71525900	-1.63687300

C	1.59319400	-0.83650200	-0.87330400
H	2.24886900	-0.55809300	-1.70548900
H	1.00952700	-1.70120600	-1.21187200
C	2.45830200	-1.20011900	0.33664400
H	1.86655700	-1.58224100	1.16919900
H	3.17537500	-1.97569800	0.05282200
H	3.01562600	-0.32891400	0.68628700

Absolute energies (Hartree): -497.183693 ZPE (Hartree): 0.162469

Harmonic Vibrational Frequencies (cm^{-1}):

-2679.3909 63.1850 87.7638 133.6624 201.2965 210.6208 217.5051 240.2948 250.9284 301.7096 316.7621 349.2668 378.7294 507.2282 607.9266 656.9824 684.7758 776.3314 828.7238 898.1921 939.4951 967.4894 997.9756 1073.7210 1115.3762 1144.8589 1150.1441 1178.8085 1225.1004 1263.6073 1301.3659 1333.4010 1372.9610 1385.0021 1395.0319 1397.1803 1424.1581 1439.3240 1496.1286 1499.4613 1512.9588 1525.3036 1532.3116 1878.0653 3069.4281 3080.5860 3083.7408 3093.7409 3130.7343 3177.3928 3179.6210 3199.3922 3210.9554 3829.0888

O_2C•(C)C(CC)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.61884000	-2.23865900	-0.10220100
H	1.17713700	-2.84936500	0.49996700
O	0.49003600	-1.41993100	-0.48058600
C	0.59317400	-0.17678300	0.24896900
H	0.70447700	-0.42258500	1.31493500
C	-0.73145400	0.48027500	0.05547400
O	-1.66312400	-0.02419400	0.93145900
O	-2.92875000	-0.24902400	0.27779500
H	-2.84770600	-1.19498600	0.09953400
C	1.78527300	0.64637800	-0.21767900
H	2.67814300	0.02798000	-0.09267500
H	1.68096100	0.84434600	-1.28931200
C	-1.17033600	1.14290800	-1.20142500
H	-1.99338500	1.83361700	-1.00261200
H	-0.33468900	1.69836700	-1.63169500
H	-1.51671900	0.41946600	-1.95050800
C	1.92689800	1.94966300	0.56827700
H	2.82644900	2.49142600	0.26325500
H	1.06499100	2.60503800	0.41430300
H	2.00299100	1.74651000	1.64137100

Absolute energies (Hartree): -497.216752 ZPE (Hartree): 0.16593

Harmonic Vibrational Frequencies (cm^{-1}):

30.9103 75.6150 100.2272 122.1714 128.9949 180.4122 207.8028 222.3515 258.7743 265.6661 283.0700 319.1944 325.9411 458.8792 504.2303 519.7201 604.2203 765.1210 849.2035 909.4275 980.2445 1008.9809

1029.9235 1079.2179 1103.7019 1132.5502 1149.4951 1198.4434 1274.4792 1298.9340 1332.6095 1357.3420 1369.6949 1389.0717 1397.8771 1422.1566 1432.5532 1434.4190 1485.7153 1505.5734 1516.6515 1520.3724 1528.3788 3057.7745 3058.5558 3074.1054 3101.8530 3142.3945 3149.6637 3164.2195 3170.7092 3189.2169 3814.7068 3831.4924

$O_2C(CCC)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-0.57555900	1.68420500	-0.55482200
H	-1.54386500	1.65969100	-0.59249700
O	-0.39759600	0.96751800	0.69184600
C	-0.09848400	-0.38448100	0.37383600
H	-0.06159100	-0.84482100	1.36954800
C	-1.21124100	-1.03867300	-0.43380800
H	-1.05103000	-2.11593200	-0.50656500
H	-1.30130600	-0.59586800	-1.42592100
O	-2.49383400	-0.90379900	0.23094900
O	-3.04155400	0.24263400	-0.01324100
C	1.24484300	-0.53887100	-0.33211000
H	1.40526700	-1.60150000	-0.55932600
H	1.19691000	-0.00120300	-1.28546000
C	2.40908800	-0.00823600	0.50345900
H	2.20217700	1.03301700	0.76776900
H	2.46245900	-0.57261400	1.44305800
C	3.74179100	-0.10954100	-0.23777200
H	4.56518700	0.27140700	0.37297000
H	3.96644600	-1.14914800	-0.49807200
H	3.71170900	0.47132200	-1.16499200

Absolute energies (Hartree): -497.232222 ZPE (Hartree): 0.168539

Harmonic Vibrational Frequencies (cm^{-1}):

55.3050 66.1618 97.7717 151.3137 155.6850 197.6443 248.6223 270.6191 295.9739 324.1050 386.6919 519.6122 531.7265 591.5053 609.9348 761.5645 849.4804 878.1252 911.2598 920.4915 978.9814 1011.1299 1075.9759 1095.7754 1131.9194 1171.8341 1187.3165 1257.2811 1270.6245 1288.5681 1330.4593 1347.7558 1348.5851 1405.4185 1411.5366 1417.9282 1422.7481 1429.7974 1491.9822 1502.5005 1513.9950 1521.3974 1527.6256 3066.4875 3069.6958 3075.9921 3096.2185 3128.4289 3134.0321 3142.2776 3161.7686 3163.7276 3211.9183 3764.6286

TS_{17}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.51911000	-0.48002500	-0.86536700
O	-2.02936200	-1.39296500	0.06337400
C	-1.33109800	-0.56103600	0.96920500

H	-0.75644900	-1.20465300	1.63958600
H	-2.01107700	0.09379700	1.52457500
C	-0.48223800	0.29505100	0.01314400
H	-1.42689900	0.25188500	-0.82057600
O	-0.31603700	1.54342400	0.59002100
O	0.48708900	2.36489800	-0.29363300
H	-0.20055800	2.96881300	-0.60238800
C	0.74667500	-0.35084800	-0.58089600
H	0.45353800	-1.35898500	-0.89528600
H	1.05557200	0.20264800	-1.47149600
C	1.91502600	-0.41557300	0.41131200
H	2.18768800	0.60225100	0.70545400
H	1.59751300	-0.93918300	1.32066800
C	3.12327800	-1.12901300	-0.19551700
H	3.46588900	-0.60794100	-1.09493300
H	3.95623200	-1.16718500	0.51224500
H	2.86806200	-2.15558800	-0.47650000

Absolute energies (Hartree): -497.180059 ZPE (Hartree): 0.163119

Harmonic Vibrational Frequencies (cm^{-1}):

-2712.4358 67.1565 85.9227 97.9814 136.7307 197.2990 230.9710 246.8369 251.9114 320.4036 348.4879 369.5724 432.2455 517.0907 687.2266 735.6266 763.6329 852.6545 884.9565 909.2544 938.7042 1007.7056 1037.3425 1072.3582 1083.7439 1142.3447 1144.1816 1220.9446 1226.8873 1276.3324 1299.8451 1321.2085 1330.8315 1350.2578 1372.4422 1389.5724 1406.0278 1428.1850 1495.3753 1509.1405 1513.8787 1520.5000 1526.1537 1876.4868 3071.3985 3083.1213 3092.5665 3097.2501 3137.2579 3157.6249 3164.6144 3167.8291 3177.2414 3825.5699

O_2C•(CCC)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.12822900	0.39087900	0.33942500
H	-3.42085900	-0.25320300	0.99503600
O	-1.69643400	0.22303800	0.45726700
C	-1.27452900	-0.48553800	-0.72296200
H	-1.55025700	0.09803400	-1.60794500
H	-1.77541800	-1.46079600	-0.75338700
C	0.19321900	-0.64367900	-0.63761400
O	0.55096200	-1.78413700	0.03386400
O	1.79958100	-1.60559800	0.73604200
H	1.46391500	-1.31944800	1.59604800
C	1.18101200	0.33397800	-1.17335600
H	2.18734300	-0.07870000	-1.06943100
H	0.98760500	0.47311500	-2.24686100
C	1.10435300	1.71109400	-0.48333100

H	1.81900300	2.38249300	-0.97396500
H	0.10548200	2.13315500	-0.63811500
C	1.39421300	1.64243200	1.01467700
H	1.38198800	2.64153400	1.45981300
H	0.62910000	1.04538200	1.51977500
H	2.37545000	1.19525100	1.20177200

Absolute energies (Hartree): -497.211015 ZPE (Hartree): 0.166449

Harmonic Vibrational Frequencies (cm^{-1}):

34.6841 59.6817 68.3897 110.3006 133.5756 161.6230 227.5321 245.0897 272.7993 278.2315 299.4300 348.5279 377.8381 422.4305 477.9641 590.6392 767.8376 815.2443 879.3280 912.3632 977.4665 997.7174 1068.5960 1076.1199 1083.2674 1112.3570 1160.7336 1240.1414 1253.9766 1296.6362 1326.5048 1340.4977 1364.6274 1382.0600 1391.8874 1418.0643 1427.4964 1433.5853 1486.4779 1509.1266 1516.3382 1520.3795 1533.0216 3047.9529 3066.9104 3070.6526 3079.1877 3128.6669 3134.1648 3159.3071 3162.2198 3165.8848 3811.0532 3835.9898

TS_{18}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.86267100	-0.60817300	0.13835900
H	2.11907100	-0.44950000	1.19072800
H	2.64207600	-1.18853500	-0.36019300
C	0.48516800	-1.27382900	-0.00917900
H	0.32272600	-1.50608500	-1.06539000
H	0.45753900	-2.20630300	0.56499400
C	-0.60151500	-0.32151500	0.43629300
H	-0.02969300	0.78515200	0.31180400
H	-0.88804400	-0.35595600	1.49245300
O	1.81719200	0.64340900	-0.52793500
O	1.03114800	1.47141500	0.25043600
O	-1.69076700	-0.44187500	-0.41721900
O	-2.71625500	0.44965600	0.07532200
H	-2.63216000	1.16148400	-0.57206400

Absolute energies (Hartree): -418.679656 ZPE (Hartree): 0.105667

Harmonic Vibrational Frequencies (cm^{-1}):

-2364.8611 69.4451 130.0250 185.4157 243.7493 325.3868 409.6377 439.6752 511.4580 539.4860 633.7595 845.1426 912.8169 929.4878 981.1601 1021.2003 1118.6130 1138.7326 1169.2575 1194.5229 1254.9846 1285.0763 1322.2314 1382.9151 1385.8127 1406.0426 1430.7106 1485.3961 1502.9186 1650.3073 3092.4836 3097.4273 3121.0799 3161.8888 3180.8418 3823.5141

TS_{19}

Cartesian Coordinates (Å)

At.	X	Y	Z

C	1.53071000	-0.10890400	0.31513600
H	1.66426500	0.20747200	1.35649300
C	0.30870700	-1.04083100	0.20296700
H	0.26027200	-1.41110900	-0.82619400
H	0.43410400	-1.89425300	0.87852300
C	-0.97213100	-0.29369200	0.49877200
H	-0.61967800	0.89167200	0.31938900
H	-1.33518700	-0.31814700	1.53143900
O	1.24235600	1.04977600	-0.46271100
O	0.28243700	1.77150400	0.21860500
O	-1.94398800	-0.68014400	-0.41714900
O	-3.15380400	0.03548200	-0.07942400
H	-3.13485700	0.71294900	-0.76768200
C	2.79734200	-0.72001900	-0.24948100
H	3.63600000	-0.02985300	-0.13607100
H	3.02917700	-1.64981600	0.27685200
H	2.66213800	-0.94117900	-1.31167900

Absolute energies (Hartree): -457.941089 ZPE (Hartree): 0.133614

Harmonic Vibrational Frequencies (cm^{-1}):

-2353.9000 52.0727 106.3282 158.4762 209.9194 244.7306 293.9731 295.8494 342.9559 408.4936 493.0267 527.4583 554.0820 637.1480 839.7229 882.1117 912.2717 944.2837 1016.1920 1083.1827 1119.3807 1150.7978 1171.6894 1193.7703 1200.8772 1269.3144 1279.9707 1356.9917 1384.4218 1386.3174 1394.2498 1426.3688 1429.4546 1481.2810 1505.4728 1520.8790 1648.3620 3084.1517 3086.3247 3093.4414 3120.0383 3155.1518 3179.4244 3187.3843 3822.0574

O_2C•CC(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.32116200	-0.33713900	-0.37146800
H	-3.43890300	-1.12961200	-0.90820800
O	-2.10703000	-0.71408800	0.32425600
C	1.43824500	0.21440000	0.00075100
H	1.64109500	1.24478600	0.27811800
O	2.52702400	-0.61315900	0.03360100
O	3.67630900	0.16876600	-0.37997600
H	4.28406500	-0.09445300	0.32127400
C	-1.05437900	0.09965500	-0.19654400
H	-1.01639300	-0.02773300	-1.28633800
C	0.20090500	-0.50433500	0.43160300
H	0.28223000	-1.55393400	0.13199000
H	0.08113000	-0.48193800	1.52548100
C	-1.26391200	1.56308200	0.15660000
H	-1.22398500	1.69182900	1.24267900

H	-0.49522000	2.18658900	-0.30837400
H	-2.24029800	1.89261100	-0.20238100

Absolute energies (Hartree): -457.955982 ZPE (Hartree): 0.13632

Harmonic Vibrational Frequencies (cm^{-1}):

51.3802 80.3907 103.9032 136.0003 174.1614 194.4279 208.2022 253.5035 294.5740 306.8020 346.2720 466.0680 517.7817 567.4343 701.8117 861.8401 905.0568 912.4750 936.3133 980.7433 1076.7176 1134.4542 1154.9211 1171.3207 1209.7191 1261.1178 1294.1798 1359.7175 1374.1696 1401.4185 1410.3201 1424.8558 1437.6915 1496.5623 1505.8544 1526.5820 3040.4432 3075.5110 3081.0949 3137.1637 3172.3014 3191.5259 3213.3165 3839.9727 3847.3487

$O_2CC(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.17202300	-0.86330900	-0.22288800
C	1.27771500	-0.89826900	0.26344000
C	-1.04565100	-0.10329400	0.77846700
O	-1.86471000	0.90888100	0.11410300
O	-1.13831700	1.85393300	-0.37568200
O	1.76935500	0.38319100	0.61358700
O	1.79271500	1.16617400	-0.60243500
H	1.91939600	-1.35543900	-0.49909700
H	1.36559600	-1.46771400	1.19690200
H	-0.44723400	0.42969200	1.51902500
H	0.94768200	1.63509200	-0.51218700
H	-0.17599400	-0.29183500	-1.15466900
H	-1.78412500	-0.73988200	1.27021900
C	-0.69528400	-2.27144800	-0.50216500
H	-0.07102300	-2.78034100	-1.24254800
H	-0.69709100	-2.87404200	0.41281100
H	-1.71810000	-2.23504700	-0.88817300

Absolute energies (Hartree): -457.974439 ZPE (Hartree): 0.140431

Harmonic Vibrational Frequencies (cm^{-1}):

64.4901 119.9406 139.3081 181.7800 245.5812 259.0107 278.2673 367.6208 405.9224 425.3598 550.3589 563.8189 616.4332 860.7714 869.4347 916.7206 936.0834 979.7044 1009.3202 1085.7852 1159.6052 1174.8193 1218.2735 1279.8302 1291.7596 1340.5127 1352.4595 1376.1659 1416.7340 1428.8496 1439.9580 1447.8463 1493.3670 1509.9054 1519.9371 1522.4158 3067.7990 3072.0256 3122.1425 3128.9785 3140.6365 3159.0349 3166.7180 3196.8175 3739.9525

TS_{20}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.82756000	0.09272500	0.00209200

H	-2.05725500	0.09783700	1.07430300
H	-2.65753900	0.52088300	-0.56624100
C	-0.51800600	0.84482700	-0.28245800
H	-0.37525200	0.83755600	-1.36936500
C	0.63450400	0.06732900	0.31300900
H	0.17515500	-1.09788200	0.34865100
O	-1.69143500	-1.24517800	-0.44800500
O	-0.82486500	-1.86808300	0.43105700
O	1.74026500	0.18712200	-0.51852800
O	2.84998900	-0.45816800	0.14685500
H	2.89091700	-1.27464700	-0.36752600
H	0.87113600	0.28845400	1.36042800
C	-0.57096200	2.28767800	0.22749000
H	-1.37591800	2.84449300	-0.26207500
H	-0.74561800	2.30735600	1.30799900
H	0.37488500	2.79506200	0.02198400

Absolute energies (Hartree): -457.936591 ZPE (Hartree): 0.134002

Harmonic Vibrational Frequencies (cm^{-1}):

-2406.1996 67.0459 109.5896 184.7383 208.5642 240.6505 247.1964 257.8917 418.1437 447.8599 472.0670 484.6925 541.6883 641.5226 892.7518 921.7642 953.4531 973.7613 1015.5774 1031.9262 1125.6041 1160.3924 1171.1686 1189.4896 1208.0199 1289.5614 1315.4119 1324.1209 1384.9362 1393.0477 1409.7854 1423.1751 1438.4254 1497.4920 1516.1700 1521.6402 1651.0387 3071.8052 3080.1300 3100.6868 3109.6979 3160.7936 3168.3652 3174.7471 3823.4271

O_2C•C(C)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.48047200	-0.58652700	0.17203600
H	3.78272300	-0.99500000	-0.64766500
O	2.33011200	0.13172000	-0.33298400
C	-1.25610000	-0.42345200	0.22113100
H	-1.41180700	-0.62438700	1.27982300
O	-2.36763400	-0.00351900	-0.45578800
O	-3.51075600	-0.68704800	0.11854900
H	-4.09507000	0.07445200	0.21482000
C	1.18900200	-0.53316200	0.18527400
H	1.24667900	-0.56666600	1.28105900
H	1.13593400	-1.55769100	-0.20236200
C	-0.02453400	0.27740500	-0.26173500
H	-0.04981700	0.27721200	-1.35846100
C	0.04840500	1.72925700	0.24001900
H	0.10339000	1.74327000	1.33385300
H	0.93373300	2.23188400	-0.15470900

H	-0.84395400	2.27964000	-0.06899600

Absolute energies (Hartree): -457.951992 ZPE (Hartree): 0.136429

Harmonic Vibrational Frequencies (cm^{-1}):

57.6620 77.0374 90.3186 105.2852 146.4796 176.6810 211.0780 236.0310 266.9646 326.3128 347.0940 398.8368 494.1900 586.7782 761.6077 888.2184 915.1897 924.2179 949.5757 1001.8557 1091.2567 1148.2130 1174.9735 1191.2115 1206.4298 1267.3710 1290.6201 1359.1646 1370.9541 1400.8019 1412.5921 1425.2035 1439.8495 1513.4603 1519.2322 1544.1974 3057.7952 3074.9376 3092.6203 3119.2466 3165.0555 3185.8288 3187.2875 3839.5404 3846.1079

$O_2CC(C)C(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.08610500	-0.49163900	-0.53718300
C	1.39059500	-0.96776100	0.09582600
C	-0.84345500	0.08380000	0.52976400
O	-1.81981000	0.96778900	-0.11787600
O	-1.26218500	2.06143400	-0.52605700
O	2.06579700	0.05719900	0.81138400
O	2.52535200	1.01068200	-0.17694500
H	2.05347500	-1.38072400	-0.67369100
H	1.21393300	-1.73368200	0.86021500
H	-0.26851800	0.72651700	1.20055700
H	1.88885400	1.72394600	-0.03508400
H	0.34633000	0.34182500	-1.19639900
C	-1.66796100	-0.91727900	1.31377200
H	-2.24187900	-0.40541800	2.08970900
H	-2.36376800	-1.44682700	0.65931100
H	-1.01278700	-1.64877400	1.79434500
C	-0.55561500	-1.59538800	-1.37550400
H	0.09122000	-1.85269200	-2.21933600
H	-0.71918100	-2.50427800	-0.78761900
H	-1.51893200	-1.26711100	-1.77610900

Absolute energies (Hartree): -497.234936 ZPE (Hartree): 0.16792

Harmonic Vibrational Frequencies (cm^{-1}):

29.7456 69.6617 118.7353 178.9082 201.9139 211.8751 247.7587 261.8580 296.6839 332.9849 350.8881 385.5371 454.5513 513.8556 590.2883 611.1657 795.0710 863.0000 881.8276 935.6841 972.1783 1024.1673 1038.0715 1081.2796 1142.1510 1183.6480 1194.2184 1225.1821 1292.4430 1306.7191 1344.9684 1370.6659 1381.3445 1393.5585 1406.2350 1427.0365 1430.2164 1444.3956 1489.2682 1501.7704 1515.2205 1524.0475 1531.7345 3072.1968 3075.5363 3089.8869 3123.0588 3140.8482 3141.8292 3161.9216 3167.9450 3182.1796 3189.0782 3811.5309

TS_{21}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.47797700	-0.15935900	0.21849900
H	-1.56258400	-0.23053400	1.31147700
C	-0.27912700	0.73744900	-0.14916500
H	-0.23419800	0.76126700	-1.24552700
C	1.00221500	0.08622500	0.32466800
H	0.69220000	-1.12407400	0.35944700
H	1.30101100	0.31494500	1.35451700
O	-1.20136600	-1.46408100	-0.28875500
O	-0.19952000	-2.00847700	0.49213400
O	2.01031100	0.35981600	-0.59163000
O	3.24496600	-0.15210500	-0.03927500
H	3.33705900	-0.95312700	-0.57106000
C	-2.78586700	0.27954700	-0.41091200
H	-3.56709400	-0.44918300	-0.18344200
H	-3.09210100	1.25249100	-0.02017800
H	-2.67517900	0.35149600	-1.49666600
C	-0.41220800	2.16232800	0.39958600
H	-1.24689400	2.69290000	-0.06568600
H	-0.57349600	2.14150400	1.48268900
H	0.50393400	2.72395100	0.19858600

Absolute energies (Hartree): -497.197561 ZPE (Hartree): 0.161956

Harmonic Vibrational Frequencies (cm^{-1}):

-2395.6927 54.0293 89.9051 164.1741 178.6547 214.6012 227.1099 240.8402 279.5450 296.3350 323.1746 434.1477 449.7439 485.8307 538.1266 561.9928 629.5160 850.9425 910.4302 924.0883 959.0519 998.0326 1029.7959 1103.7739 1126.2641 1161.0878 1170.4788 1190.3148 1193.2861 1210.5911 1285.8912 1315.1704 1368.9179 1382.3475 1388.9091 1392.9230 1419.7730 1427.3627 1435.9465 1506.3061 1512.7122 1517.6636 1528.2607 1652.2933 3071.5158 3072.9636 3086.1045 3091.4351 3107.1271 3164.2551 3173.9220 3180.6785 3188.9219 3823.0118

$O_2C•C(C)C(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.31629500	-0.28722800	-0.66197500
H	3.38093200	-0.20813900	-1.62107400
O	2.12191300	0.50601400	-0.45034100
C	-1.41164100	-0.38292800	0.03409900
H	-1.62217500	-0.85818900	0.98973000
O	-2.50393600	0.16848300	-0.57971200
O	-3.64893900	-0.66376900	-0.26301700
H	-4.25995200	0.03392400	0.00238300
C	1.06544400	-0.40097800	-0.12371500
H	0.99383200	-1.15161800	-0.92224500

C	-0.19794600	0.47137500	-0.16963100
H	-0.25900500	0.87711500	-1.18724000
C	-0.15495400	1.65099300	0.81813600
H	-0.15225400	1.29658300	1.85266000
H	0.73769000	2.25949800	0.65572400
H	-1.04123000	2.27580700	0.67697200
C	1.32433700	-1.09082200	1.20676200
H	0.52345300	-1.79971900	1.43539800
H	2.26524200	-1.64098500	1.15049800
H	1.39935700	-0.35811200	2.01365700

Absolute energies (Hartree): -497.211167 ZPE (Hartree): 0.164802

Harmonic Vibrational Frequencies (cm^{-1}):

49.8010 64.0620 91.5689 121.9832 149.8795 177.1589 212.1918 222.8008 237.4930 272.2123 297.6429 315.2830 341.2349 382.8460 500.9090 538.5711 627.1388 772.5783 841.1800 893.2693 918.8137 931.3660 968.1010 1023.5837 1050.0858 1122.5562 1160.2145 1182.2097 1198.6318 1215.2004 1286.9061 1353.2342 1360.3875 1364.8532 1401.3245 1407.0859 1415.8206 1432.3110 1436.3587 1503.6380 1514.8528 1519.1969 1530.8216 3067.6977 3079.8474 3089.0372 3091.9301 3168.8733 3179.8628 3182.4574 3192.2420 3196.9396 3837.3075 3845.9465

$O_2CCC(C)(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.00288400	-0.77376700	-0.87946900
C	1.24613600	-1.32018200	-0.17917700
C	-1.11310000	-0.16818800	-0.00975100
O	-1.12047800	1.31702800	-0.13914700
O	0.01468800	1.88410800	0.05234400
O	1.97443500	-0.38001500	0.58558300
O	2.51121000	0.58225300	-0.34682400
H	1.90410600	-1.76978400	-0.93266800
H	0.97794100	-2.08768100	0.55378400
H	1.83083400	1.26535200	-0.24944000
H	0.30264200	-0.03589000	-1.62886800
H	-0.42894000	-1.61659500	-1.43347400
C	-2.48583200	-0.51806500	-0.56604300
H	-3.26584100	0.03600200	-0.03695700
H	-2.54004400	-0.27634300	-1.63143600
H	-2.66449000	-1.58890100	-0.43811000
C	-1.01178700	-0.47084000	1.47761400
H	-1.09828200	-1.54902200	1.64288100
H	-0.05683700	-0.12463300	1.87384400
H	-1.82973700	0.02675700	2.00575500

Absolute energies (Hartree): -497.237335 ZPE (Hartree): 0.168095

Harmonic Vibrational Frequencies (cm^{-1}):

81.5262 95.4778 161.8387 191.2315 228.3657 256.3593 284.8941 313.2366 317.6929 355.0259 404.7693 436.1868 457.2347 554.4012 568.9023 583.0688 730.8350 826.5315 846.9545 898.3545 948.8276 964.5863 1027.2747 1036.6147 1070.9845 1139.7968 1181.8995 1254.6313 1281.0783 1294.4422 1336.9429 1387.3025 1403.6704 1414.4404 1421.4564 1429.0112 1435.9027 1484.1820 1492.1651 1500.7071 1506.1777 1520.6608 1534.7149 3074.7509 3078.8009 3082.8726 3087.5858 3143.1470 3157.0747 3170.9868 3175.9322 3182.3984 3205.3021 3766.1554

TS_{22}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.34638500	-0.17407000	0.01411900
C	0.08469200	-1.05225800	0.19192500
H	-0.08884500	-1.58914400	-0.74606300
H	0.26156200	-1.78491000	0.98769600
C	-1.14360800	-0.21918000	0.48146600
H	-0.79277400	0.90157600	0.05400100
H	-1.40288700	-0.05285900	1.53188900
O	0.98137000	0.85266100	-0.92304300
O	0.09367400	1.71964200	-0.31828700
O	-2.21121500	-0.72527400	-0.25279800
O	-3.36523800	0.08643800	0.06362000
H	-3.39784000	0.63237800	-0.73262700
C	2.44989500	-0.94502300	-0.69203900
H	3.34696400	-0.32602500	-0.77689000
H	2.69494900	-1.84779900	-0.12529300
H	2.12230600	-1.23352800	-1.69448800
C	1.82812000	0.41584900	1.33355000
H	2.20689800	-0.38760200	1.97280000
H	2.63676300	1.12578100	1.13916300
H	1.03127400	0.94248400	1.85975600

Absolute energies (Hartree): -497.201022 ZPE (Hartree): 0.161364

Harmonic Vibrational Frequencies (cm^{-1}):

-2354.8799 50.9564 101.5537 153.4626 197.4592 237.1879 254.2388 273.8934 290.4416 316.6497 341.6297 388.8121 435.2441 515.2922 548.0173 554.1036 647.5516 796.1866 850.5482 896.0581 927.2185 960.9539 981.9888 1015.7038 1071.7272 1109.7591 1138.9042 1170.8757 1215.1422 1250.6140 1253.9211 1305.8551 1326.0641 1366.0814 1385.0529 1417.3923 1421.5638 1428.6917 1479.4759 1495.7518 1505.6404 1511.6682 1529.0282 1647.9042 3078.5879 3081.6757 3085.0256 3120.9980 3152.7120 3171.4567 3177.6768 3179.0715 3195.8956 3821.2307

$O_2C•CC(C)(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z

O	3.25410400	-0.23832800	-0.17407300
H	3.47571000	-1.06242200	0.27504400
O	1.95441000	-0.60513900	-0.70197900
C	-1.56675200	0.24853000	-0.14545800
H	-1.78257400	1.28960100	-0.36843600
O	-2.64899800	-0.58669900	-0.19758200
O	-3.79493900	0.16133100	0.28400200
H	-4.41684100	-0.06934100	-0.41636200
C	0.94091200	0.09162100	0.04750100
C	-0.33090200	-0.43602400	-0.63160700
H	-0.42156700	-1.50910600	-0.43078100
H	-0.20553200	-0.31328000	-1.71775100
C	1.10046800	1.59588100	-0.13884800
H	0.98691300	1.85863300	-1.19497400
H	0.35440100	2.13777900	0.44921400
H	2.09448900	1.90221500	0.19334000
C	0.99021000	-0.30870600	1.51680500
H	0.98522100	-1.40030600	1.60301400
H	1.89247300	0.08393100	1.99104500
H	0.11708000	0.08515900	2.04335100

Absolute energies (Hartree): -497.21654 ZPE (Hartree): 0.164332

Harmonic Vibrational Frequencies (cm^{-1}):

38.5330 73.6179 102.1543 149.4827 172.9840 198.3285 240.4995 262.9218 271.7349 300.1003 303.0838 346.7138 357.7250 391.4501 468.9885 539.0383 588.9543 702.7533 781.5560 890.9120 897.2704 934.6041 941.6477 964.1908 1030.3222 1035.9922 1107.9624 1164.9801 1182.6736 1226.1660 1303.7838 1317.1687 1325.8938 1367.4560 1406.5996 1409.5184 1417.4327 1431.3979 1491.5659 1496.1317 1513.1565 1518.5332 1532.9021 3043.5691 3074.9584 3079.7796 3129.4703 3167.6887 3171.7566 3182.0786 3186.9557 3211.2198 3840.5029 3846.7610

$O_2C(C)CCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.07747300	-0.72167500	0.88454900
C	-1.35607500	-0.03490900	0.39262500
C	0.81677500	-1.16529400	-0.27364600
O	2.19150300	-0.69529000	-0.10182300
O	2.26590500	0.58853500	-0.16121300
O	-1.05260500	1.00582600	-0.52856400
O	-0.31032700	2.01729000	0.19106000
H	-1.87679400	0.39934100	1.25505900
H	0.47654800	-0.75214400	-1.22425500
H	0.93469300	-2.24623700	-0.34999800
H	0.59334900	1.75719600	-0.04947100

H	0.47710100	-0.01157000	1.50121800
H	-0.34481500	-1.56914500	1.52306600
C	-2.28975200	-0.96471400	-0.36788200
H	-2.61407100	-1.77798500	0.28732800
H	-3.16877000	-0.41457000	-0.71013600
H	-1.79389900	-1.39621800	-1.24237100

Absolute energies (Hartree): -457.978456 ZPE (Hartree): 0.140332

Harmonic Vibrational Frequencies (cm^{-1}):

87.6617 118.9713 144.1526 197.1746 213.3202 274.4056 291.8076 318.6685 391.0780 501.5630 547.6740 571.4501 638.9655 786.8132 851.3692 912.1634 938.1749 974.5735 1013.9799 1040.9666 1122.4643 1148.6735 1214.7747 1269.7433 1302.4763 1331.0094 1359.6288 1379.9833 1399.2310 1429.1286 1439.6721 1451.1392 1499.7833 1504.8126 1516.1572 1524.8645 3082.3754 3085.9273 3111.1194 3133.4952 3172.2944 3173.2103 3186.0430 3209.0507 3736.8491

TS_{23}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.97087100	0.54506200	-0.24115600
H	-2.15285800	0.96576300	0.75308500
H	-2.78133200	0.81630200	-0.92154600
C	-0.60395500	0.98113100	-0.79462400
H	-0.52126400	0.63634400	-1.82893200
H	-0.52829400	2.07496600	-0.77745900
C	0.51300300	0.35181900	0.01577900
H	-0.07885900	-0.62465200	0.51202700
O	-1.98242700	-0.87122600	-0.16098600
O	-1.14664000	-1.20940400	0.88526900
O	1.47599400	-0.09827800	-0.89552400
O	2.46013500	-0.87036300	-0.16590700
H	2.14299100	-1.75858000	-0.37593600
C	1.04946200	1.15585500	1.17874700
H	1.75657900	0.56862100	1.76471000
H	1.55879000	2.04757000	0.79594700
H	0.22191200	1.46462500	1.82281800

Absolute energies (Hartree): -457.942695 ZPE (Hartree): 0.133808

Harmonic Vibrational Frequencies (cm^{-1}):

-2253.5273 64.3670 128.3644 152.5681 217.0769 256.3911 285.3901 306.1890 375.1924 427.0381 469.8686 527.3419 549.6857 654.2894 830.4531 891.8651 896.5682 959.9507 989.2162 1020.9102 1040.8067 1133.0343 1174.6836 1215.9619 1240.0455 1268.3129 1298.5976 1362.7151 1369.9894 1390.3915 1405.7341 1417.3961 1479.6085 1494.7440 1501.8497 1516.4724 1643.3509 3074.9275 3084.0220 3095.9439 3158.2380 3167.4456 3178.3462 3202.5595 3816.8977

$O_2C•(C)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.67200800	0.10153200	-0.40312500
H	-4.00297400	-0.76994500	-0.64965100
O	-2.55054000	-0.29664300	0.42083400
C	1.09082700	0.14017500	-0.00952400
O	2.02218200	-0.85916100	0.18359100
O	3.22422500	-0.54699200	-0.55992100
H	3.84266400	-0.47710200	0.17700600
C	-1.38258400	0.05836000	-0.30292800
H	-1.40256700	1.12951600	-0.53221300
H	-1.32470400	-0.50513200	-1.24169700
C	-0.20819000	-0.28972100	0.60552600
H	-0.18605700	-1.37036800	0.77225300
H	-0.36073600	0.20076700	1.57764800
C	1.54585600	1.56100700	0.09902800
H	0.69631100	2.23109100	-0.04954700
H	1.95877500	1.75647600	1.10187200
H	2.31295900	1.79588600	-0.63931900

Absolute energies (Hartree): -457.956858 ZPE (Hartree): 0.136871

Harmonic Vibrational Frequencies (cm^{-1}):

42.0985 82.7868 98.7752 133.0030 154.4120 192.2815 208.5292 212.4439 288.8172 314.2013 350.2264 385.3369 503.8296 580.4299 810.7220 843.8131 922.3581 983.7974 1001.6376 1048.6811 1081.1930 1110.0515 1127.0384 1231.5310 1259.3599 1298.5327 1326.3147 1354.3292 1371.8399 1399.2994 1425.7016 1432.8831 1490.7446 1499.2991 1512.8486 1547.9542 3022.4443 3052.4121 3071.2531 3125.5488 3146.7810 3152.6586 3197.7130 3841.5290 3842.0568

$O_2C(C)CC(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.00682800	0.38749000	0.94981200
C	1.43866800	0.40921600	0.40418900
C	-1.04010500	0.45588900	-0.16354800
O	-2.01696400	-0.63916100	-0.01110700
O	-1.48194800	-1.79912700	-0.16386400
O	1.62546300	-0.60165100	-0.57975100
O	1.46296100	-1.88054700	0.07541100
H	2.13325800	0.22548300	1.23361400
H	-0.57338200	0.27023000	-1.13369700
H	0.53130400	-2.05268800	-0.13687900
H	-0.12902300	-0.53943200	1.51060800
H	-0.12454900	1.21688000	1.65393700
C	1.80291700	1.70495800	-0.30522600

H	1.70568200	2.54635400	0.38678400
H	2.83388400	1.65822600	-0.66254100
H	1.15153400	1.88043100	-1.16632700
C	-1.87692100	1.71763300	-0.17415000
H	-2.60754700	1.69811000	-0.98632300
H	-2.40423900	1.82750100	0.77768600
H	-1.22134800	2.58167000	-0.30884200

Absolute energies (Hartree): -497.240057 ZPE (Hartree): 0.168444

Harmonic Vibrational Frequencies (cm^{-1}):

75.3886 115.2511 125.9551 184.5891 210.5345 226.2609 241.5353 267.7869 321.1844 334.0607 391.6005 456.2108 502.8363 550.9176 578.0092 636.6125 834.7814 855.4350 875.0931 908.1582 942.1465 982.4350 1039.8651 1057.0227 1138.7540 1174.6810 1187.3057 1215.8852 1264.2087 1323.3274 1350.3095 1371.1068 1385.8603 1407.8017 1419.0431 1430.0679 1436.2596 1453.8897 1498.3147 1502.2079 1508.9669 1520.2781 1527.0206 3081.0729 3082.2700 3084.0085 3098.0383 3141.5815 3167.9197 3172.6635 3180.5281 3184.0657 3186.1273 3730.9580

TS_{24}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.66681700	-0.18233500	0.20229700
H	1.71640500	-0.28509200	1.29303700
C	0.45578000	-0.96379200	-0.34374800
H	0.49168400	-0.92262200	-1.43704100
H	0.52299800	-2.01134300	-0.02563700
C	-0.84683400	-0.34547500	0.12509300
H	-0.47096700	0.80175200	0.42010000
O	1.44871700	1.19330100	-0.09984300
O	0.43763500	1.63839500	0.72756300
O	-1.69335000	-0.28064000	-0.98947200
O	-2.86329400	0.48970500	-0.62116000
H	-2.61063400	1.34139500	-1.00137100
C	-1.46928300	-0.92584800	1.37509300
H	-2.33224800	-0.33828900	1.68907400
H	-1.79270700	-1.95352000	1.17364500
H	-0.73009200	-0.93441200	2.18062900
C	2.97379300	-0.57982000	-0.45419700
H	3.80295700	-0.01134600	-0.02742200
H	3.15825800	-1.64645200	-0.30043000
H	2.92506000	-0.38255600	-1.52851700

Absolute energies (Hartree): -497.204191 ZPE (Hartree): 0.161711

Harmonic Vibrational Frequencies (cm^{-1}):

-2244.3005 52.0021 96.1556 133.1931 208.9844 215.0160 254.9636 261.1271 285.2996 310.5703 333.4731 373.0656 452.8170 487.3786 545.0407 563.8869 651.1652 859.1519 877.9186 890.1695 920.1494 946.6481

984.1911 1045.8111 1106.6962 1147.4509 1174.6844 1190.1017 1222.2632 1243.1123 1281.7287 1316.1337 1366.7648 1382.3224 1387.4215 1394.1586 1415.0943 1428.2061 1476.1296 1494.4382 1504.8682 1515.9209 1521.0367 1640.9303 3073.4759 3077.2619 3084.6614 3091.2261 3150.4165 3165.9053 3179.1922 3186.3278 3201.1716 3815.5016

O_2C•(C)CC(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.50967700	0.13508500	0.35922200
H	3.89556400	-0.56214600	-0.18360000
O	2.37519200	0.48419100	-0.47208900
C	-1.27692000	0.45691000	0.03842300
O	-1.84847800	-0.64104600	-0.57278700
O	-2.95279600	-1.11364100	0.23170900
H	-3.65136600	-1.06899600	-0.43192800
C	1.19924600	0.05795100	0.21935300
H	1.22074000	0.48361100	1.23066600
C	0.06495400	0.70674800	-0.58000000
H	0.08648000	0.30794500	-1.60339500
H	0.25519500	1.78340200	-0.63580700
C	-2.16920400	1.57352200	0.47422100
H	-1.58440200	2.31716000	1.02013400
H	-2.62602500	2.07211800	-0.39604200
H	-2.96958100	1.21103800	1.12013600
C	1.09727200	-1.45648000	0.28434400
H	1.10309900	-1.86994300	-0.72930600
H	1.93981400	-1.86538800	0.84642500
H	0.16963500	-1.75741800	0.77622400

Absolute energies (Hartree): -497.218069 ZPE (Hartree): 0.165459

Harmonic Vibrational Frequencies (cm^{-1}):

44.0167 56.6695 81.4541 128.4855 147.7071 195.3536 213.2128 239.4719 277.9028 279.8350 302.0129 325.1721 369.4824 403.3657 467.1135 534.5704 581.8593 835.4285 856.6346 900.9444 917.7829 964.2380 991.4436 1049.9191 1055.1718 1138.3527 1173.2545 1183.5133 1245.4892 1271.9240 1329.2429 1342.6212 1368.7161 1392.0082 1396.6596 1405.1775 1427.8375 1435.1295 1487.9704 1492.7052 1503.1135 1512.2512 1526.0194 3019.4399 3062.8872 3079.5819 3083.9561 3140.6346 3145.2051 3174.2982 3187.8792 3197.0014 3842.8355 3843.2477

O_2C(C)C(C)COO•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.11472100	0.68405300	-0.44954500
C	-1.31121200	-0.24638600	-0.20334600
C	0.77830400	0.75098100	0.79043700

O	2.18865400	0.60808400	0.43141000
O	2.44197100	-0.58131300	0.00420100
O	-0.87308900	-1.51629600	0.27397100
O	-0.06724700	-2.12390700	-0.76269500
H	-1.83638000	-0.39300000	-1.15690500
H	0.56262100	-0.05572800	1.49232500
H	0.74311900	1.71793400	1.29642400
H	0.81922600	-1.87897600	-0.45256100
H	0.47340100	0.20196100	-1.23507800
C	-2.28403200	0.24007400	0.86052400
H	-2.77739900	1.15798800	0.53273500
H	-3.04674200	-0.52262000	1.03265300
H	-1.77338100	0.43451700	1.80852500
C	-0.53231600	2.06812800	-0.94400600
H	0.34854500	2.65074300	-1.23037300
H	-1.18483700	1.98872800	-1.81926600
H	-1.06662200	2.62480300	-0.16795900

Absolute energies (Hartree): -497.234776 ZPE (Hartree): 0.168715

Harmonic Vibrational Frequencies (cm^{-1}):

67.4912 99.5989 142.8651 178.8727 198.4606 228.1707 250.3993 278.0594 291.0234 314.9894 389.4211 454.9710 542.7268 549.0705 554.3609 642.3218 822.2239 891.5186 911.4751 922.6541 965.3257 996.1852 1022.6850 1056.7969 1142.6308 1180.2362 1191.0397 1239.8596 1283.4591 1325.9501 1353.4896 1354.3251 1380.7124 1400.7342 1425.9515 1430.6852 1441.5937 1446.1610 1504.3886 1510.8161 1518.0357 1521.7500 1527.8311 3069.4751 3072.8078 3084.8604 3122.9804 3130.0580 3161.0354 3162.4356 3175.2725 3187.9261 3198.8318 3740.3563

TS_{25}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.93199400	-0.00357500	-0.04762600
H	-2.10250100	0.09907000	1.03067600
H	-2.80847100	0.34169300	-0.60287000
C	-0.67120700	0.75955700	-0.48675800
H	-0.58742300	0.62076500	-1.57101200
C	0.55200200	0.09039600	0.12242100
H	0.13310100	-1.07389100	0.26527300
O	-1.77509700	-1.37352400	-0.37816900
O	-0.82847900	-1.88183500	0.49009400
O	1.55379700	0.13285900	-0.85530900
O	2.68854200	-0.63518800	-0.38478400
H	2.53294100	-1.45219700	-0.87652900
C	0.98511400	0.52334000	1.50541300
H	1.77551600	-0.13000900	1.87526400

H	1.36521200	1.54987600	1.47290400
H	0.13652200	0.47438200	2.19248200
C	-0.78511300	2.25359300	-0.17164200
H	0.12475900	2.77846900	-0.47480500
H	-1.62906400	2.69053800	-0.71423600
H	-0.94350800	2.42295400	0.89735400

Absolute energies (Hartree): -497.199011 ZPE (Hartree): 0.162352

Harmonic Vibrational Frequencies (cm^{-1}):

-2281.7748 66.0031 120.9946 155.8360 213.0103 235.4838 251.8510 255.7663 274.3216 301.1115 323.0579 419.8733 455.5898 477.6262 554.4220 564.2400 667.7902 819.7901 885.0170 930.1395 958.9321 971.4546 1014.0610 1060.8963 1073.2351 1151.5989 1161.9238 1176.3254 1217.0257 1265.6994 1300.3213 1322.0797 1374.6754 1381.4517 1397.9265 1400.0018 1422.2892 1423.7161 1490.3276 1496.8517 1511.7763 1521.4695 1527.1868 1641.2449 3074.4624 3078.9826 3081.9494 3100.9595 3162.3760 3166.6064 3172.3442 3173.5642 3201.0714 3817.5298

O_2C•(C)C(C)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.61370500	0.56867000	-0.38877300
H	-3.99503800	-0.18951700	-0.84697300
O	-2.53123000	-0.09398100	0.30630500
C	1.10785900	0.31612100	-0.00813900
O	2.11866300	-0.62061900	-0.03728500
O	3.27615200	-0.04998400	-0.68967300
H	3.89629000	-0.07972200	0.04870600
C	-1.33397800	0.32985700	-0.33004900
H	-1.27550000	1.42254800	-0.29919900
H	-1.31847200	-0.00014700	-1.37730200
C	-0.18363800	-0.32204200	0.44006500
H	-0.34103900	-0.08295800	1.50533300
C	1.46613200	1.69058500	0.46821300
H	0.57323300	2.31605600	0.51947700
H	1.90017800	1.63808900	1.47957800
H	2.19218800	2.16874700	-0.19038500
C	-0.21504000	-1.84276100	0.26236400
H	-0.04130100	-2.10363700	-0.78570500
H	0.55543400	-2.32935500	0.86291600
H	-1.19301900	-2.22334000	0.56423700

Absolute energies (Hartree): -497.211829 ZPE (Hartree): 0.16564

Harmonic Vibrational Frequencies (cm^{-1}):

42.2541 88.5675 89.5086 120.0785 143.8092 184.9661 208.9790 215.8244 242.9591 274.4479 299.2291 325.1626 363.5968 391.8814 454.6343 521.7485 596.8028 809.8336 916.7358 924.5753 951.6861 980.4920 1020.2548 1069.3404 1099.9973 1131.8378 1166.0874 1184.4198 1257.9203 1274.6005 1295.1527 1331.6175 1371.0863

1381.0027 1401.4555 1413.6195 1420.2827 1435.4549 1492.6042 1511.4378 1517.3468 1523.3905 1540.2966 3018.9544 3025.3980 3061.8243 3087.1279 3131.2345 3150.6574 3177.2997 3191.3277 3198.4400 3837.9789 3840.1975

$O_2C(CC)CCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.39928400	-0.70444400	0.94608300
C	-0.89376200	0.02292900	0.56314100
C	1.17059300	-1.18719700	-0.28267800
O	2.56973700	-0.76006000	-0.24123600
O	2.67833100	0.52053400	-0.31362800
O	-0.63634500	1.04192200	-0.39536200
O	0.19195000	2.04106300	0.24346500
H	-1.32139900	0.48593400	1.46298500
H	0.75903400	-0.77200400	-1.20361000
H	1.24707000	-2.27209300	-0.35619000
H	1.06467500	1.74619800	-0.06293800
H	1.03082800	-0.00968500	1.50381700
H	0.16041100	-1.53717700	1.61471500
C	-1.93422700	-0.88319800	-0.08709400
H	-2.11496100	-1.71831300	0.60029500
H	-1.51964200	-1.30914000	-1.00915800
C	-3.24425800	-0.15601000	-0.39093100
H	-3.07458200	0.66342100	-1.09118100
H	-3.97902600	-0.84117800	-0.82262000
H	-3.66756900	0.26387600	0.52685700

Absolute energies (Hartree): -497.232542 ZPE (Hartree): 0.169159

Harmonic Vibrational Frequencies (cm^{-1}):

70.9072 94.3252 104.6358 141.6613 167.9312 215.6591 258.2523 278.8551 284.4313 346.2336 420.5472 503.3367 544.3156 571.7024 666.8421 772.9038 796.1198 868.3901 911.3285 954.0234 989.2824 1013.6170 1051.2884 1076.8778 1119.3786 1155.7737 1204.4301 1263.8947 1300.0041 1318.9797 1324.3861 1343.1980 1359.8323 1399.0844 1417.9886 1430.2755 1439.1507 1451.3340 1492.8654 1502.1886 1515.7097 1517.1347 1528.7630 3068.3010 3074.6689 3081.2638 3109.3188 3125.6792 3134.7245 3165.1836 3170.5686 3190.8829 3209.4322 3734.1548

TS_{26}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.02406200	-0.91682200	-0.31084100
H	1.98791400	-1.53328900	0.59324500
H	2.75977800	-1.31604800	-1.01292100
C	0.63630600	-0.79528400	-0.96293000

H	0.74466700	-0.28431200	-1.92366300
H	0.22447000	-1.79538100	-1.14072500
C	-0.28666000	0.02315300	-0.07930400
H	0.53811300	0.65244400	0.60505400
O	2.47011500	0.38648400	0.02738700
O	1.70592300	0.79285300	1.10279900
O	-0.97095300	0.91102500	-0.91935400
O	-1.75673900	1.79787500	-0.08649900
H	-1.16305400	2.56035300	-0.06805200
C	-1.15461400	-0.73458700	0.90921800
H	-1.52085300	-0.04131600	1.67016800
H	-0.51310700	-1.46526000	1.41473700
C	-2.33985200	-1.42476600	0.22658500
H	-2.00453700	-2.12612800	-0.54314600
H	-2.92779100	-1.98332400	0.96008100
H	-2.98781700	-0.68379900	-0.24580900

Absolute energies (Hartree): -497.197564 ZPE (Hartree): 0.162988

Harmonic Vibrational Frequencies (cm^{-1}):

-2241.7782 59.3616 86.7976 134.2452 138.5141 210.3077 250.3327 284.6549 291.3934 315.4512 384.2702 434.5455 486.9485 536.2047 592.0003 693.5852 796.2193 810.0863 898.9292 912.9159 971.6390 1008.8716 1017.6379 1041.9469 1052.8899 1117.4848 1175.0669 1207.8245 1229.5145 1257.4564 1295.9741 1321.9796 1366.3244 1366.9169 1380.4398 1391.0220 1407.5367 1426.4310 1480.8124 1496.5336 1502.8645 1518.1878 1524.9586 1645.2006 3081.7680 3088.2192 3094.6620 3097.5663 3153.9014 3157.7906 3169.6007 3177.4846 3187.0997 3813.2372

O_2C•(CC)CCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.78204700	-0.01514300	-0.51190600
H	-4.14772000	-0.81403700	-0.11456000
O	-2.70915900	0.24467700	0.42369700
C	0.96172400	-0.07440300	0.14889500
O	1.12098400	-1.43636200	0.30702800
O	2.19181500	-1.89712400	-0.54651100
H	2.72275700	-2.35561400	0.11558100
C	-1.50195600	-0.05884100	-0.25946700
H	-1.43137100	0.53373100	-1.17769500
H	-1.45964500	-1.12437900	-0.51236900
C	-0.37742900	0.30228900	0.70548700
H	-0.54724800	-0.22200300	1.65721500
H	-0.40511600	1.37604000	0.90845600
C	2.15407000	0.82139100	0.29907000
H	2.30454300	1.04452000	1.36902300

H	3.03894200	0.28562700	-0.04973200
C	2.00474000	2.13016600	-0.48235400
H	1.90082700	1.92423600	-1.55077200
H	1.12406000	2.69139300	-0.15789000
H	2.88033100	2.76848600	-0.33550700

Absolute energies (Hartree): -497.210885 ZPE (Hartree): 0.166325

Harmonic Vibrational Frequencies (cm^{-1}):

30.9486 65.3611 72.4947 87.2534 121.2049 181.1198 208.2864 214.4507 217.3028 243.1549 296.6156 325.4356 374.3541 460.3989 503.9300 580.7649 792.7371 804.4291 829.1656 922.4830 996.2989 1020.8526 1077.0213 1085.9342 1096.5296 1125.7215 1187.8704 1235.3441 1257.1671 1280.2673 1311.4653 1320.5734 1355.9249 1371.3339 1385.3261 1419.9932 1430.0002 1437.1041 1491.6004 1494.9034 1522.1734 1525.5501 1551.4409 3010.5559 3052.9438 3076.5707 3080.0144 3133.9342 3154.2441 3157.7786 3170.8831 3175.9208 3839.9773 3843.0180

$O_2C(C)C(C)C(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.00980600	-0.37040600	0.69169700
C	-1.45394400	-0.32246900	0.16786100
C	0.98743500	-0.18305100	-0.46105600
O	2.02076500	0.79036700	-0.05438000
O	1.53535400	1.97541400	0.08209300
O	-1.67974300	0.86732900	-0.58550000
O	-1.51136200	1.99621400	0.30324100
H	-2.12908500	-0.32039300	1.03457400
H	0.48045900	0.29783500	-1.30073300
H	-0.58841700	2.22671700	0.10954200
H	0.08390100	0.51874900	1.32096400
C	-1.83486500	-1.44254200	-0.78830700
H	-1.72476300	-2.41466400	-0.30142300
H	-2.87598900	-1.32269800	-1.09632900
H	-1.21059100	-1.42231100	-1.68607400
C	1.76719600	-1.39822600	-0.91993000
H	2.43062000	-1.12461000	-1.74406500
H	2.36981000	-1.80805200	-0.10622900
H	1.07961900	-2.17246000	-1.26826300
C	0.24901700	-1.58632400	1.57991000
H	1.22938100	-1.51661100	2.06048000
H	-0.50630800	-1.63237800	2.37100600
H	0.21105300	-2.52560400	1.02186500

Absolute energies (Hartree): -536.494904 ZPE (Hartree): 0.197075

Harmonic Vibrational Frequencies (cm^{-1}):

69.9646 89.1408 137.6027 169.6549 215.1076 224.0301 235.3187 248.5948 261.7872 287.7089 300.5562

316.3236 354.2449 466.4884 488.9862 543.0129 556.0268 581.9449 640.8760 789.3490 853.9694 876.9066 906.3673 963.1138 999.3968 1028.4293 1036.9881 1066.2055 1148.3794 1159.1848 1189.1598 1207.1677 1234.2402 1325.4205 1343.8120 1354.5175 1377.3621 1387.7000 1407.2065 1416.1250 1429.4870 1431.4239 1443.8940 1446.8068 1500.8791 1504.1109 1513.5699 1523.8272 1526.6319 1534.1626 3069.0786 3074.6872 3085.8743 3090.8016 3127.9599 3140.7976 3159.1566 3169.4567 3177.3932 3184.5731 3185.8928 3190.7415 3736.1345

TS_{27}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.59925400	-0.18077800	0.19346800
H	-1.61163700	-0.15012900	1.29133400
C	-0.43835700	0.68251000	-0.34281300
H	-0.45570100	0.56305800	-1.43377300
C	0.88718800	0.09905100	0.12598500
H	0.58506000	-1.09918100	0.25665600
O	-1.34576000	-1.52595600	-0.20984500
O	-0.28114400	-1.99066200	0.53657200
O	1.78592200	0.26443400	-0.93611900
O	3.02370700	-0.41097700	-0.60200400
H	2.89119300	-1.22657100	-1.10278900
C	1.41016900	0.52262100	1.48082300
H	2.28045600	-0.07483300	1.75334800
H	1.70395100	1.57726500	1.45590300
H	0.63447200	0.38203200	2.23784700
C	-2.95272800	0.19052000	-0.38188700
H	-3.70116200	-0.53533000	-0.05567900
H	-3.25703100	1.18201200	-0.03937800
H	-2.91191200	0.18890600	-1.47494400
C	-0.59461800	2.16556600	0.01053800
H	-1.45520300	2.59798300	-0.50588000
H	-0.73521400	2.30245700	1.08733000
H	0.29653500	2.72067000	-0.29549800

Absolute energies (Hartree): -536.459912 ZPE (Hartree): 0.190315

Harmonic Vibrational Frequencies (cm^{-1}):

-2273.5206 62.3288 91.1539 137.3822 186.0576 213.2396 224.7198 253.6242 254.5262 274.5573 284.5120 308.8293 321.5605 344.3638 447.8418 472.6572 484.5659 551.8017 617.8128 653.0182 834.8651 860.1024 903.1589 921.8132 956.0347 985.3006 1050.8523 1072.7839 1116.1684 1151.5914 1162.6383 1179.0189 1187.2469 1218.9662 1272.2935 1307.6054 1355.5393 1369.0224 1376.8484 1385.3138 1396.3798 1420.0998 1421.6235 1426.3148 1489.6049 1505.4819 1510.9222 1516.4826 1523.6138 1530.7123 1642.4424 3072.8410 3075.3641 3081.3462 3085.3625 3090.6855 3167.1917 3171.8587 3173.2742 3179.7604 3188.4444 3200.0739 3817.1552

$O_2C•(C)C(C)C(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.42009400	-0.39554600	-0.33676200
H	3.61476100	0.10168600	-1.14002000
O	2.35035900	0.42798300	0.18881100
C	-1.31356100	0.11723800	0.37801200
O	-1.55226000	-0.52437900	-0.82293100
O	-2.73004100	-1.35456000	-0.69828500
H	-3.28562700	-0.93083100	-1.36350600
C	1.12637800	-0.28537500	-0.01510300
H	1.05596700	-0.55901900	-1.07612100
C	0.04613600	0.75291700	0.31820000
H	0.26574900	1.12422300	1.32822800
C	-2.46066100	0.81252000	1.03966400
H	-2.11667200	1.28159500	1.96423700
H	-2.87844000	1.59860900	0.39067600
H	-3.26194400	0.11119700	1.27737200
C	0.07978800	1.93751100	-0.66569500
H	-0.14155400	1.58589400	-1.67798600
H	-0.66607900	2.69006300	-0.39249500
H	1.06507200	2.40790400	-0.66124500
C	1.06721700	-1.52651600	0.85866600
H	1.06639700	-1.23709900	1.91403700
H	0.16349300	-2.10136800	0.64380600
H	1.94188500	-2.15060300	0.66388800

Absolute energies (Hartree): -536.474609 ZPE (Hartree): 0.193565

Harmonic Vibrational Frequencies (cm^{-1}):

57.8048 61.0750 81.4678 118.7808 151.7531 168.1314 203.5699 212.7442 218.4109 222.3989 247.5297 270.5205 279.9730 325.6430 358.3127 396.1041 464.9154 517.9080 558.1794 625.2944 801.4424 867.8054 902.8457 940.4655 960.2401 993.4586 1038.0908 1043.6637 1083.3836 1125.6813 1141.0991 1173.8434 1197.3901 1237.6390 1299.6703 1311.4217 1356.4631 1362.1769 1391.0446 1398.5464 1404.3413 1408.6136 1424.3718 1429.8707 1489.8584 1502.9230 1509.6126 1517.5979 1522.0009 1523.9256 3024.1246 3072.0966 3076.4470 3082.4092 3086.3242 3142.6687 3164.0464 3176.9975 3183.6523 3189.9302 3191.9338 3834.9285 3839.5716

TS_{28}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.83461500	-0.57015200	-0.23327500
H	2.56849700	-1.09297300	-1.00061900
O	1.84742700	0.48378900	-0.30686600
C	0.89931500	0.22362000	0.67771800
H	1.35574900	0.03562200	1.65549300

H	0.29054400	-0.82398900	0.37201700
C	-0.16194200	1.30366300	0.61030000
H	-0.75505800	1.26938400	1.52898800
H	0.34267100	2.27615600	0.57408900
C	-1.05975800	1.11783800	-0.62409800
H	-0.43153200	0.81868700	-1.46634600
H	-1.53584300	2.06573300	-0.89530200
C	-2.16256700	0.08015700	-0.39604500
H	-3.00323600	0.51562800	0.15296100
H	-2.52224300	-0.33161600	-1.34539500
O	-1.74264200	-0.98301800	0.46359500
O	-0.61438000	-1.56615600	-0.07134700

Absolute energies (Hartree): -457.935433 ZPE (Hartree): 0.134638

Harmonic Vibrational Frequencies (cm^{-1}):

-2499.4036 79.4506 111.3021 159.9535 217.0443 256.5784 291.4172 308.9753 365.2446 427.1636 530.1052 600.7987 704.8536 818.7413 860.4794 881.3859 937.3641 974.1859 1008.2015 1076.7527 1088.3188 1128.1008 1181.8177 1197.7554 1253.0602 1266.3145 1316.5118 1324.7252 1363.6177 1385.5040 1399.2973 1406.0478 1419.4128 1482.4464 1503.5046 1515.3060 1579.1346 3083.2914 3085.7759 3103.1855 3117.0344 3146.5568 3152.1295 3168.0044 3822.2252

$O_2CCC(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.50140500	-1.76179400	0.29232900
H	-1.19394500	-2.30416400	0.94525000
C	0.30291800	-0.75464600	1.10866600
H	0.78857100	-1.31110600	1.92107700
H	-0.38460300	-0.05028400	1.58717500
C	1.39771500	0.00743500	0.34354600
H	2.00983900	0.53300200	1.08863700
C	0.86232600	1.07808000	-0.60077400
H	0.12555300	0.69052800	-1.30367900
H	1.68214700	1.57169400	-1.12942200
O	-1.23215400	-1.18375500	-0.78098400
O	-2.34209600	-0.47397600	-0.18365300
H	-1.99076900	0.43146100	-0.18474100
O	0.23524700	2.15694400	0.15617700
O	-1.04896900	2.06727400	0.20013400
H	0.15128300	-2.48738700	-0.20298600
C	2.31550600	-0.92350600	-0.45679500
H	3.19427700	-0.38261100	-0.82108800
H	2.66244600	-1.75207200	0.16797800

H	1.79661300	-1.34436700	-1.32343500

Absolute energies (Hartree): -497.231507 ZPE (Hartree): 0.169727

Harmonic Vibrational Frequencies (cm^{-1}):

64.3341 81.6999 148.1931 166.2952 202.2657 229.9424 261.2623 277.6254 354.3952 371.5825 435.3580 487.8802 562.7567 578.1885 596.6113 788.2263 832.4205 895.1989 917.7569 945.7178 983.8872 1012.9400 1026.1962 1081.3432 1142.3112 1173.1769 1206.6477 1258.4354 1283.5210 1321.3136 1334.9832 1369.6507 1400.7957 1409.0089 1423.2654 1432.4962 1436.2417 1470.9550 1490.4416 1502.1244 1512.9712 1518.9531 1531.6103 3070.1242 3071.2173 3080.1004 3090.1862 3119.2303 3139.7042 3154.5245 3162.0189 3164.9202 3211.3229 3717.0192

TS_{29}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.12401100	-0.20533300	-0.39759600
H	-2.95761500	0.21026900	-1.25351900
O	-1.85662100	-0.87472200	-0.20546600
C	-1.13694900	-0.12828800	0.72270300
H	-1.72345300	0.09832700	1.61967800
H	-0.85065500	0.97416900	0.20957000
C	0.20470600	-0.80107300	0.92873900
H	0.66969300	-0.39813900	1.83462700
H	0.02769300	-1.87205200	1.09186200
C	1.12877300	-0.60384900	-0.28530400
H	0.50280700	-0.64617600	-1.18230800
C	1.82024600	0.76374300	-0.24256600
H	2.69395400	0.72692700	0.41833000
H	2.13554400	1.07313900	-1.24632200
O	1.01523200	1.78540700	0.34848500
O	-0.17341300	1.86894200	-0.34455600
C	2.18903700	-1.70091800	-0.37544200
H	1.72437800	-2.67699500	-0.54245500
H	2.88561000	-1.51061700	-1.19889400
H	2.76767400	-1.75089900	0.55370700

Absolute energies (Hartree): -497.19243 ZPE (Hartree): 0.162905

Harmonic Vibrational Frequencies (cm^{-1}):

-2493.6611 80.4053 105.0909 117.5335 171.6076 253.4064 260.4851 287.4286 300.4389 319.1916 350.7913 403.9932 416.8199 560.0768 618.2211 704.2059 830.0866 846.9131 921.9002 943.1820 965.2040 1005.1432 1031.0924 1069.1570 1120.0546 1142.5048 1186.3917 1198.4149 1213.6319 1265.4730 1312.5235 1324.3005 1328.6443 1355.7339 1383.8529 1400.1255 1410.4567 1423.9960 1427.9815 1477.2852 1500.6796 1518.3658 1521.4411 1583.0708 3063.0840 3070.5939 3072.4977 3109.2399 3115.5958 3139.5834 3142.7692 3151.9391 3162.4767 3821.8911

$O_2C•CC(C)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.67939900	-0.92887700	-0.29008800
H	3.50033500	-1.86812900	-0.41615200
O	2.34421100	-0.40692500	-0.49233500
C	-1.87312500	0.18648000	-0.00989700
H	-2.14467400	1.01308700	-0.66041700
O	-2.79832200	-0.82197100	0.04580700
O	-4.11180700	-0.21445800	-0.05489300
H	-4.47560700	-0.78108400	-0.74540600
C	1.89969600	0.05678100	0.77407900
H	2.61223700	0.79287500	1.16574800
H	1.83027600	-0.78453600	1.47778800
C	-0.48139800	-0.35215400	0.06825300
H	-0.48806100	-1.20202500	0.76203000
H	-0.15152000	-0.73867200	-0.90766400
C	0.53202300	0.69529600	0.55564700
H	0.20306900	1.04750200	1.54238500
C	0.62798600	1.89615500	-0.38946400
H	0.87607200	1.56821400	-1.40242700
H	-0.31302000	2.45171600	-0.41952200
H	1.41195300	2.58355200	-0.05601200

Absolute energies (Hartree): -497.206224 ZPE (Hartree): 0.165295

Harmonic Vibrational Frequencies (cm^{-1}):

52.7381 54.4134 75.6926 112.6258 129.7531 166.4857 189.9337 206.3858 213.1505 242.0383 306.5381 322.2471 387.8678 455.8319 510.1127 626.3253 693.0954 847.1788 897.8281 918.0279 927.1999 988.9830 998.1781 1026.7074 1097.0119 1133.9372 1164.4269 1192.0628 1204.1629 1260.8000 1274.3622 1295.3741 1361.8074 1376.0103 1382.9631 1406.3802 1413.0306 1426.0888 1438.5848 1494.8732 1518.0463 1520.8884 1543.8002 3040.5266 3047.3674 3076.8042 3080.6921 3109.0087 3112.0919 3162.0861 3176.1339 3210.9983 3839.0803 3847.3573

$O_2CCC(C)C(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.79882200	1.09485700	0.09335900
H	1.65253200	2.05939400	-0.40275900
H	2.77670900	1.10166300	0.58737300
C	0.70109100	0.82223000	1.11771800
H	0.80813500	1.57334600	1.91153000
H	0.88175500	-0.14915700	1.58729600
C	-0.74330300	0.90386700	0.59068500
H	-1.40935200	0.88788300	1.46557500
C	-1.14712800	-0.30153600	-0.26065300

H	-0.42222900	-0.48720900	-1.05421500
O	1.83101700	0.16860000	-0.98402000
O	2.35986600	-1.06605400	-0.44615900
H	1.53646900	-1.56207900	-0.30523100
O	-1.10983800	-1.48606800	0.61602600
O	-0.10404700	-2.25953300	0.40054300
C	-2.56761500	-0.25477900	-0.79366000
H	-2.65816600	0.51741100	-1.56024700
H	-2.82573300	-1.21711200	-1.24212700
H	-3.27516100	-0.03930000	0.01256400
C	-0.99451000	2.20710900	-0.17808500
H	-2.06299200	2.39726700	-0.30416400
H	-0.56732100	3.05386300	0.36833900
H	-0.53476800	2.17798400	-1.17123300

Absolute energies (Hartree): -536.491518 ZPE (Hartree): 0.197983

Harmonic Vibrational Frequencies (cm^{-1}):

61.8930 76.2937 109.6486 158.3230 187.4003 215.5583 226.8798 274.0786 291.4672 329.5231 360.1127 378.4853 417.3962 446.0396 497.9760 550.6342 578.6147 608.1855 794.5627 847.8490 863.2715 903.1402 910.3684 976.8173 1003.9215 1020.4420 1069.0978 1096.8916 1149.9861 1160.2406 1174.7595 1208.8566 1276.4270 1296.1973 1327.2014 1350.6363 1383.9296 1399.4446 1404.6434 1414.9311 1428.4553 1430.1359 1433.5863 1473.2927 1490.3018 1503.8122 1506.7136 1515.5040 1525.0094 1534.1706 3058.2917 3072.4949 3076.7930 3084.0807 3089.3473 3142.8808 3155.7622 3159.4509 3166.2792 3172.1368 3182.7702 3191.4838 3709.8102

TS_{30}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.42998400	-0.16537300	-0.33580500
H	4.12862200	0.42768200	-0.03408600
O	2.28643100	0.68932200	-0.07693800
C	1.41665100	-0.04583000	0.71944100
H	1.90227900	-0.43676400	1.62132200
H	1.02434400	-1.05185500	0.08047500
C	0.15630300	0.77380800	0.90862900
H	-0.39862600	0.37632700	1.76367400
H	0.44893700	1.80307000	1.15484000
C	-0.70863400	0.76515800	-0.36655800
H	-0.02091700	0.69227000	-1.21502400
C	-1.61768200	-0.47664700	-0.41388100
H	-1.88543900	-0.68446100	-1.45881500
O	-0.93347700	-1.62721200	0.11433400
O	0.26137900	-1.80575400	-0.54902200
C	-2.87321600	-0.38753300	0.43923900

H	-3.57995100	0.32613300	0.01047000
H	-3.35099400	-1.36973000	0.47633100
H	-2.63765200	-0.08000700	1.46215100
C	-1.51410700	2.05540800	-0.52010500
H	-0.83731400	2.90394800	-0.65920500
H	-2.17861800	2.00744400	-1.38961900
H	-2.12508200	2.25190400	0.36634800

Absolute energies (Hartree): -536.45049 ZPE (Hartree): 0.191084

Harmonic Vibrational Frequencies (cm^{-1}):

-2544.8720 71.5012 96.7735 118.6852 134.3530 177.8717 231.9666 258.2511 281.0993 301.0374 305.8061 318.8777 351.7410 362.3001 448.5801 537.9310 584.7455 604.7022 696.7817 785.9707 853.3365 887.5322 932.9081 961.7504 994.1526 1031.1679 1048.6465 1072.2149 1124.3533 1142.9672 1164.0076 1183.4642 1188.9759 1230.4954 1260.9238 1318.9669 1324.3493 1349.4406 1376.6605 1381.6399 1388.6724 1404.6654 1422.0082 1427.2117 1432.2578 1477.8371 1504.8232 1516.1340 1525.4469 1528.0018 1581.8414 3065.5117 3067.5505 3071.2801 3085.2608 3101.1744 3112.3061 3147.6109 3154.3075 3161.1625 3175.3117 3186.8019 3842.0034

O_2C•CC(C)C(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.04440200	-1.75428300	0.12030600
H	2.60215700	-2.45222100	0.61794100
O	1.87743900	-1.10423100	-0.44405100
C	-2.06223800	-0.01163200	-0.28793000
H	-2.18024600	-0.05519200	-1.36885700
O	-3.09246100	-0.55473200	0.43047700
O	-4.32276500	-0.25047300	-0.27651900
H	-4.70875000	-1.13436200	-0.27224000
C	1.73952900	0.16166600	0.20873500
H	1.74350500	-0.00824300	1.29667300
C	-0.74032800	-0.25923200	0.36168700
H	-0.83608800	-0.07354800	1.43973600
H	-0.43900600	-1.30819000	0.23480100
C	0.35318300	0.65526800	-0.21362200
H	0.31955200	0.59344500	-1.31094700
C	2.88290100	1.08396500	-0.18394000
H	2.86691400	2.00527500	0.40373400
H	3.83266000	0.57615400	-0.00556200
H	2.81010000	1.33502200	-1.24672000
C	0.12205900	2.10680100	0.21307700
H	0.30019900	2.21901600	1.28919300
H	0.77896100	2.79890300	-0.31891800
H	-0.91351700	2.39268100	0.01142100

Absolute energies (Hartree): -536.466742 ZPE (Hartree): 0.19347

Harmonic Vibrational Frequencies (cm^{-1}):

45.8433 58.6296 70.8524 98.5712 122.4742 162.1465 186.3620 205.1292 220.6297 241.1286 275.9175 296.5782 318.2767 348.9659 393.4314 424.8956 495.6138 545.3548 563.2448 693.0670 857.7266 886.8902 906.1505 924.3171 944.1101 968.7394 992.8701 1083.6056 1118.1671 1130.4127 1158.2951 1172.1205 1195.3267 1219.9463 1244.1965 1282.7103 1323.0095 1356.9138 1362.9093 1395.1221 1397.7561 1407.3024 1419.4524 1425.1289 1427.7768 1496.7499 1504.8842 1515.3138 1524.8684 1531.7521 3039.6297 3048.8526 3064.6961 3069.9801 3081.7251 3105.1213 3156.5726 3173.5000 3178.1503 3189.1713 3190.8138 3836.6026 3847.2362

$O_2CC(C)C(C)C(C)OO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.88651800	-0.00209100	-0.50965500
H	-2.09196900	-0.80167700	-1.22997700
H	-2.84076900	0.35842800	-0.10827200
C	-1.00440700	-0.50433600	0.63278100
H	-0.80591700	0.34688000	1.29248900
C	0.34990700	-1.08848400	0.16879500
H	0.77424700	-1.62769200	1.02930100
C	1.38107900	-0.01887200	-0.19952000
H	0.98409500	0.67045500	-0.94544500
O	-1.29994300	1.02486800	-1.29624200
O	-1.35565100	2.23226500	-0.49963700
H	-0.45893000	2.24347400	-0.12512400
O	1.63712500	0.78460000	1.00833700
O	1.11178300	1.95935800	0.96572200
C	2.74009200	-0.56195400	-0.60404300
H	2.67568200	-1.05861000	-1.57412100
H	3.45636800	0.25926600	-0.68508500
H	3.10544600	-1.27815200	0.13808600
C	-1.79062800	-1.53499300	1.45096800
H	-2.71624400	-1.09598900	1.83600100
H	-2.06177500	-2.40677300	0.84616500
H	-1.20028900	-1.88305500	2.30383100
C	0.20159300	-2.07854500	-0.99474600
H	0.02426600	-1.55114600	-1.93774800
H	1.09961000	-2.69013000	-1.11000900
H	-0.63703700	-2.75835400	-0.82302700

Absolute energies (Hartree): -575.747633 ZPE (Hartree): 0.226199

Harmonic Vibrational Frequencies (cm^{-1}):

58.3666 79.7439 108.8292 138.0013 179.0473 183.9761 204.5153 222.4268 225.5389 271.1949 286.5354 329.0382 354.6440 374.4766 390.7471 433.2417 473.4092 540.4793 567.7154 573.8469 593.0536 807.1846 861.0457 865.9317 903.8391 945.7847 968.3203 974.8733 1031.3306 1063.4767 1083.4261 1094.8763 1120.3356

1162.3670 1184.4268 1213.5498 1216.8518 1292.2884 1300.0399 1347.2822 1350.3121 1383.9625 1387.1730 1404.1717 1411.8394 1421.2409 1428.0769 1430.3772 1438.2769 1474.9695 1488.0518 1506.6597 1513.8296 1518.2300 1521.4999 1526.4990 1535.2469 3049.4453 3068.2471 3076.0450 3080.4857 3083.9618 3113.7711 3143.4470 3156.8057 3162.1123 3166.2021 3168.0049 3174.0615 3183.3195 3192.3601 3705.0329

TS_{31}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.37511500	-0.60036600	0.36516700
H	-3.15432600	-1.16038100	1.12089600
O	-2.22926900	0.28233400	0.37878800
C	-1.37045500	-0.14771100	-0.62846300
H	-1.89203000	-0.29134300	-1.58256100
H	-0.91972800	-1.26393000	-0.29871500
C	-0.15285200	0.76357800	-0.66110100
H	0.40945200	0.48215200	-1.55984400
C	0.72559700	0.48581000	0.58706600
H	0.04547200	0.18909800	1.39269800
C	1.68025000	-0.70245400	0.34524800
H	1.96630900	-1.12709900	1.31768600
O	1.05148500	-1.73815600	-0.42936600
O	-0.13285700	-2.11570200	0.16368600
C	2.92412200	-0.36891600	-0.46461100
H	3.61424300	0.24223900	0.12044200
H	3.43079800	-1.29771300	-0.73859300
H	2.66743600	0.16814500	-1.38243300
C	-0.60742100	2.22250900	-0.81576800
H	0.24788600	2.88545800	-0.96746900
H	-1.26717000	2.31448100	-1.68459300
H	-1.16352900	2.55683000	0.06301000
C	1.52157800	1.69392600	1.08739700
H	2.16758900	1.39772800	1.92150900
H	2.15581200	2.12013100	0.30468200
H	0.85291200	2.47887300	1.44848500

Absolute energies (Hartree): -575.705789 ZPE (Hartree): 0.220154

Harmonic Vibrational Frequencies (cm^{-1}):

-2468.7633 70.7559 85.5486 110.1653 169.5592 190.8334 233.4619 256.7710 265.0730 273.7763 295.3175 315.2034 319.4970 345.0230 350.4012 372.0309 446.2194 452.7828 554.4329 602.5361 649.3838 719.0415 776.1194 858.5912 913.9190 930.8420 971.4351 981.0814 1016.6839 1033.3039 1035.3502 1071.2307 1119.2297 1151.5069 1154.0312 1189.7004 1199.5602 1206.6025 1229.0482 1303.2371 1321.8347 1339.2167 1358.5886 1374.2185 1381.7947 1384.6862 1401.6826 1417.3246 1423.7528 1429.8215 1433.3605 1503.8923 1512.4590 1515.9802 1519.9342 1530.5817 1537.4444 1576.1317 3061.6307 3070.5789 3078.7432 3084.4107 3090.8835

3103.3123 3107.2746 3153.8811 3164.3932 3173.3398 3174.4829 3184.6577 3188.4159 3818.4114

$O_2C•C(C)C(C)C(C)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.20355000	-1.53227100	0.06694300
H	-2.77114200	-2.36885100	-0.14300200
O	-2.06482500	-0.83586900	0.64013300
C	2.02526600	0.14736900	0.31856400
H	2.11194400	0.02132900	1.39742800
O	3.11063500	-0.27169600	-0.40210400
O	4.29603500	0.03010100	0.37940700
H	4.73420800	-0.82608500	0.30506700
C	-1.78212200	0.27861700	-0.21192000
H	-1.74963700	-0.07779500	-1.25225900
C	0.73657600	-0.15293700	-0.38645600
H	0.85808400	0.15697800	-1.43522800
C	-0.38012700	0.72909100	0.22064600
H	-0.35183800	0.62156900	1.31558300
C	-2.88034300	1.32075000	-0.06048800
H	-2.74893500	2.14546700	-0.76532100
H	-3.84486500	0.84697800	-0.25580500
H	-2.88420600	1.71590600	0.95970900
C	-0.11778200	2.19646300	-0.13813300
H	-0.26042600	2.35832200	-1.21303500
H	-0.78297400	2.87291400	0.40309900
H	0.91407600	2.45934300	0.10744400
C	0.47035400	-1.67030200	-0.37235600
H	0.30960600	-2.02523900	0.64881500
H	-0.40732400	-1.92976100	-0.97043600
H	1.33613400	-2.18748800	-0.79624400

Absolute energies (Hartree): -575.719361 ZPE (Hartree): 0.222211

Harmonic Vibrational Frequencies (cm^{-1}):

44.0708 63.5488 75.4238 86.1744 103.1834 167.1235 173.5883 179.3703 223.1876 261.8422 275.8186 284.9584 302.8609 321.9490 342.0439 356.1262 381.1771 398.5001 484.7791 499.6083 550.7966 576.9787 757.3213 837.4417 877.7995 899.9781 920.2348 949.5362 977.9915 982.4063 1021.4369 1075.7140 1105.5775 1129.2498 1157.9080 1171.7598 1191.1505 1205.7494 1222.5576 1257.7861 1310.1600 1325.7027 1357.6209 1371.4971 1391.4738 1399.6268 1404.5697 1414.4095 1419.8837 1424.6172 1426.9399 1502.2596 1509.5883 1516.1228 1524.6529 1529.7181 1530.4741 3046.1239 3051.2096 3062.6785 3070.5744 3075.6167 3082.2386 3158.0557 3164.1361 3175.3988 3177.0416 3178.6961 3179.1573 3185.8310 3833.4656 3845.2265

$O_2C(C)CCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.57700500	0.12770000	0.34630600
H	-2.14251500	0.70258300	1.09033300
C	-0.47837700	-0.64589100	1.08198300
H	-0.96582300	-1.22799700	1.87388100
H	0.17378400	0.07211900	1.58842900
C	0.35666100	-1.60445200	0.22610600
H	0.96175500	-2.24175200	0.88138600
H	-0.29502100	-2.27673300	-0.34317600
C	1.29930400	-0.93814300	-0.76546900
H	0.81410400	-0.17617000	-1.37291800
H	1.80354800	-1.67689200	-1.39233500
O	-1.05641000	1.05123100	-0.61046500
O	-0.42308200	2.12202600	0.12705700
H	0.50611100	1.85479700	0.03815700
O	2.39637200	-0.29565200	-0.04380700
O	2.21021400	0.96337200	0.15179700
C	-2.52854300	-0.74919300	-0.45481100
H	-2.92376900	-1.54979000	0.17733300
H	-3.36025300	-0.14948300	-0.83007800
H	-2.02092200	-1.19862100	-1.31236200

Absolute energies (Hartree): -497.235207 ZPE (Hartree): 0.169407

Harmonic Vibrational Frequencies (cm^{-1}):

62.6474 79.1794 144.6462 160.6850 198.6832 226.6274 249.0291 298.0826 338.2249 367.6790 437.9303 505.4330 527.7922 576.5850 607.1692 786.9397 825.8617 862.0536 889.7484 929.9627 978.3226 989.6109 1046.4896 1074.3396 1121.3931 1156.6657 1217.0896 1237.4951 1264.2704 1321.4052 1365.6131 1375.6410 1395.7822 1408.4903 1417.0580 1426.3336 1436.1662 1466.3739 1487.6529 1500.3170 1507.0353 1514.2314 1529.0093 3077.1604 3081.9513 3084.7478 3091.2995 3127.5519 3135.6503 3147.5022 3175.0262 3185.3558 3220.1561 3723.0003

TS_{32}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.45677700	-0.64616800	-0.98150200
H	1.96800700	-1.08676200	-1.68882800
O	1.59178300	0.49851500	-0.78068000
C	0.80033100	0.25166600	0.35149800
H	0.16264900	-0.78972800	0.12604000
C	-0.26394500	1.33821200	0.35736600
H	-0.71557200	1.38234100	1.35342900
H	0.24068200	2.29581100	0.17710200
C	-1.33367800	1.08533400	-0.71509100
H	-0.83475400	0.73522500	-1.62182100

H	-1.84990100	2.01740600	-0.96830500
C	-2.38387400	0.06724400	-0.26461000
H	-3.12265900	0.53156700	0.39608400
H	-2.89465100	-0.38269400	-1.12318000
O	-1.82532300	-0.96102300	0.55845400
O	-0.79656100	-1.56690200	-0.12889100
C	1.57298400	0.04222000	1.63180600
H	2.33620000	-0.72480400	1.49761200
H	2.05727600	0.98317000	1.92039900
H	0.88841000	-0.26496200	2.42660600

Absolute energies (Hartree): -497.199279 ZPE (Hartree): 0.16271

Harmonic Vibrational Frequencies (cm^{-1}):

-2354.5162 68.3633 110.4533 128.0289 214.6102 222.9505 253.2636 288.6650 295.2729 306.1460 374.2354 404.2079 444.5169 538.9182 600.7574 634.9180 816.2607 844.4538 894.5378 921.4303 936.3321 969.7013 1012.9146 1079.3146 1094.5153 1125.3855 1183.3947 1206.8811 1233.8518 1258.5004 1279.3735 1310.4321 1327.9688 1368.8521 1385.0675 1404.5174 1411.2697 1418.4325 1479.7417 1493.9589 1503.5212 1513.4611 1515.0780 1577.3420 3068.2271 3076.7358 3082.2569 3101.1739 3142.8625 3147.5447 3162.9137 3166.7703 3202.3956 3818.6016

$O_2C(CC)CCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.13627600	0.09718800	0.55149400
H	-1.63511000	0.66658300	1.34763800
C	0.03750400	-0.66528700	1.17183900
H	-0.36406700	-1.25749300	2.00345900
H	0.72877900	0.05722100	1.61686400
C	0.79403200	-1.60815000	0.22966600
H	1.46429000	-2.24713400	0.81646200
H	0.09495600	-2.27898400	-0.28238800
C	1.63169400	-0.92220300	-0.83972300
H	1.08159900	-0.16369900	-1.39377600
H	2.08647900	-1.64962300	-1.51575600
O	-0.71998800	1.02759300	-0.44959600
O	-0.04729000	2.11664600	0.22387100
H	0.87554200	1.86304600	0.05936700
O	2.78151100	-0.26778600	-0.21750900
O	2.59428700	0.98598100	0.00852300
C	-2.16229100	-0.78667600	-0.15126700
H	-2.36356800	-1.65353300	0.48999900
H	-1.72503000	-1.16796700	-1.08133100
C	-3.45843900	-0.03688200	-0.45910000

H	-3.24629400	0.84555200	-1.06598400
H	-4.16302800	-0.67390600	-1.00108500
H	-3.94005800	0.29253000	0.46676400

Absolute energies (Hartree): -536.489471 ZPE (Hartree): 0.198226

Harmonic Vibrational Frequencies (cm^{-1}):

51.4054 79.4871 96.0494 130.4271 163.6635 180.3989 207.2151 233.5802 276.6634 311.0539 335.9235 398.6182 441.6486 511.4978 525.2229 576.0460 620.0839 769.0311 817.9091 830.6555 874.1582 908.3363 921.1035 985.4955 1017.3276 1030.2225 1069.3027 1094.8580 1123.8029 1156.0951 1209.1867 1235.1476 1261.9475 1315.6480 1320.8654 1329.9663 1371.1868 1396.5487 1403.8561 1409.0523 1425.6990 1427.9523 1432.4242 1465.9125 1486.1072 1495.4405 1506.9737 1513.8794 1518.7404 1529.8939 3065.4683 3075.0681 3079.3868 3081.1418 3088.1825 3125.4304 3128.7869 3136.2021 3145.5483 3164.4096 3185.8177 3220.6282 3721.5253

TS_{33}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	1.75851000	1.96358400	0.21752900
H	1.05646000	2.62302200	0.29498100
O	1.13977400	0.87619900	0.94881100
C	0.58254900	-0.01537000	0.01772800
H	-0.24564000	0.62290200	-0.64920600
C	-0.26456100	-0.98183600	0.83380700
H	-0.45487700	-1.87779700	0.23369600
H	0.31977400	-1.28562600	1.71059300
C	-1.58457600	-0.33281000	1.27673200
H	-1.37521100	0.69320300	1.58890800
H	-1.99623900	-0.85838500	2.14504200
C	-2.64285500	-0.34193200	0.17174300
H	-3.11581000	-1.32559300	0.08968600
H	-3.41128300	0.41817300	0.35181100
O	-2.07272600	-0.15451400	-1.12687400
O	-1.34851700	1.01671600	-1.12527400
C	1.56904600	-0.60930800	-0.96629000
H	2.05254300	0.20581100	-1.51007400
H	0.99674700	-1.19867700	-1.69110000
C	2.62192800	-1.47717300	-0.26688400
H	2.16409200	-2.34104600	0.22379300
H	3.35175900	-1.84911800	-0.99136300
H	3.15215900	-0.89217500	0.48869300

Absolute energies (Hartree): -536.454002 ZPE (Hartree): 0.191833

Harmonic Vibrational Frequencies (cm^{-1}):

-2350.6838 61.0988 78.4363 108.5667 121.1054 215.1093 221.6022 230.2574 264.0100 291.5387 302.2868 328.4223 378.6688 437.9895 469.0361 538.7184 607.5945 671.8816 802.5439 819.7088 846.3003 912.3740 922.5440 949.2648 980.8959 1017.2984 1042.8513 1083.7733 1098.0202 1107.9765 1179.2916 1202.3518

1221.3912 1255.9182 1268.6871 1305.4550 1317.0906 1337.6747 1369.6885 1376.1624 1382.9035 1404.2049 1417.5780 1422.0660 1478.5473 1500.2056 1503.4005 1514.4487 1519.9239 1525.5712 1577.9491 3078.0660 3080.5346 3081.6081 3099.0356 3099.6971 3141.8347 3146.5840 3156.2658 3165.3901 3170.0592 3180.0691 3815.5206

O_2C•(CC)CCCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.25558200	0.38670400	-0.19017700
H	4.22570200	0.77855300	-1.07068100
O	2.84883400	0.45506400	0.14468300
C	-1.39321200	-0.02949700	-0.09472100
O	-1.85913600	-1.30678800	-0.33792000
O	-3.14128300	-1.48504800	0.30387700
H	-3.65217300	-1.77404200	-0.46148200
C	2.37569000	-0.88442400	0.16818200
H	2.96006200	-1.46835900	0.88795100
H	2.48287000	-1.33567200	-0.82808000
C	0.06876700	0.00014200	-0.41559100
H	0.22767800	-0.40234700	-1.43101100
H	0.41020800	1.03798200	-0.42847400
C	0.91396500	-0.81005600	0.57512200
H	0.83909400	-0.36493000	1.57254500
H	0.52160700	-1.82996900	0.63723100
C	-2.28550000	1.13423600	-0.41027200
H	-2.18866600	1.38113600	-1.48158100
H	-3.32161700	0.83624500	-0.23787100
C	-1.96168800	2.37115300	0.43302400
H	-2.09027400	2.14927200	1.49557400
H	-0.93124000	2.70233500	0.27839200
H	-2.62335300	3.20101500	0.16932700

Absolute energies (Hartree): -536.465859 ZPE (Hartree): 0.195171

Harmonic Vibrational Frequencies (cm^{-1}):

30.4626 50.2021 57.8660 73.6464 108.1789 128.8460 198.5008 203.9326 210.8785 225.9213 244.8992 267.8886 303.6297 347.9523 415.1513 462.7017 527.5350 593.4176 749.2978 792.1806 834.7422 887.8292 921.9578 952.6020 1011.9326 1042.2341 1091.1236 1097.4742 1112.4052 1130.2874 1182.1456 1226.9298 1246.6138 1277.0552 1288.2329 1313.9239 1331.5051 1353.7423 1372.2038 1384.1973 1403.6218 1425.2897 1429.2982 1431.0477 1483.3395 1494.6555 1498.0188 1521.4712 1526.3096 1546.1390 3006.4004 3011.2341 3051.7198 3079.9575 3095.6949 3120.1910 3147.1816 3152.9009 3163.0563 3170.0212 3176.0481 3841.3351 3843.1776

O_2C(C)C(C)CCOO•

Cartesian Coordinates (Å)

At.	X	Y	Z

C	1.38039400	0.55466300	-0.06445100
H	1.96198300	0.94833900	-0.90870600
C	0.60177700	-0.67120500	-0.56986100
H	-0.10493700	-0.29757700	-1.31915500
C	-0.18371200	-1.41540100	0.51791200
H	-0.54825100	-2.36418500	0.10428400
H	0.48125200	-1.67862600	1.34957600
C	-1.38308600	-0.68084400	1.09789500
H	-1.15871900	0.34083700	1.39815900
H	-1.83245000	-1.24234100	1.92015400
O	0.52400000	1.60216100	0.39324900
O	-0.14183700	2.15559000	-0.76568100
H	-1.01084500	1.73289500	-0.67017200
O	-2.45001400	-0.62438700	0.09935800
O	-2.47782700	0.48347000	-0.55620500
C	2.30553300	0.29434100	1.11621400
H	2.97875900	-0.54009700	0.90463600
H	2.90401400	1.18608800	1.31405400
H	1.73337500	0.06443400	2.01901700
C	1.54701800	-1.64673400	-1.27972500
H	0.97641700	-2.42427500	-1.79654300
H	2.16181100	-1.12770500	-2.02180300
H	2.21547600	-2.14138400	-0.56718100

Absolute energies (Hartree): -536.491265 ZPE (Hartree): 0.197625

Harmonic Vibrational Frequencies (cm^{-1}):

57.5138 76.5819 121.9884 146.2456 183.3502 203.1616 223.5896 235.4521 262.5616 285.6376 320.7980 357.8370 427.8339 477.8144 521.6529 559.1638 575.1699 593.0472 766.4397 840.3527 864.8971 906.7843 944.1523 966.5473 1019.4776 1027.9545 1063.2554 1065.4703 1144.0409 1155.2674 1185.7055 1223.2384 1256.0920 1285.1175 1340.3407 1360.4662 1373.1383 1396.8775 1399.6902 1420.0765 1423.0627 1427.6460 1439.6318 1465.2492 1483.6753 1502.8789 1513.6164 1519.2630 1522.3049 1527.9334 3066.7489 3070.6357 3074.2119 3088.1006 3105.7768 3123.9383 3131.5537 3156.3767 3160.7678 3178.7979 3187.1066 3222.1381 3721.3301

TS_{34}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.25242200	-1.28775600	-0.94897100
H	1.67879400	-1.72604200	-1.59137800
O	1.54386700	-0.02982200	-0.82724200
C	0.75745200	-0.08417300	0.33346400
H	-0.00104400	-1.05540900	0.19797000
C	-0.18123100	1.12113000	0.28503600
H	-0.65258400	1.18056900	1.27396900

C	-1.27275200	0.89437200	-0.77583000
H	-0.81036900	0.43511000	-1.65376800
H	-1.68646500	1.85794800	-1.09592400
C	-2.43124100	0.02981000	-0.27294200
H	-3.11825600	0.61628200	0.34518400
H	-2.98333600	-0.41760700	-1.10718000
O	-1.99649600	-0.99700000	0.62323300
O	-1.03377400	-1.75267300	-0.00684000
C	1.52896000	-0.30517500	1.61413000
H	2.17843700	-1.17612500	1.52064800
H	2.14456800	0.57437400	1.83565000
H	0.82815000	-0.46682200	2.43750800
C	0.59102100	2.42183100	0.02371300
H	1.00852800	2.42109200	-0.98608300
H	-0.08185700	3.27899900	0.12381100
H	1.41401900	2.54888300	0.73272300

Absolute energies (Hartree): -536.455081 ZPE (Hartree): 0.19117

Harmonic Vibrational Frequencies (cm^{-1}):

-2339.1001 69.0829 100.0905 131.4864 183.7040 204.7200 214.0748 245.9780 258.9833 269.4410 296.4934 318.5068 341.7428 421.2627 438.4278 457.4867 563.9525 628.2540 673.4056 832.9813 838.9087 888.5352 915.1906 964.1944 988.4021 996.1475 1053.0224 1074.4833 1092.9302 1143.9113 1173.0531 1187.9398 1208.2708 1238.4334 1280.8479 1291.6014 1312.5731 1339.3751 1375.7550 1389.6448 1404.4996 1408.5676 1415.9559 1423.8822 1493.7636 1500.7715 1510.0169 1511.9067 1518.9543 1520.7193 1568.2595 3072.2747 3077.0650 3079.1093 3088.0598 3091.6704 3142.2109 3160.0327 3162.7240 3166.3026 3178.5953 3200.3068 3814.9587

O_2C•(C)C(C)CCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.00846600	-0.24287100	-0.63952200
H	3.95565300	-1.18402800	-0.84241200
O	2.59558200	0.07987500	-0.67622200
C	-1.59085600	0.23990600	0.11669700
O	-2.37106900	-0.72921600	-0.48736100
O	-3.76260600	-0.51145700	-0.16359700
H	-4.11102900	-0.41882700	-1.05817200
C	2.24378000	0.46142200	0.64477000
H	2.86899500	1.30275300	0.96498400
H	2.40519900	-0.37621300	1.33322300
C	-0.15427000	-0.21166700	0.04279500
H	0.10036000	-0.36600900	-1.01878700
C	0.78151400	0.87692700	0.58994700
H	0.70551700	1.77923400	-0.02492600

H	0.47388200	1.14323400	1.60969600
C	-1.99704800	1.66503400	-0.10142400
H	-1.47042400	2.33089300	0.58363400
H	-1.76735300	1.98380100	-1.13152500
H	-3.06832600	1.78021500	0.06417500
C	0.03492900	-1.54866300	0.77223900
H	-0.07611600	-1.40999100	1.85335100
H	-0.71354400	-2.26977600	0.44024200
H	1.02590700	-1.96368800	0.56998500

Absolute energies (Hartree): -536.466731 ZPE (Hartree): 0.194906

Harmonic Vibrational Frequencies (cm^{-1}):

35.7064 53.0202 86.1183 108.2541 128.9313 159.9699 187.1682 199.3738 221.0784 239.5362 292.8641 302.1712 331.4840 346.3409 375.0259 433.7539 483.1930 524.4025 604.4238 777.2355 847.8785 887.9001 931.4797 957.9763 993.5170 1019.7762 1030.4465 1091.2753 1118.3610 1130.5347 1173.5852 1192.9061 1247.5090 1264.5419 1292.2362 1297.9159 1348.9558 1363.3993 1375.0632 1399.6197 1402.9127 1417.8065 1419.8230 1432.3574 1487.7718 1497.9651 1511.4585 1516.0994 1528.9874 1558.2656 3016.8913 3024.6034 3069.2769 3073.9430 3078.0705 3122.0751 3143.9229 3155.1310 3162.9267 3188.8691 3203.5800 3842.6098 3843.5637

$O_2C(C)C(C)C(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.63860500	-0.12473700	-0.03369600
H	-2.35647500	-0.20791800	-0.86033200
C	-0.43157400	0.67703200	-0.56264000
H	0.04350100	0.05009000	-1.32734200
C	0.62543600	1.02658400	0.50477800
H	0.11194500	1.50461700	1.35094900
C	1.32675400	-0.19354800	1.10196300
H	0.64431700	-0.99788000	1.36923600
H	1.94493600	0.09994600	1.95456200
O	-1.31155900	-1.45276000	0.37459900
O	-0.97251800	-2.20031500	-0.81578500
H	-0.00408200	-2.18147300	-0.74302400
O	2.30354600	-0.73586000	0.15780800
O	1.83400300	-1.67920300	-0.58230300
C	-2.33031200	0.47585600	1.18266600
H	-2.58131700	1.52482600	1.00618100
H	-3.25027400	-0.07548500	1.38881700
H	-1.69243700	0.41250600	2.06838900
C	-0.95142200	1.93938300	-1.26563500
H	-0.18313000	2.39234000	-1.89589300
H	-1.80221100	1.69120600	-1.90812400
H	-1.28136900	2.69247500	-0.54142400

C	1.68406800	2.01075800	-0.01341300
H	1.25211800	2.99402100	-0.20799500
H	2.48292700	2.13594300	0.72540700
H	2.13770300	1.64192500	-0.93808600

Absolute energies (Hartree): -575.745153 ZPE (Hartree): 0.226395

Harmonic Vibrational Frequencies (cm^{-1}):

50.7484 73.4515 100.3751 147.0213 187.5328 204.1008 221.9707 233.9504 249.8889 267.9683 279.0313 295.5819 338.7540 374.8757 407.2479 442.1306 518.8053 549.3087 585.9858 605.7253 627.5222 769.4451 847.4744 889.8965 909.8064 952.5284 968.3290 984.7168 994.3655 1034.1025 1051.2204 1090.0502 1127.5509 1164.5938 1176.0812 1211.4166 1221.5538 1283.3045 1312.7861 1328.4519 1348.6354 1370.8619 1384.1260 1402.4780 1416.6888 1419.4915 1425.9447 1427.8455 1441.7687 1468.4136 1501.9335 1509.2641 1514.2865 1519.6074 1520.0814 1524.8833 1540.5396 3066.8951 3068.9399 3073.1337 3075.4913 3087.5285 3096.7176 3122.1561 3152.8165 3157.8202 3172.9170 3177.6772 3185.4373 3186.1459 3219.9320 3715.9051

TS_{35}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.67659100	0.14033000	-1.28666800
H	-2.24898800	0.65746400	-1.98200500
O	-1.54195300	-0.65290900	-0.85832800
C	-1.01619400	-0.06685000	0.30424300
H	-0.72019000	1.09505800	0.00715000
C	0.32469400	-0.75509800	0.57162700
H	0.63143800	-0.44930800	1.58088500
C	1.38403000	-0.24892500	-0.43542000
H	0.87925600	-0.13080600	-1.40074900
C	1.95342000	1.11318100	-0.01304200
H	2.72283200	0.97615000	0.75574500
H	2.38983100	1.63082900	-0.87624900
O	1.00500100	1.96439200	0.62860700
O	-0.06032100	2.14806800	-0.22413000
C	-1.98255400	0.02858000	1.46303400
H	-2.90836800	0.50955000	1.14552100
H	-2.21499100	-0.97263800	1.84337000
H	-1.52855700	0.61849600	2.26376600
C	0.14426200	-2.28132500	0.55880400
H	-0.09103000	-2.63793900	-0.44687200
H	1.05083400	-2.78125900	0.90821800
H	-0.67608400	-2.57458100	1.21994600
C	2.57024000	-1.19735500	-0.62648800
H	3.04801300	-1.42302900	0.33366300
H	2.26732800	-2.13801600	-1.09115100
H	3.32219500	-0.73225900	-1.27363400

Absolute energies (Hartree): -575.710235 ZPE (Hartree): 0.219768

Harmonic Vibrational Frequencies (cm^{-1}):

-2321.4696 66.9875 90.2030 120.7323 140.6084 197.6126 205.5228 252.9701 269.2105 272.8006 283.7413 303.4791 320.3017 336.0376 353.4893 407.2737 410.5560 430.8623 475.5902 594.3031 632.0102 676.3927 804.5040 871.3508 911.5127 932.6989 959.3747 968.3049 987.9651 1032.1398 1062.5894 1064.1193 1107.5062 1159.3600 1173.4656 1193.5410 1206.6000 1213.2651 1243.7155 1286.6019 1302.7406 1341.9578 1349.6096 1359.8511 1384.8375 1405.3801 1407.1419 1417.4547 1420.7054 1430.1661 1494.1277 1497.5794 1509.5321 1514.5921 1516.6670 1525.8906 1534.6852 1572.4093 3063.7365 3068.2404 3073.4324 3077.4771 3084.1043 3101.8220 3137.6084 3146.5437 3164.2035 3170.7699 3176.5315 3182.4839 3199.6942 3815.5232

O_2C•(C)C(C)C(C)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.03144400	-0.32052000	-0.18615100
H	4.06391300	-1.28349100	-0.14741500
O	2.62149900	-0.14663900	-0.47321700
C	-1.60682200	-0.20768300	-0.40578900
O	-2.17609200	0.33252100	0.73160200
O	-3.48383200	0.86246000	0.41333100
H	-4.02147400	0.28337900	0.96669400
C	2.04957200	0.45469500	0.67996200
H	2.58185500	1.38530200	0.91039600
H	2.14104500	-0.22285700	1.53798100
C	-0.15935300	-0.50972200	-0.13032900
H	0.27702700	-0.81787400	-1.08872300
C	0.59195400	0.75270800	0.34260500
H	0.12722900	1.08941900	1.27850200
C	-2.44488900	-1.13078100	-1.23274600
H	-1.85589600	-1.49676700	-2.07685100
H	-2.78116600	-2.00093900	-0.64607200
H	-3.33142100	-0.62290000	-1.61614900
C	-0.01810600	-1.68468800	0.85706200
H	-0.33752000	-1.38271800	1.85966500
H	-0.63882600	-2.52877800	0.54058200
H	1.01642500	-2.03474500	0.90551200
C	0.48939800	1.87932200	-0.68902000
H	0.93199100	1.56662500	-1.63926800
H	-0.55439300	2.15338800	-0.86046300
H	1.02653200	2.76726600	-0.33938400

Absolute energies (Hartree): -575.724553 ZPE (Hartree): 0.222689

Harmonic Vibrational Frequencies (cm^{-1}):

34.8972 60.5673 71.6824 93.0209 118.2959 157.5560 170.3725 186.9260 194.1074 201.1456 211.4826 223.6735 226.1007 290.1101 332.0234 344.3776 386.1045 432.8906 470.2072 512.4980 565.2560 656.0442 788.2156

848.3826 914.9941 933.6048 968.4344 979.9091 993.4859 1019.4682 1042.9834 1051.1310 1091.0815 1128.5275 1155.7036 1185.1505 1207.6628 1233.3024 1273.2002 1302.1710 1311.3733 1351.8454 1365.1605 1374.5184 1390.0570 1405.0296 1405.8349 1411.8823 1426.5123 1431.8019 1490.0988 1510.9174 1511.6836 1513.5950 1518.7181 1523.1181 1555.2640 3020.0248 3061.7979 3071.1230 3073.0354 3082.6225 3096.0987 3116.6350 3140.2957 3158.5394 3159.7716 3168.8452 3175.9676 3189.6726 3839.4508 3841.0810

TS_{36}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.08530100	0.30721500	0.24817100
H	-1.12070400	-0.00433400	1.30059300
H	-0.45779100	-0.65318400	-0.24810200
C	-0.34961800	1.60229000	-0.00477200
H	-0.45180200	1.86221800	-1.06446800
H	-0.84986900	2.39139500	0.57220500
C	1.97895200	0.65848600	-0.56053900
H	1.44066700	0.48697200	-1.49754100
H	2.91518100	1.16419800	-0.82374500
C	2.36470800	-0.68799000	0.03908100
H	2.87583700	-1.30709600	-0.70700200
H	3.01567300	-0.55713700	0.90957300
O	1.25539400	-1.41256100	0.57144800
O	0.33260000	-1.60696500	-0.43174300
O	-2.34664800	0.40530200	-0.32210100
O	-3.06265200	-0.80567700	0.03242200
H	-3.83228900	-0.40251400	0.45155900
C	1.13736400	1.55135600	0.37149900
H	1.51951500	2.57648800	0.33568600
H	1.23941000	1.21406500	1.41040100

Absolute energies (Hartree): -497.189137 ZPE (Hartree): 0.163271

Harmonic Vibrational Frequencies (cm^{-1}):

-2513.4095 55.1039 92.6006 145.2226 172.0848 189.1497 218.1020 249.0037 269.5536 358.2679 429.9745 465.9886 482.1799 588.1225 614.6837 771.0577 810.7436 893.1808 912.0697 915.9174 1005.8663 1027.4714 1050.4628 1097.7137 1133.6829 1152.8779 1176.4458 1197.0435 1243.1379 1256.6682 1297.7165 1303.1605 1320.4087 1336.6112 1369.7517 1393.3397 1408.4777 1411.5314 1424.2642 1498.1584 1502.8895 1506.2317 1510.3381 1617.8972 3064.8585 3076.6815 3078.6935 3085.2532 3089.0197 3125.7575 3135.8593 3139.3474 3154.2846 3842.9838

$O_2CC(C)CCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.42531100	-1.10814600	-0.49312700
H	1.01276400	-0.41847400	-1.22845100

H	1.55784500	-2.09792500	-0.93554000
C	0.61715100	-1.14505600	0.79224300
H	1.00188400	-1.95081500	1.42737900
H	0.75825000	-0.20239800	1.32085600
C	-0.87725400	-1.37560900	0.52361400
H	-1.39326200	-1.46241500	1.48955400
H	-1.00378000	-2.34526400	0.02172200
C	-1.59613800	-0.30668300	-0.31387500
H	-1.08019300	-0.17221100	-1.27036600
C	-1.66684300	1.06112200	0.36526900
H	-2.16439200	0.97067000	1.33953700
H	-2.24493800	1.75284200	-0.26186100
O	-0.42862400	1.66248200	0.69982700
O	0.22547000	1.96892200	-0.56389400
H	1.12016400	1.66066600	-0.34441200
O	2.78950400	-0.65806900	-0.22393100
O	2.83524800	0.61762900	-0.04585200
C	-3.02858500	-0.76240200	-0.61272400
H	-3.59108900	-0.89710000	0.31853000
H	-3.55871800	-0.02787600	-1.22701400
H	-3.02917000	-1.71677500	-1.14753500

Absolute energies (Hartree): -536.485477 ZPE (Hartree): 0.19844

Harmonic Vibrational Frequencies (cm^{-1}):

66.4312 87.2215 132.1016 141.9080 148.2478 170.9500 216.6258 256.7379 263.3703 306.7498 318.7637 370.1297 423.5601 469.4275 564.6936 569.9116 621.0805 757.3597 842.8792 849.2810 869.4350 939.1697 957.8446 963.9624 1014.1765 1063.4701 1086.8359 1103.0955 1154.5773 1168.0680 1206.2885 1247.0253 1276.7323 1313.3643 1325.0331 1329.8876 1354.8097 1371.2490 1383.6838 1414.4467 1421.8528 1435.2877 1437.0956 1461.4764 1481.3558 1499.0139 1515.3853 1520.0649 1520.8745 1526.8085 3048.2588 3055.5592 3064.1680 3093.5902 3099.1995 3110.4161 3126.0629 3131.4106 3151.9940 3161.9240 3187.4214 3211.6710 3723.6237

TS_{37}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.97598200	-0.15359500	0.15592600
H	-1.05150600	-0.29997200	1.24170900
H	-0.08914300	-0.97444000	-0.14472600
C	-0.57176600	1.24700700	-0.24952700
H	-0.66008600	1.31512000	-1.34204900
C	1.92425700	0.75543000	-0.69388300
H	1.44435500	0.32140700	-1.57619400
H	2.70224800	1.43305800	-1.06375300
C	2.63622700	-0.35421100	0.07054600

H	3.28514500	-0.92778200	-0.60124600
H	3.23300400	0.05346200	0.89264800
O	1.73882000	-1.24717800	0.73408600
O	0.87780000	-1.77826800	-0.19737900
O	-2.15145200	-0.50220600	-0.50104400
O	-2.66373300	-1.69711800	0.12821800
H	-2.27896100	-2.37065200	-0.44821500
C	0.88702300	1.53805500	0.13590100
H	1.04788200	2.61407600	0.00752000
H	1.01837200	1.32802400	1.20590200
C	-1.52866900	2.26120600	0.39039800
H	-1.41110700	2.25328300	1.47951000
H	-1.31147300	3.27141300	0.02941100
H	-2.56674300	2.01779900	0.15227400

Absolute energies (Hartree): -536.448117 ZPE (Hartree): 0.191719

Harmonic Vibrational Frequencies (cm^{-1}):

-2461.2944 52.2182 90.5720 116.2120 161.1277 199.4256 218.8487 232.1443 244.1843 273.6398 310.0979 333.8395 408.9768 456.7768 472.7789 491.3744 592.4008 619.3232 778.4481 883.4494 909.5138 916.0585 936.7615 957.6677 1004.0744 1027.8935 1074.6070 1104.9843 1123.5937 1160.4803 1180.4552 1193.8532 1204.9128 1249.3173 1275.2633 1298.4176 1321.3901 1332.0284 1337.7973 1378.9090 1389.8269 1405.1594 1407.5997 1418.4919 1421.9430 1499.6028 1503.8937 1509.9775 1514.6351 1523.5270 1598.3893 3064.4136 3068.7240 3077.4117 3078.9691 3089.6062 3092.4418 3123.9355 3138.9835 3155.2351 3156.6132 3178.0229 3813.7584

O_2C•C(C)CCCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.89628300	-0.48417400	0.13874600
H	5.23771100	-0.67501900	-0.74248000
O	3.73020600	0.29418500	-0.22677300
C	-2.36614000	-0.49410200	0.16762600
H	-2.48444000	-0.83576200	1.19502100
O	-3.51990200	-0.07955600	-0.44009400
O	-4.59439000	-0.92944900	0.03891300
H	-5.23915500	-0.24001900	0.23750100
C	2.60185900	-0.48766800	0.13189500
H	2.63916500	-0.72481200	1.20215000
H	2.59632900	-1.42655200	-0.43782200
C	-1.18823700	0.33437000	-0.24260100
H	-1.17726500	0.37137100	-1.34084000
C	1.37783300	0.35326900	-0.19233400
H	1.47382900	1.31366700	0.32280300
H	1.35297500	0.55473600	-1.26986300

C	0.09434000	-0.36391200	0.22995300
H	0.06839900	-0.45069100	1.32512200
H	0.10021400	-1.38550900	-0.16971400
C	-1.29857500	1.77372100	0.29034100
H	-1.24093100	1.77426000	1.38475500
H	-0.49645300	2.40754700	-0.09809700
H	-2.25442800	2.21467200	-0.00415000

Absolute energies (Hartree): -536.4604 ZPE (Hartree): 0.194059

Harmonic Vibrational Frequencies (cm^{-1}):

42.5481 56.9116 65.8061 82.5344 99.9153 129.8565 141.8177 174.6931 184.6678 203.8978 239.6827 261.3227 288.2687 362.0555 399.4182 481.6099 495.2510 576.8962 745.4708 775.5888 865.7708 892.2256 914.6566 922.6172 990.2204 1011.7949 1070.1290 1091.6244 1103.1822 1148.3479 1180.2055 1190.6199 1202.6907 1239.6495 1268.5198 1301.5454 1314.7442 1332.7476 1360.9568 1368.9430 1390.8634 1408.5222 1416.8009 1428.5951 1438.1196 1500.5376 1513.0431 1519.8985 1525.4420 1551.8644 3052.3143 3056.3224 3066.5581 3070.9880 3084.5434 3110.0073 3111.4508 3152.2693 3158.8525 3172.1137 3183.7983 3843.3319 3846.2818

TS_{38}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.51751400	0.26208500	0.22802500
H	-1.62981600	0.07657300	1.30335000
H	-0.67263600	-0.59697900	-0.07941600
C	-0.99565400	1.63372100	-0.12484100
H	-1.04638900	1.76620400	-1.21154900
H	-1.66644200	2.37670000	0.32546400
C	1.49821400	1.06412400	-0.43093000
H	1.06856900	0.69371400	-1.36814200
H	2.33253700	1.71853400	-0.70757500
C	2.10615200	-0.11730800	0.32172000
H	2.59917100	0.24661300	1.23156800
O	1.09996600	-0.98788500	0.87120800
O	0.27414000	-1.42415700	-0.13877700
O	-2.69504500	0.02603000	-0.47185800
O	-3.28848800	-1.17261000	0.07363300
H	-2.94916900	-1.82775800	-0.55015100
C	0.44315900	1.86549300	0.35797100
H	0.65610200	2.93514000	0.26579500
H	0.51031100	1.62348300	1.42591700
C	3.08355300	-0.91120500	-0.53176400
H	3.89179600	-0.26479000	-0.88680100
H	3.51421600	-1.72930300	0.05070600
H	2.55970700	-1.33061700	-1.39390100

Absolute energies (Hartree): -536.451438 ZPE (Hartree): 0.191454

Harmonic Vibrational Frequencies (cm^{-1}):

-2458.8206 45.8805 92.5783 133.5897 159.9842 181.9845 216.7016 222.8535 230.0491 263.2092 329.5014 349.7943 384.3635 466.6403 488.9906 509.0767 605.2105 622.0948 769.6177 819.9984 873.0707 913.6038 932.9261 947.1342 990.2909 1056.7585 1075.1046 1094.2717 1127.2845 1157.0859 1159.1776 1186.3955 1209.3387 1248.3004 1261.3013 1300.3824 1309.3589 1328.2940 1339.3047 1381.0018 1387.7680 1400.0860 1408.6841 1410.8654 1420.6014 1496.4218 1502.4554 1506.1977 1508.9470 1521.6759 1607.3349 3069.0560 3076.9127 3079.9636 3083.8768 3095.0846 3100.1797 3127.0987 3135.9122 3138.9788 3174.3019 3186.4601 3817.2330

O_2C•CCCC(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-4.50257100	-0.33087300	-0.39231300
H	-4.62852300	-1.09233600	-0.97031400
O	-3.26895500	-0.74173300	0.25182600
C	2.80458200	0.24960900	-0.06826300
H	2.93178800	1.29116600	0.21864000
O	3.93378300	-0.51775500	0.01906000
O	5.05676900	0.31840700	-0.36254200
H	5.65199700	0.09037900	0.36127600
C	-2.23499300	0.12280700	-0.22257900
H	-2.22784100	0.08333500	-1.32190000
C	1.57729400	-0.52004700	0.29343500
H	1.60541300	-1.49119500	-0.21444600
H	1.54946300	-0.72952300	1.37512100
C	-0.95787900	-0.51087900	0.31817100
H	-1.02488100	-0.54918400	1.41263000
H	-0.90678900	-1.54524900	-0.04195800
C	0.30677500	0.23815800	-0.10306500
H	0.32428800	1.23189200	0.35866800
H	0.30427700	0.38933200	-1.18940700
C	-2.45857400	1.55131600	0.24715600
H	-2.38156900	1.59803700	1.33798200
H	-1.71947700	2.22709300	-0.19210700
H	-3.45358800	1.88611600	-0.05155700

Absolute energies (Hartree): -536.464754 ZPE (Hartree): 0.193818

Harmonic Vibrational Frequencies (cm^{-1}):

37.5829 52.6948 66.0737 92.2527 115.1886 142.7940 150.1621 183.6662 197.7780 206.0934 237.0295 256.0597 320.0470 348.9084 458.5498 486.9794 499.2221 570.8221 681.9295 760.8936 856.5364 888.5256 904.3081 922.8380 966.3186 1004.3033 1061.4366 1079.8082 1108.9396 1145.2002 1163.8849 1175.2615 1195.9564 1231.6536 1258.9771 1301.6347 1320.5635 1342.0144 1357.7012 1373.0219 1402.4594 1405.7517 1413.8796 1431.8905 1433.5600 1499.8657 1501.1513 1506.7115 1519.9367 1526.6772 3021.7929 3049.6667 3068.7378 3076.9020 3080.0794 3106.4552 3120.8094 3141.4997 3170.8254 3189.2409 3195.3435 3841.3439 3848.2374

$O_2C(C)CCCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.78946900	0.83501200	0.42208800
H	1.39154400	0.20071400	1.21320200
H	2.29864000	1.70058200	0.85155300
C	0.73445100	1.22707300	-0.59795100
H	1.15985300	1.97613900	-1.27494500
H	0.47489800	0.34607700	-1.18601400
C	-0.52384900	1.79277700	0.07728000
H	-1.18938400	2.18319800	-0.70007100
H	-0.24142100	2.65767000	0.69260800
C	-1.28987600	0.80191800	0.96582500
H	-2.11535900	1.33954100	1.45052600
H	-0.65379300	0.43373900	1.77570200
C	-1.91118900	-0.41040200	0.26543100
H	-2.45747500	-0.99072300	1.02223500
O	-0.96063000	-1.27756300	-0.34692300
O	-0.14089600	-1.83502400	0.71909400
H	0.72742000	-1.74191600	0.29377300
O	2.86346100	0.07743700	-0.21653800
O	2.51275700	-1.14362800	-0.43344000
C	-2.85316600	-0.04679700	-0.87392900
H	-3.33483100	-0.94615200	-1.26355400
H	-3.62344800	0.64089000	-0.51330500
H	-2.30921500	0.43298200	-1.69172000

Absolute energies (Hartree): -536.488745 ZPE (Hartree): 0.198608

Harmonic Vibrational Frequencies (cm^{-1}):

56.0182 98.8148 116.1068 141.7081 149.8497 194.7254 227.0744 255.7144 286.5889 305.1005 344.9742 377.1262 425.7010 498.2277 569.4503 593.5889 611.7244 753.1888 804.9833 853.2540 879.9491 917.7092 938.1940 962.1169 989.8592 1038.5097 1060.8164 1093.8365 1149.2589 1156.2616 1215.5026 1237.1651 1255.9031 1303.8198 1326.0051 1357.3533 1369.9154 1371.7050 1398.5218 1401.6077 1413.6802 1431.8442 1437.0798 1464.6767 1498.2150 1501.0058 1507.7984 1515.9268 1525.4426 1530.5117 3059.0794 3064.5425 3080.9375 3085.4497 3096.3742 3122.2286 3130.2641 3146.5915 3177.1415 3182.3065 3184.6554 3211.7337 3723.3144

TS_{39}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.00234100	0.35466000	0.12808700
H	-0.31745500	-0.61562700	-0.22658000
C	-0.22720700	1.62876000	-0.15355000

H	-0.32959600	1.86511700	-1.21884000
H	-0.70740400	2.44144000	0.40858800
C	2.06827800	0.62046200	-0.71740400
H	1.48365000	0.38860200	-1.61290800
H	2.98320000	1.11674800	-1.06117700
C	2.49902700	-0.68645200	-0.06336800
H	2.97341100	-1.34648600	-0.79865300
H	3.19352000	-0.50348400	0.76277900
O	1.42302400	-1.38338100	0.56871700
O	0.44206100	-1.62381300	-0.36279400
O	-2.12534400	0.40080700	-0.71301500
O	-2.91613600	-0.79396400	-0.50824100
H	-2.57450100	-1.33717300	-1.23051300
C	1.26466100	1.55956800	0.20476700
H	1.66559100	2.57565800	0.13080600
H	1.38348600	1.25505100	1.25098000
C	-1.30418800	0.07659500	1.58383400
H	-1.91842500	0.89178700	1.98441700
H	-1.84248800	-0.86428100	1.69174300
H	-0.37120500	0.01388900	2.14783500

Absolute energies (Hartree): -536.454077 ZPE (Hartree): 0.191674

Harmonic Vibrational Frequencies (cm^{-1}):

-2344.6175 56.5918 97.1194 119.4540 160.9440 204.7542 218.1775 238.6866 251.4239 274.3277 317.9350 365.6893 397.8040 435.0283 465.5171 526.2748 595.3833 618.3379 764.9034 833.1129 863.1512 894.6671 938.4631 943.6620 987.9795 1017.3702 1046.7564 1071.8102 1119.6051 1157.2492 1168.9125 1188.5715 1224.7319 1252.9010 1259.5503 1295.9112 1315.4347 1334.3156 1369.7920 1382.0580 1388.0613 1407.5159 1410.5797 1421.9913 1487.8055 1495.5410 1502.1959 1505.7085 1509.6482 1517.1929 1571.3922 3060.7084 3074.6281 3078.7040 3083.1432 3089.2669 3123.7875 3136.6462 3139.2065 3154.9459 3174.2684 3211.3279 3816.5986

$O_2C(CC)CCCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.09343300	0.95369600	0.40071300
H	1.79358600	0.26573600	1.19027800
H	2.53686300	1.85377900	0.83220600
C	0.96003700	1.26703800	-0.56103400
H	1.27700800	2.07441200	-1.23039100
H	0.76237300	0.38109500	-1.16568400
C	-0.31583700	1.68241700	0.18694000
H	-1.04972100	2.03194900	-0.54765700
H	-0.09130600	2.54909700	0.82349300
C	-0.94057100	0.58867000	1.06484600

H	-1.78167600	1.02320000	1.61857800
H	-0.23212300	0.24644400	1.82440900
C	-1.46930500	-0.64917900	0.33534800
H	-1.95129200	-1.30050400	1.08015700
O	-0.45438300	-1.40634600	-0.31912200
O	0.44260700	-1.91292900	0.71008500
H	1.28544800	-1.72339300	0.26599100
O	3.20409100	0.31762600	-0.30399100
O	2.96734300	-0.92958500	-0.52645500
C	-2.46628500	-0.35290200	-0.78227100
H	-2.76383000	-1.31196400	-1.21811100
H	-1.96396300	0.21183800	-1.57558200
C	-3.70087700	0.40419900	-0.29088600
H	-3.44988100	1.41393400	0.04558200
H	-4.43843900	0.49406900	-1.09302500
H	-4.17388800	-0.12345800	0.54368000

Absolute energies (Hartree): -575.74257 ZPE (Hartree): 0.227622

Harmonic Vibrational Frequencies (cm^{-1}):

50.7958 83.0402 97.8149 118.9013 138.6461 153.4036 192.9261 221.2656 247.8851 258.9993 300.8578 327.5911 366.6011 415.1502 431.5358 496.9446 568.6915 589.7592 607.9746 748.7406 788.5036 835.7736 861.5564 888.4444 914.1199 942.8000 959.8520 1006.9216 1044.0386 1060.2759 1083.1070 1100.8308 1144.9481 1161.1599 1209.2188 1234.4436 1254.6201 1294.2517 1304.8206 1326.9374 1330.9368 1360.7243 1372.0219 1389.0055 1402.0822 1407.8429 1424.7079 1430.8887 1436.5883 1463.3399 1497.7718 1504.9118 1514.9635 1519.8242 1523.1279 1525.3746 1531.1921 3045.0397 3062.9395 3074.6412 3089.7419 3091.3344 3096.2779 3119.9104 3129.9067 3138.8239 3147.2439 3163.3086 3169.2893 3181.4858 3211.3322 3723.7206

TS_{40}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.96799000	-0.00016000	-0.40181900
H	0.17593200	0.23315200	0.52541100
C	0.27277400	-0.80512800	-1.49484800
H	0.35375300	-0.22596300	-2.42279200
H	0.81455600	-1.74489100	-1.65013000
C	-2.01201300	0.19460900	-0.94124400
H	-1.36736200	1.06799300	-1.07538900
H	-2.83179200	0.30100300	-1.66034800
C	-2.61755700	0.24091500	0.45932900
H	-3.02109900	1.23511300	0.68229900
H	-3.40529200	-0.50970000	0.57673000
O	-1.67383500	-0.12751700	1.46803600
O	-0.59763100	0.72124700	1.41277500
O	1.21515700	1.26766300	-0.96089600

O	1.70382100	2.14425200	0.08458300
H	0.85900700	2.46367300	0.43271900
C	-1.20807300	-1.09611500	-1.20361000
H	-1.62846000	-1.64817000	-2.05066600
H	-1.27174800	-1.75444000	-0.33048600
C	2.15566100	-0.65081000	0.28144100
H	2.88709700	-0.91337300	-0.49598700
H	2.62130300	0.08235100	0.94335800
C	1.73329400	-1.88789800	1.07539500
H	1.00056200	-1.61620100	1.84066600
H	1.28454400	-2.64868200	0.42930600
H	2.59644200	-2.33949500	1.57145000

Absolute energies (Hartree): -575.707416 ZPE (Hartree): 0.221253

Harmonic Vibrational Frequencies (cm^{-1}):

-2345.7896 34.4883 88.6145 122.2346 130.9893 171.0862 218.3870 221.6818 235.0121 288.2282 303.4534 324.9811 336.2291 368.0823 425.7751 440.9167 457.5529 567.8445 595.6379 610.6869 764.0606 797.0742 844.2042 874.9620 895.2055 942.9535 958.8991 1006.6208 1021.0759 1050.8562 1078.1490 1094.2726 1114.4738 1136.5925 1176.4540 1200.1308 1217.3915 1240.4849 1263.8741 1287.0861 1308.2415 1314.9586 1323.6243 1363.9126 1374.7096 1381.1252 1394.9241 1413.5781 1416.5483 1432.1024 1494.6335 1501.2186 1503.8521 1513.4379 1517.7418 1524.4406 1526.6197 1567.6479 3062.8817 3073.9335 3076.6356 3081.5640 3084.5818 3094.9147 3129.6707 3140.3021 3144.7237 3154.2498 3159.4847 3170.7756 3173.4651 3791.4645

O_2C•(CC)CCCCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-5.26440500	0.49614800	-0.22317400
H	-5.65688500	-0.04820800	-0.91539800
O	-4.18191600	-0.38008700	0.17647000
C	2.01387300	-0.28859900	0.07083800
O	2.93450500	-1.28911300	-0.15022600
O	4.16627800	-0.68843800	-0.62722600
H	4.78444000	-1.17779100	-0.07159000
C	-2.98139700	0.26687100	-0.21537100
H	-2.92873200	1.26082000	0.24515400
H	-2.95334300	0.38166400	-1.30736900
C	0.68165600	-0.90267300	0.37212000
H	0.62076100	-1.87512700	-0.12899500
H	0.58016400	-1.08752300	1.45500000
C	-1.84140300	-0.61500100	0.26649100
H	-1.92337400	-0.73814000	1.35212000
H	-1.93875800	-1.60829600	-0.18632500
C	-0.48046200	-0.01515100	-0.08929300
H	-0.39012300	0.97710800	0.36987700

H	-0.40688300	0.12807300	-1.17382000
C	2.46234900	0.97767900	0.74532300
H	1.68512700	1.27608200	1.46015400
H	3.36829600	0.76604200	1.32629700
C	2.73339400	2.13757600	-0.22252100
H	1.83228300	2.37452800	-0.79521600
H	3.04101600	3.03564800	0.32279100
H	3.52225700	1.86283100	-0.92494200

Absolute energies (Hartree): -575.718904 ZPE (Hartree): 0.223526

Harmonic Vibrational Frequencies (cm^{-1}):

37.1492 44.2615 46.9525 81.6973 94.0361 126.0212 137.4187 146.6515 160.3789 193.7286 201.8377 219.4982 242.1114 266.6006 325.0110 352.3475 429.3475 485.1724 503.6042 591.7587 751.2728 777.7508 800.8088 823.2680 912.1599 940.0164 1010.9844 1024.0744 1054.5969 1076.3108 1082.3213 1094.8465 1098.4529 1138.2907 1142.8182 1219.7347 1232.6781 1267.7995 1273.8245 1296.7717 1319.2609 1324.7933 1342.0222 1364.6590 1370.3619 1378.4045 1414.0415 1419.6930 1425.0755 1438.8646 1484.3227 1495.2404 1507.9696 1515.9672 1521.4553 1528.3187 1552.1485 3010.9003 3052.7010 3061.8196 3069.4076 3076.5028 3083.6471 3108.5139 3112.2063 3118.1712 3127.1707 3148.3793 3161.8644 3188.1255 3843.3768 3846.9758

$O_2C(C)CCC(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.68259300	0.11349000	0.78110800
H	1.09702300	-0.59418900	1.36677900
H	2.30563400	0.72954200	1.43595100
C	0.83297500	0.96083800	-0.15303500
H	0.44653500	0.29668400	-0.92997500
C	-0.35549200	1.55888400	0.61578600
H	-0.86457500	2.26840700	-0.04740700
H	0.03705800	2.15977700	1.44941200
C	-1.37183800	0.55534500	1.17823600
H	-2.12130100	1.11184600	1.75647500
H	-0.89480500	-0.12968500	1.88475400
C	-2.14424400	-0.28292700	0.15537800
H	-2.86353500	-0.90490500	0.70661500
O	-1.32355300	-1.15025400	-0.62213500
O	-0.72844400	-2.11257100	0.29331800
H	0.18058100	-2.08928700	-0.04851600
O	2.64966600	-0.67689700	0.02117500
O	2.09389600	-1.70650800	-0.52028500
C	-2.88171400	0.54557900	-0.88729500
H	-3.48715700	-0.10411100	-1.52295900
H	-3.53636200	1.26841400	-0.39197500
H	-2.17704100	1.08817300	-1.52298200

C	1.68139800	2.05780300	-0.79674400
H	2.02913400	2.76753700	-0.03682000
H	2.55689100	1.63566200	-1.29887000
H	1.09732800	2.61190800	-1.53765700

Absolute energies (Hartree): -575.746641 ZPE (Hartree): 0.226724

Harmonic Vibrational Frequencies (cm^{-1}):

53.1475 80.3243 107.9788 136.2197 146.1881 171.1620 203.5707 235.2081 240.4856 256.2423 290.4524 312.0767 362.6912 385.5188 413.6577 454.5352 498.3811 573.8378 600.7996 613.3140 793.1628 815.7001 874.7930 905.6218 912.5075 928.6993 969.7747 973.7151 981.0429 1032.5436 1066.9121 1088.7989 1168.4433 1174.5700 1202.5273 1214.5262 1244.0824 1277.3835 1289.8061 1341.3287 1358.1408 1372.1271 1379.3455 1397.9122 1408.8027 1413.6222 1427.0727 1430.3129 1434.4242 1467.0140 1495.9677 1499.6149 1506.4961 1510.2660 1519.9621 1522.1858 1529.6195 3049.3415 3058.6361 3063.6750 3079.3207 3084.3092 3108.5263 3116.9376 3138.9726 3145.5482 3157.4958 3165.8041 3176.2304 3184.1475 3205.7763 3720.9854

TS_{41}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.29002600	-0.40440500	0.16473100
H	0.72177400	0.60836500	-0.26915700
C	0.29547400	-1.55074400	0.19142400
H	0.23060100	-1.97448600	-0.81749300
H	0.70373200	-2.33141900	0.84791400
C	-1.87412800	-0.28363800	-0.35934900
H	-1.30804400	-0.26966900	-1.29795800
C	-2.01711400	1.16472800	0.10016600
H	-2.44144600	1.77874500	-0.70347300
H	-2.66174200	1.22576400	0.98459200
O	-0.79358900	1.75255200	0.54252200
O	0.11673200	1.70380400	-0.48632300
O	2.26639700	-0.77021800	-0.77500300
O	3.25343900	0.28506600	-0.86250700
H	2.91008500	0.76048300	-1.63028900
C	-1.11253200	-1.15690700	0.66129800
H	-1.67335900	-2.08343000	0.83152400
H	-1.05557200	-0.64749000	1.63059200
C	1.82667100	0.02959200	1.51076600
H	2.36301900	-0.80917400	1.97017200
H	2.50695600	0.87321800	1.40014200
H	0.99835900	0.32845600	2.15687700
C	-3.26970500	-0.84265300	-0.65052400
H	-3.81087600	-0.21509700	-1.36647100
H	-3.19904900	-1.85125300	-1.06836700
H	-3.86041500	-0.89848900	0.27081000

Absolute energies (Hartree): -575.710501 ZPE (Hartree): 0.219975

Harmonic Vibrational Frequencies (cm^{-1}):

-2354.5330 43.5101 95.8060 107.1723 148.1726 164.1668 193.0567 222.7039 251.2396 255.3207 277.6070 295.9966 338.9986 347.2920 388.6649 401.0923 428.6157 520.1950 530.0564 608.5076 618.7959 797.5684 836.0201 893.4129 914.5475 932.5813 945.0081 972.9507 986.5872 1027.1348 1067.6452 1088.9984 1114.1727 1169.0544 1172.1667 1184.5379 1212.2780 1230.3396 1255.3757 1289.4838 1301.3619 1330.4914 1351.1137 1360.7908 1381.3638 1386.6550 1408.7712 1413.0244 1419.5806 1429.0242 1488.2262 1495.7726 1499.0782 1503.1367 1515.6114 1519.2973 1522.0263 1569.3591 3059.0952 3062.1744 3070.7824 3073.5347 3075.6347 3092.3574 3119.4029 3129.9973 3140.4486 3151.9016 3159.8664 3173.3407 3210.7067 3817.1983

O_2C•(C)CCC(C)COO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.82859900	-0.78737900	-0.23316200
H	5.04753500	-0.99500500	-1.14908700
O	3.72247900	0.12045600	-0.45728100
C	-2.43001600	-0.22605300	-0.04324600
O	-3.41756100	0.57689300	-0.58118900
O	-4.61676400	-0.20331600	-0.80400600
H	-5.21736300	0.27741200	-0.22233400
C	2.55423800	-0.55653800	-0.01922200
H	2.68224400	-0.87756100	1.02306100
H	2.37697900	-1.44112400	-0.64628700
C	-1.15746300	0.56767100	-0.01411300
H	-1.09220200	1.14223700	-0.94592300
H	-1.19235700	1.29674700	0.81106700
C	1.39780400	0.42984000	-0.13542400
H	1.38223000	0.79742500	-1.17091200
C	0.08544100	-0.31919400	0.12487200
H	0.12314600	-0.75540000	1.13200700
H	-0.00060900	-1.15249800	-0.58373300
C	-2.80056900	-1.11541600	1.10182300
H	-1.96276400	-1.76520400	1.36155700
H	-3.05275000	-0.51443200	1.99140200
H	-3.65992100	-1.73816900	0.85301000
C	1.59722600	1.61227000	0.81428700
H	0.84543500	2.38911900	0.65203900
H	1.52098100	1.27306700	1.85456400
H	2.58542500	2.05467900	0.67080400

Absolute energies (Hartree): -575.721315 ZPE (Hartree): 0.222819

Harmonic Vibrational Frequencies (cm^{-1}):

25.9341 48.3737 67.5277 84.7986 100.7973 115.2095 122.8546 167.6072 204.3755 208.8481 223.9289 229.7006 251.9282 291.6952 333.4955 363.5628 386.2323 428.0373 497.8074 514.9848 589.8973 777.1873 837.6214

880.4474 920.8791 948.2243 950.2889 973.3896 995.2015 1037.7778 1054.2062 1078.3338 1109.9828 1153.7175 1170.8851 1196.3254 1222.4441 1248.6907 1276.3800 1294.8419 1306.8554 1334.8255 1356.0621 1368.7910 1393.2942 1395.3043 1409.8189 1422.8307 1424.3902 1432.0356 1489.5251 1495.3022 1506.7185 1513.4135 1514.1001 1528.2544 1543.4630 3014.4874 3026.3329 3044.3667 3057.9735 3066.1191 3071.5693 3102.0439 3107.6283 3122.8925 3150.8544 3156.5333 3180.8367 3201.7383 3840.3939 3842.9936

O_2CCCCCCOO•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.40391300	-1.03173800	-0.51843900
H	0.95926600	-0.35544000	-1.24762700
H	1.64351900	-1.99534000	-0.97433200
C	0.55654500	-1.17805200	0.73169900
H	1.11861300	-1.77802400	1.45724200
H	0.42263100	-0.18804400	1.16713800
C	-0.78853500	-1.87064600	0.45702400
H	-1.33480500	-1.95583200	1.40526000
H	-0.57126100	-2.89904500	0.14010400
C	-1.70692200	-1.23067400	-0.59817100
H	-2.41789900	-1.99719400	-0.92877700
H	-1.12985200	-0.95111700	-1.48456700
C	-2.52868000	-0.01999600	-0.13293000
H	-3.24408100	-0.33436800	0.63744300
H	-3.11244800	0.35379400	-0.98135300
O	-0.68157500	1.39024800	-0.49406300
O	2.71369300	-0.48197000	-0.17299100
O	2.64990400	0.77359000	0.10510300
C	-1.70624300	1.12221500	0.44674000
H	-2.32282900	2.01650300	0.59715500
H	-1.26684300	0.84523200	1.41174300
O	0.17580000	2.39209700	0.11150000
H	1.01294900	1.90049400	0.08863200

Absolute energies (Hartree): -536.482891 ZPE (Hartree): 0.199585

Harmonic Vibrational Frequencies (cm^{-1}):

56.8827 104.3972 122.1108 133.1534 166.1519 190.3454 230.6479 238.6693 263.1915 315.7548 339.5886 406.1282 463.7998 533.0230 549.9984 591.3533 752.1985 790.2942 825.1725 859.8718 907.5172 936.8621 955.3939 984.3158 1037.7818 1070.9004 1093.9013 1145.6261 1153.3291 1162.8466 1228.5832 1253.6458 1267.7342 1310.3830 1312.9119 1331.1591 1355.3682 1377.8308 1390.8848 1406.3565 1410.0528 1429.8814 1436.2890 1472.5772 1491.1088 1500.5924 1512.3934 1513.6544 1521.4695 1563.0108 3058.8448 3068.6915 3075.9782 3084.0574 3093.6648 3109.7055 3115.3233 3126.6511 3132.9108 3145.8503 3189.1913 3213.4933 3726.0133

TS_{42}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.33865200	-0.29391100	0.35087100
O	-1.76995300	-1.27691100	-0.52840700
C	0.32779100	1.72325900	0.31396000
O	-0.80933500	-2.01421200	0.15030900
C	0.79569400	0.58006700	1.22361700
C	1.22954500	-0.67000900	0.48798000
H	-1.86025700	-0.39456900	1.32572600
H	-0.03566000	2.54270500	0.94754600
H	0.03216600	0.30150600	1.95738500
H	-3.40468500	-0.52138800	0.46501000
H	1.20791100	2.11257800	-0.21163700
H	1.65707100	0.93600100	1.80791400
H	1.74208400	-1.40885100	1.11354400
C	-2.14780700	1.09156100	-0.26074700
H	-2.47268400	1.84480400	0.47003700
H	-2.82295700	1.17286500	-1.12010200
C	-0.72725700	1.39732200	-0.75082400
H	-0.38037200	0.57118600	-1.37929200
H	-0.79273600	2.27279900	-1.40786600
H	0.15897500	-1.35933400	0.16035500
O	1.90673800	-0.46640200	-0.71819900
O	3.27125200	-0.21147400	-0.36415300
H	3.34563900	0.71195300	-0.63415700

Absolute energies (Hartree): -536.440498 ZPE (Hartree): 0.192571

Harmonic Vibrational Frequencies (cm^{-1}):

-2210.8201 39.9303 71.8204 99.9738 163.7306 179.0031 199.0413 219.2206 237.5393 297.5427 331.7215 394.6710 415.3584 501.4249 516.7095 579.8956 638.4816 744.1686 800.2921 811.3123 876.0831 918.7586 955.6261 991.2287 1046.0486 1049.7481 1096.2666 1114.7334 1130.5617 1157.5200 1172.2632 1198.7889 1214.2700 1248.8507 1289.1232 1311.9569 1335.2181 1368.6484 1373.9204 1387.8508 1398.4542 1410.9971 1417.9415 1422.5045 1484.6909 1492.8372 1501.2424 1505.0821 1511.7066 1526.9214 1529.5717 3050.2427 3063.6225 3066.5459 3081.2184 3088.8943 3109.9054 3119.0229 3121.0556 3131.1755 3143.3156 3179.3398 3831.3016

O_2C•CCCCCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	5.26039400	-0.14781700	0.08369100
H	5.52163800	-0.71204500	0.82049200
O	3.95971700	-0.72104000	-0.19807400
C	-3.34845600	0.60280200	-0.28815200
H	-4.20154500	1.26476100	-0.41186000

O	-3.62892700	-0.56471800	0.37906900
O	-4.98882900	-0.94386600	0.08345300
H	-4.83074100	-1.56345200	-0.63966300
C	3.00525200	0.27197600	0.14295000
H	3.20689200	1.18956100	-0.42282700
H	3.06394900	0.49869100	1.21618700
C	1.64354200	-0.29890700	-0.21689400
H	1.63489900	-0.54748900	-1.28391200
H	1.48563700	-1.22984800	0.33943500
C	0.51673300	0.68678300	0.09563900
H	0.68060400	1.61753200	-0.46375200
H	0.54365200	0.94862500	1.16174300
C	-0.86254600	0.12743500	-0.24990800
H	-1.03130600	-0.80004400	0.30831700
H	-0.89673900	-0.12905200	-1.31602000
C	-1.99019400	1.11909300	0.06192100
H	-1.83128100	2.04739900	-0.49847600
H	-1.95049300	1.37980100	1.13188700

Absolute energies (Hartree): -536.459487 ZPE (Hartree): 0.19452

Harmonic Vibrational Frequencies (cm^{-1}):

33.9609 45.0464 62.1709 84.6766 100.5357 103.0315 134.8848 151.0415 198.0775 200.4356 240.2501 253.2396 298.7321 383.8627 431.3760 517.0975 577.0254 740.8031 749.8048 778.6477 849.9340 911.9064 921.8183 976.6724 1004.0109 1058.8208 1068.7692 1091.7321 1100.3702 1135.7319 1152.0851 1213.7892 1232.9805 1248.1501 1281.4939 1313.8820 1319.0500 1338.3534 1343.2999 1367.8080 1373.9334 1387.4149 1388.2021 1420.4042 1439.1043 1485.0968 1506.1987 1512.9112 1524.8884 1552.5637 3025.4705 3050.9765 3055.8340 3075.3115 3083.7787 3100.6461 3108.4401 3114.7518 3137.4991 3147.8459 3206.1321 3827.7360 3843.8152

$O_2CCCCCCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.36931200	-1.54937500	-0.42917500
H	1.08552900	-0.98751000	-1.32073700
H	1.51715200	-2.60257000	-0.68050100
C	0.40640700	-1.37050100	0.73151800
H	0.85295000	-1.85556600	1.60751600
H	0.32966400	-0.30562500	0.95759700
C	-0.96504300	-2.01086700	0.45748400
H	-1.55256500	-1.98481300	1.38386100
H	-0.79693800	-3.07298900	0.23658700
C	-1.80105500	-1.39262900	-0.67902100
H	-2.45239000	-2.17141400	-1.09296800
H	-1.15105800	-1.08628900	-1.50592400
C	-2.70518400	-0.22441700	-0.25165400

H	-3.48871800	-0.61974200	0.40680600
H	-3.21594300	0.16728000	-1.14098400
O	2.70618800	-1.09924100	-0.05609700
O	2.79576700	0.18551400	-0.02469700
C	-1.99785200	0.92226300	0.47879100
H	-2.73320600	1.67284100	0.78559300
H	-1.53714000	0.54675500	1.39785500
C	-0.91637400	1.57998000	-0.37015300
H	-1.32858700	2.35174800	-1.03113400
H	-0.39655100	0.84113500	-0.99100700
O	0.01173200	2.15104300	0.53814500
O	1.08833800	2.69120400	-0.26232800
H	1.71033600	1.95188600	-0.19948900

Absolute energies (Hartree): -575.731845 ZPE (Hartree): 0.227997

Harmonic Vibrational Frequencies (cm^{-1}):

42.4873 66.8025 93.3661 98.6522 134.8701 161.0545 171.5999 189.4280 238.2445 260.9939 295.6366 312.7263 389.9763 424.5993 465.6604 471.1551 510.2070 577.6997 749.2137 784.4001 811.4677 858.9382 875.8811 912.1268 944.4920 969.1239 974.0950 1048.0446 1074.6265 1082.3845 1098.3557 1147.2667 1148.7259 1160.3847 1215.7413 1242.2764 1258.2166 1294.9602 1300.6570 1313.8930 1328.7135 1353.1432 1356.7517 1372.1879 1393.2244 1405.4560 1408.8219 1424.5056 1436.9221 1439.5785 1497.9862 1505.0144 1508.4755 1514.6636 1521.7295 1529.1755 1553.5202 3059.9766 3062.5851 3069.3446 3080.1992 3092.1034 3095.7486 3111.3766 3112.2618 3115.8014 3118.2278 3132.6632 3149.8954 3175.5710 3196.1067 3786.9396

TS_{43}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.48988100	0.74940700	0.51980100
H	0.73254300	-0.14970800	0.95419900
H	1.86070900	1.21317500	1.44124600
C	0.75143800	1.70876500	-0.38938100
H	1.45073300	2.52603100	-0.61652500
H	0.52635300	1.22303000	-1.33889500
C	-0.51150900	2.29356000	0.25216000
H	-0.91984000	3.04690100	-0.43324500
H	-0.22583600	2.83309500	1.16535700
C	-1.63128100	1.30141800	0.60538400
H	-2.44797000	1.89236900	1.03836300
H	-1.30671300	0.61306500	1.38994500
C	-2.20612900	0.51296400	-0.58087000
H	-2.32140600	1.19661200	-1.43322600
H	-3.22096600	0.18658300	-0.31787700
O	2.59298500	0.09403600	-0.02157200
O	2.13185700	-0.67510700	-1.16124900

C	-1.44009400	-0.73102400	-1.06209000
H	-1.95653400	-1.10356300	-1.95490600
H	-0.42533500	-0.48830600	-1.38307300
C	-1.34091100	-1.88668500	-0.05545500
H	-1.53568200	-2.84466000	-0.54576900
H	-2.03450600	-1.76871600	0.78389800
O	-0.02179100	-2.07891500	0.47927200
O	0.21492900	-1.16455400	1.48103200
H	1.81224300	-1.47002200	-0.70665900

Absolute energies (Hartree): -575.695676 ZPE (Hartree): 0.222335

Harmonic Vibrational Frequencies (cm^{-1}):

-2506.0169 77.6974 92.0485 131.1706 150.1210 166.9007 214.6092 221.8714 269.1881 288.1752 325.2085 376.2888 402.8723 430.2462 439.0086 500.8616 523.1710 560.2207 617.4115 733.8436 786.0412 824.5864 842.3442 865.8173 902.1501 956.9032 966.7787 1024.9916 1045.7726 1049.0609 1090.3227 1121.1201 1127.9348 1147.8431 1168.0574 1178.0215 1219.3371 1232.3451 1264.5921 1306.5548 1316.3102 1330.0269 1337.9259 1351.6455 1375.3940 1398.9791 1409.3176 1415.2865 1420.2053 1423.8368 1434.9721 1489.2394 1495.7999 1498.1678 1504.9909 1515.5915 1516.9416 1526.6429 3051.7591 3055.3260 3065.6964 3079.0526 3084.3289 3091.8516 3102.2142 3107.3291 3123.3175 3154.0001 3159.5314 3166.4642 3186.7852 3763.5192

O_2C•CCCCCCOO

Cartesian Coordinates (Å)

At.	X	Y	Z
O	4.96061800	-1.55243900	-0.11312600
H	5.49589300	-1.54897000	0.68881600
O	3.80067200	-0.83856100	0.37866700
C	-3.83750200	0.40954100	-0.21932600
H	-4.79273800	0.92590400	-0.26891000
O	-3.90440300	-0.85531700	0.31217200
O	-5.18141600	-1.42939100	-0.03617200
H	-4.92458800	-1.93011600	-0.82039600
C	3.78337300	0.41076300	-0.29620400
H	3.77693800	0.24376800	-1.38028700
H	4.67694800	0.99108600	-0.03108800
C	-0.03311300	1.11196900	0.16030500
H	-0.04113700	2.11606700	-0.28659000
H	-0.02536300	1.25155000	1.24995000
C	-1.30573500	0.36903300	-0.24357400
H	-1.29949900	-0.63246500	0.20071900
H	-1.32186900	0.23564900	-1.33267000
C	-2.57959400	1.10718800	0.18679800
H	-2.59470500	2.10831000	-0.25905500
H	-2.56061500	1.24374700	1.28011600
C	1.23881700	0.37823300	-0.26305400

H	1.24463500	-0.62678600	0.17178800
H	1.23716900	0.25153600	-1.35428000
C	2.51238200	1.11604500	0.15097200
H	2.51664000	2.12243600	-0.28663100
H	2.53674800	1.23731600	1.24068500

Absolute energies (Hartree): -575.713651 ZPE (Hartree): 0.223333

Harmonic Vibrational Frequencies (cm^{-1}):

28.1129 35.4235 56.0809 82.8297 87.9086 102.6753 113.4372 137.1728 152.2964 195.3791 207.6128 253.4758 260.8057 306.4668 320.4151 397.8397 432.2826 545.7297 586.4761 734.9010 746.9158 755.5177 810.8613 890.6566 921.9482 924.0162 955.0347 1000.0639 1021.8705 1063.1970 1075.4671 1098.5386 1115.7516 1135.8152 1148.6023 1201.9321 1227.0246 1241.4080 1270.5435 1292.4382 1313.3999 1331.6243 1339.1952 1347.7317 1368.8987 1371.5127 1379.7093 1386.5083 1411.8835 1423.8124 1428.3876 1484.9557 1491.8015 1504.3043 1510.8235 1523.9726 1546.8983 3025.4401 3047.7111 3053.4345 3063.6006 3072.2546 3073.9450 3094.9085 3110.1647 3113.0474 3122.0432 3136.1311 3143.9332 3204.0521 3828.1583 3842.7261

TS_{44}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	2.73311100	-0.14738100	-0.06953900
O	1.57477700	-0.89648300	0.18356700
C	0.55636200	-0.05614300	-0.34776500
H	0.59565100	-0.05217700	-1.44324700
C	0.94958400	1.31792400	0.19134000
H	2.17130600	0.95776500	0.12145300
H	0.74119500	1.46224600	1.25263400
H	0.75077700	2.18892800	-0.42882500
C	-0.77793600	-0.58921900	0.14490000
H	-0.98864600	-1.57372700	-0.28429500
H	-0.77038000	-0.65661000	1.23946000
O	-1.72909500	0.36164600	-0.30153600
O	-3.02608000	-0.17264000	0.04996100
H	-3.28966900	0.47706400	0.71234700

Absolute energies (Hartree): -418.656138 ZPE (Hartree): 0.104556

Harmonic Vibrational Frequencies (cm^{-1}):

-2795.5977 78.8626 101.3132 145.3070 193.0534 232.4306 360.9491 381.8030 436.2091 550.3753 652.7928 717.9727 892.2023 922.6666 965.6588 1038.1561 1093.7454 1138.4372 1163.5281 1170.7422 1202.8069 1241.9528 1255.4839 1337.2657 1376.7480 1386.0362 1437.0199 1478.3640 1551.2778 1835.6003 3074.4014 3100.2062 3143.2008 3145.9097 3252.2510 3840.1394

$O_2CC(C•)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z

C	-0.64130500	0.45365200	-0.24550200
H	-0.70192200	0.25301400	-1.32703400
C	-0.56124100	1.91379000	0.02843900
H	-1.46739100	2.50444400	0.03539700
H	0.40397600	2.39973000	0.04008600
C	0.54635500	-0.32293600	0.32126100
H	0.63220600	-0.13110700	1.39791000
H	0.41178100	-1.39192200	0.14057700
O	-1.84848100	0.00386200	0.36889100
O	-2.09770000	-1.33494900	-0.13119400
H	-2.88440900	-1.15564700	-0.65946400
O	1.68338900	0.15877400	-0.37708500
O	2.79722900	-0.66656500	0.03398600
H	3.26740600	-0.03451900	0.59056400

Absolute energies (Hartree): -418.689787 ZPE (Hartree): 0.106174

Harmonic Vibrational Frequencies (cm^{-1}):

86.3869 109.0122 138.3935 168.0136 181.3536 211.7357 218.0681 278.2875 352.3524 414.0729 465.2945 512.0685 568.3953 875.2749 916.1477 944.0695 961.8801 1072.1083 1107.7786 1167.5833 1194.2675 1249.9484 1342.4881 1359.2933 1373.0443 1378.5007 1427.3955 1473.4807 1546.8271 3026.3545 3076.2353 3163.8790 3219.9044 3347.1399 3836.8457 3841.1899

TS_{45}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.30535300	-0.06409700	-0.16942100
O	2.19214400	-0.86545500	0.11819300
C	1.11081300	-0.04357600	-0.31495800
H	1.11429700	0.01815600	-1.41202400
C	1.49433600	1.31908300	0.26720500
H	2.72207500	1.00636900	0.10772300
H	1.34433100	1.40556900	1.34486500
H	1.23881100	2.21501400	-0.29602700
C	-0.18180500	-0.64896300	0.20037100
H	-0.29176100	-1.66142300	-0.20082200
H	-0.13643900	-0.71402500	1.29137300
O	-2.52024100	-0.48690100	0.26740900
C	-1.37666200	0.19484000	-0.21641900
H	-1.42800500	0.29384800	-1.30904800
H	-1.33075900	1.19679500	0.22700400
O	-3.65148200	0.35938800	-0.05538400
H	-4.11883800	-0.23209100	-0.65661400

Absolute energies (Hartree): -457.913762 ZPE (Hartree): 0.133441

Harmonic Vibrational Frequencies (cm^{-1}):

-2831.9105 63.5617 77.8282 109.5117 139.7720 188.5521 232.1049 295.9202 316.0332 418.5281 497.4477 550.2355 651.9891 712.0286 824.8195 894.6206 921.8854 978.1961 1031.2699 1080.3717 1089.0757 1149.0668 1166.8211 1168.7903 1203.5940 1239.6159 1259.5629 1302.2229 1312.4516 1370.5734 1374.3006 1405.6181 1446.0966 1475.6642 1518.7165 1550.7569 1832.5714 3053.3099 3068.2375 3100.5435 3110.6604 3137.2272 3165.9121 3242.7169 3845.0799

$O_2CCC(C•)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.11488700	0.12358500	-0.22738500
H	-1.12096100	0.09790400	-1.32375800
C	-1.31423500	1.51913300	0.26385800
H	-1.34277900	2.36613300	-0.40806700
H	-1.39871500	1.68727600	1.33194100
C	0.16991400	-0.51768000	0.30249900
H	0.16086900	-0.49453800	1.39653600
H	0.19745700	-1.56258300	-0.02058300
O	-2.14309000	-0.75438200	0.24681300
O	-3.37334900	-0.34315100	-0.39313100
H	-3.77571800	0.15789100	0.32631300
O	2.51342300	-0.52450200	0.27231700
C	1.40155800	0.20950100	-0.21343100
H	1.44547100	1.23795700	0.16094800
H	1.41336200	0.23062700	-1.31167500
O	3.69003100	0.21084200	-0.14558500
H	4.07079900	-0.43835700	-0.74820600

Absolute energies (Hartree): -457.946255 ZPE (Hartree): 0.135002

Harmonic Vibrational Frequencies (cm^{-1}):

55.9868 62.5561 78.8901 114.0281 132.6047 160.8584 194.9013 246.3883 275.5805 294.9616 329.6562 440.0758 462.9617 527.6856 604.8708 829.8320 890.7024 914.9136 934.7512 980.7584 1046.2888 1088.4238 1118.3390 1177.9329 1190.3738 1251.2822 1299.5718 1311.2245 1359.4455 1371.7751 1376.8207 1401.9380 1439.6347 1485.6473 1518.1104 1550.7632 3054.5687 3090.0357 3101.1576 3120.3914 3166.5694 3199.7720 3326.0759 3835.2050 3844.6422

TS_{46}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	3.90161700	-0.08550300	-0.11886400
O	2.77277000	-0.88281700	0.11657700
C	1.70949900	-0.03849200	-0.32007400
H	1.73694800	0.05133900	-1.41504500
C	2.09252100	1.30475900	0.30569200
H	3.32027900	0.98395300	0.16965200

H	1.91743400	1.36588500	1.38152100
H	1.85935300	2.21720800	-0.24015900
C	0.39686000	-0.63791600	0.14698900
H	0.29760100	-1.64170200	-0.28249300
H	0.43480600	-0.74535300	1.23698400
C	-0.79434400	0.23010900	-0.26190300
H	-0.79675100	0.37614900	-1.34807500
H	-0.72142100	1.21884800	0.20427500
O	-3.12810100	0.49570300	-0.24372600
C	-2.10976700	-0.40565300	0.15790700
H	-2.14523700	-0.54753000	1.24456700
H	-2.24921100	-1.37881700	-0.33137100
O	-4.37597500	-0.07061400	0.22516600
H	-4.78490700	-0.27097700	-0.62474700

Absolute energies (Hartree): -497.169172 ZPE (Hartree): 0.162298

Harmonic Vibrational Frequencies (cm^{-1}):

-2812.9877 50.8510 60.2155 83.2680 120.1822 143.0487 200.4377 205.5713 242.7501 283.5944 390.6203 436.8997 515.6759 534.6078 652.6870 709.6277 778.6379 868.0313 912.5526 917.1071 993.9252 1036.2172 1070.4774 1084.0921 1097.9158 1143.7514 1171.5287 1172.7573 1205.3421 1238.9855 1246.5179 1276.3763 1306.3869 1330.3750 1355.0345 1371.4282 1382.3533 1415.0714 1442.7102 1475.3742 1509.9087 1521.0734 1552.7408 1832.2069 3055.9673 3066.2582 3076.8153 3085.8164 3112.3264 3130.9390 3136.1359 3151.1647 3242.7647 3843.3141

$O_2CCCC(C\bullet)OO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.71807000	0.12883400	-0.22512300
H	-1.73783100	0.13038900	-1.32203200
C	-1.94968200	1.50477000	0.30477300
H	-1.84917600	2.38251400	-0.31934600
H	-2.11108200	1.62980500	1.37016000
C	-0.40326900	-0.48680800	0.26262900
H	-0.41344500	-0.50784900	1.35871600
H	-0.36714300	-1.52369000	-0.09035300
O	-2.71279200	-0.78733500	0.24378300
O	-3.96312400	-0.41224200	-0.37930200
H	-4.36008500	0.09985200	0.33547500
C	0.81622100	0.28698900	-0.23861600
H	0.80987600	1.30677600	0.15877500
H	0.79071000	0.35684000	-1.33216300
O	3.16217800	0.41918000	-0.30418600
C	2.10747200	-0.39355400	0.18518600
H	2.17837100	-1.40294700	-0.24155100

H	2.17021200	-0.46649100	1.27751100
O	4.39157800	-0.19051100	0.15957800
H	4.75083800	-0.47931300	-0.68726600

Absolute energies (Hartree): -497.201298 ZPE (Hartree): 0.163978

Harmonic Vibrational Frequencies (cm^{-1}):

49.8950 56.0443 84.3773 109.3807 125.9870 144.0897 159.0648 202.6258 219.2265 244.4519 261.7938 312.0518 394.9748 461.5625 483.0344 517.0345 602.3266 782.0714 882.0762 892.9149 911.3594 929.9585 1001.2843 1053.4230 1086.5665 1093.3130 1114.8035 1178.8612 1191.0569 1236.4709 1276.7314 1301.4870 1329.0329 1340.9810 1369.2306 1373.7064 1390.8116 1403.6569 1440.4447 1483.0281 1509.5838 1521.0593 1552.6559 3054.9322 3076.3710 3084.6954 3089.6218 3112.0263 3132.7811 3154.7136 3197.9215 3323.9960 3833.1310 3843.2502

TS_{47}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-1.98977700	-1.21013400	-0.24703200
O	-2.59686800	-0.00385900	0.11937200
C	-1.56706900	0.93093600	-0.16314400
H	-1.85496800	1.88173700	0.29247600
H	-1.43156900	1.04501600	-1.24597400
C	-0.33154500	0.26588000	0.44849400
H	-0.85450900	-0.86345800	0.17644100
H	-0.28221400	0.31318800	1.53830200
C	0.98638700	0.47248000	-0.23802700
H	1.29692500	1.52526900	-0.16698400
H	0.92040200	0.19996000	-1.29939700
O	1.92164000	-0.35142800	0.43423100
O	3.20161500	-0.07988500	-0.18564200
H	3.38639900	-0.95503900	-0.54623900

Absolute energies (Hartree): -418.655841 ZPE (Hartree): 0.105132

Harmonic Vibrational Frequencies (cm^{-1}):

-2783.7455 66.1583 91.9388 156.7419 172.0595 200.1891 349.2442 379.7605 442.3195 621.0567 702.0789 823.9015 918.8129 955.5314 1002.5763 1058.5487 1114.3949 1123.2252 1161.3839 1188.8979 1256.9853 1268.4817 1292.4158 1308.3826 1377.6101 1393.6989 1449.5129 1518.0657 1532.9215 1834.8854 3040.1099 3073.5432 3096.1873 3159.6748 3172.3225 3843.8108

$O_2CC•COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.12646300	-0.54528000	-0.48795700
H	1.81755500	-1.26382700	-0.94892800

H	0.76217900	0.14270400	-1.26031200
C	-0.00455100	-1.24084900	0.18893200
H	0.22282000	-1.89992100	1.01764700
C	-1.41417700	-0.86577000	-0.11367400
H	-1.61382400	-0.91925900	-1.19322500
H	-2.12860400	-1.50725500	0.41067600
O	-1.57203400	0.49019900	0.31410500
O	-2.91935400	0.86467600	-0.05918500
H	-2.71695000	1.56000100	-0.69545700
O	1.82673100	0.17664200	0.52305900
O	2.99251500	0.73446100	-0.13088200
H	2.78755500	1.67113300	-0.03099000

Absolute energies (Hartree): -418.68878 ZPE (Hartree): 0.107851

Harmonic Vibrational Frequencies (cm^{-1}):

16.1525 67.6006 103.7099 119.7487 185.4776 198.5263 240.4832 279.7455 342.3577 459.3609 512.7846 558.0575 942.5463 957.5541 991.5257 1012.1389 1069.5608 1073.9062 1153.8198 1185.1499 1252.1422 1278.0184 1355.1609 1364.2884 1376.8260 1418.9222 1463.4628 1530.5317 1537.5751 3047.2456 3050.4207 3108.8842 3133.3803 3261.2443 3845.8664 3846.8942

TS_{48}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.46688900	-1.28937300	-0.30888400
O	-3.16858600	-0.17110600	0.15203700
C	-2.24176900	0.87220900	-0.10538600
H	-2.60712800	1.76721400	0.40567100
H	-2.14402200	1.05136000	-1.18322200
C	-0.93087000	0.29998400	0.44163300
H	-1.35068000	-0.85190700	0.09537000
H	-0.90303500	0.26322000	1.53489800
C	0.36774000	0.68313500	-0.21612300
H	0.58129000	1.74331500	-0.02197500
H	0.28512000	0.56076300	-1.30150300
O	2.67949900	0.31332800	-0.37941500
C	1.52897200	-0.15106500	0.30486300
H	1.36564800	-1.21687800	0.09820600
H	1.65527300	-0.01398900	1.38520200
O	3.79736800	-0.42659600	0.16746800
H	4.04195300	-0.93870400	-0.61221800

Absolute energies (Hartree): -457.912657 ZPE (Hartree): 0.134053

Harmonic Vibrational Frequencies (cm^{-1}):

-2760.0562 52.6399 69.9726 108.8360 134.5038 171.8498 205.3173 286.7064 324.4485 401.1911 505.7887

600.6735 698.2465 786.4066 855.1709 918.0940 987.4805 1001.9192 1041.3953 1085.1375 1119.3139 1140.7318 1160.8972 1194.1220 1247.9825 1261.5964 1280.7258 1288.8521 1313.4323 1362.3307 1374.6833 1413.4160 1446.3919 1498.6687 1519.7010 1551.9651 1842.8824 3057.3448 3064.8415 3075.0453 3113.4617 3131.2169 3142.5714 3162.5088 3842.1661

$O_2CCC•COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.94678000	0.45851100	0.05509000
H	-2.29494200	1.16232900	0.82804700
H	-1.89514100	1.00203000	-0.89892400
C	-0.62838900	-0.13610100	0.40753100
H	-0.62899900	-0.93760600	1.14029200
C	0.64098600	0.60096500	0.13035300
H	0.56853600	1.14249300	-0.81974900
H	0.83779400	1.35443400	0.90928400
O	2.97440000	0.47303500	-0.12418500
O	-2.87039400	-0.61896300	-0.03294900
O	-4.17715500	-0.00963300	-0.17523200
H	-4.40082400	-0.33197500	-1.05574100
C	1.83430700	-0.34492900	0.08170500
H	1.72833900	-1.06620800	-0.73795300
H	1.93359300	-0.89166600	1.02656300
O	4.11760800	-0.41484400	-0.09561900
H	4.39521400	-0.34127900	-1.01600800

Absolute energies (Hartree): -457.944814 ZPE (Hartree): 0.135707

Harmonic Vibrational Frequencies (cm^{-1}):

26.8512 31.4016 73.3466 107.7806 126.9957 157.1651 179.9161 198.3495 230.2387 287.0729 393.8155 483.1722 514.5013 520.8195 805.5406 907.7082 921.2438 969.7003 1037.7514 1072.1761 1093.5890 1102.3895 1161.6410 1174.3889 1235.5905 1251.3196 1270.2730 1306.5953 1361.1145 1371.4025 1379.2146 1430.6896 1466.7983 1497.9531 1530.1354 1552.3553 3015.4247 3030.9504 3065.5256 3070.4352 3108.3121 3129.8324 3225.7683 3843.6533 3847.4644

TS_{49}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.03731200	-1.31507000	-0.34246600
O	-3.77711800	-0.20684100	0.08233000
C	-2.85981400	0.85204700	-0.14445900
H	-3.26111000	1.74227700	0.34791000
H	-2.72586700	1.02914400	-1.21904600
C	-1.55884500	0.30737500	0.45255600
H	-1.94446000	-0.85501500	0.10670400

H	-1.56185300	0.28379100	1.54661700
C	-0.24323100	0.69664600	-0.16679600
H	-0.07615700	1.77210300	-0.00168000
H	-0.30131100	0.55160300	-1.25299400
C	0.93450800	-0.09453000	0.40706900
H	0.76308100	-1.16661900	0.26076200
H	1.01443300	0.08437100	1.48456900
O	3.25322300	-0.47529600	0.36760900
C	2.24405400	0.29890400	-0.25752700
H	2.45066900	1.36635300	-0.11269600
H	2.21652400	0.08697200	-1.33477500
O	4.50762600	-0.05114100	-0.22074400
H	4.75466900	-0.87085900	-0.66426100

Absolute energies (Hartree): -497.167185 ZPE (Hartree): 0.162815

Harmonic Vibrational Frequencies (cm^{-1}):

-2736.9425 43.8563 51.9606 87.5328 107.7029 135.7653 170.5692 196.0629 220.7924 288.4683 370.4852 438.3158 510.7246 598.6736 695.2329 762.6487 814.9981 898.5428 914.0758 991.8446 1013.1817 1039.6165 1068.5096 1094.1034 1122.1248 1142.7861 1165.2595 1197.1385 1239.1011 1249.6012 1274.9401 1284.7136 1309.8437 1326.8417 1335.0259 1371.1463 1386.3742 1426.6436 1443.6435 1491.9520 1518.3593 1518.9714 1552.4658 1840.7589 3039.5985 3053.9453 3071.7158 3087.7295 3100.9439 3109.1370 3137.8917 3150.5856 3160.2317 3844.2674

$O_2CCCC•COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.67663500	0.66014800	0.36419900
H	3.37467100	1.49688700	0.26324900
H	2.65579500	0.33476600	1.41401500
C	1.30884600	1.01032000	-0.11100300
H	1.18303100	1.85211800	-0.78418400
C	0.19809600	0.02103700	0.02042800
H	0.28782600	-0.73666400	-0.77509400
H	0.30986800	-0.52528600	0.96701600
O	3.11901900	-0.43541300	-0.44782800
O	4.43134000	-0.79674800	0.04321300
H	4.22455800	-1.65644100	0.42764600
C	-1.19002900	0.66459500	-0.04963900
H	-1.29511500	1.21291400	-0.99230600
H	-1.30883100	1.38349200	0.76718000
O	-3.51836100	0.32561000	-0.02619700
C	-2.28994200	-0.37965300	0.04481800
H	-2.23046400	-0.92612700	0.99384300
H	-2.21863100	-1.09931400	-0.78195200

O	-4.56318300	-0.66517700	0.13490400
H	-4.95486200	-0.62119500	-0.74496500

Absolute energies (Hartree): -497.200194 ZPE (Hartree): 0.165244

Harmonic Vibrational Frequencies (cm^{-1}):

32.5518 44.5035 64.5586 99.9630 118.9670 123.7578 146.2797 198.2844 212.0421 233.3305 275.7485 315.4168 423.2267 460.0362 489.9743 602.3198 765.2377 873.6228 909.4406 941.9650 991.8321 1045.7087 1055.1555 1072.0223 1094.1234 1113.6277 1160.8934 1187.7194 1230.2862 1253.2660 1282.0682 1305.1653 1324.3171 1357.7204 1363.2301 1371.5346 1406.6535 1438.2255 1452.2067 1486.1421 1519.5193 1535.5384 1552.4112 3021.1657 3046.6841 3052.6587 3082.4853 3090.0003 3109.1599 3129.7660 3152.1314 3233.0886 3841.6889 3844.1276

TS_{50}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.33714300	-0.61072200	0.88579300
O	-2.37415600	-0.44656400	-0.50037800
C	-0.99988400	-0.56234600	-0.83885300
H	-0.88725400	-0.23612700	-1.87648700
H	-0.65306700	-1.59520300	-0.71350900
C	-0.32137700	0.35136600	0.19364500
H	-1.23628800	0.01085600	1.00925300
C	-0.44544600	1.82812700	-0.09276300
H	-0.18836900	2.42380900	0.78756100
H	0.24491200	2.09938400	-0.90048500
H	-1.46512000	2.06895200	-0.40407800
C	1.01773500	-0.11385700	0.70529700
H	1.38684100	0.53227600	1.50950700
H	0.96397500	-1.15059300	1.06199000
O	1.88685600	-0.03005600	-0.42048400
O	3.20253500	-0.40369000	0.05158500
H	3.30345500	-1.24484300	-0.40983800

Absolute energies (Hartree): -457.919152 ZPE (Hartree): 0.133822

Harmonic Vibrational Frequencies (cm^{-1}):

-2752.5889 68.7863 101.2349 117.3216 181.6910 210.8161 234.2481 279.1462 331.6542 371.4817 403.6743 433.4113 694.9992 705.2154 856.7033 953.9675 969.2690 994.6336 997.6831 1032.3467 1068.9198 1119.5610 1142.3066 1190.5449 1233.6100 1270.8999 1301.6082 1331.4565 1371.0419 1374.4551 1417.8148 1422.2432 1503.8455 1507.0812 1513.7311 1543.1932 1827.0658 3061.2533 3065.7932 3076.8984 3127.7173 3152.5545 3162.7400 3178.9954 3837.3877

$O_2CC•(C)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z

C	-1.29289400	0.21361000	0.74391300
H	-1.18944900	-0.50135000	1.56955300
H	-2.07150800	0.94478600	0.99425500
C	0.00002300	0.89154200	0.43450000
C	0.00016900	1.99214600	-0.57424700
H	0.89223400	2.61807600	-0.47607100
H	0.00034200	1.57526400	-1.59029000
H	-0.89196200	2.61803400	-0.47637000
C	1.29279100	0.21335300	0.74396800
H	1.18902500	-0.50166500	1.56954200
H	2.07150400	0.94434700	0.99451800
O	1.68193500	-0.47611300	-0.44933800
O	3.00557800	-1.00333100	-0.19081000
H	2.80338100	-1.94562900	-0.21550000
O	-1.68198600	-0.47594900	-0.44934900
O	-3.00555600	-1.00337200	-0.19039400
H	-2.80386000	-1.94564500	-0.21931700

Absolute energies (Hartree): -457.95122 ZPE (Hartree): 0.136725

Harmonic Vibrational Frequencies (cm^{-1}):

31.4711 34.4367 102.6284 109.1927 130.4974 141.4311 185.3776 201.0252 238.9059 339.4058 346.4386 424.9740 522.6413 537.1131 835.7896 982.4086 988.8888 995.7559 1024.6967 1044.7683 1047.6678 1066.7976 1072.6856 1243.4727 1243.4854 1323.0968 1352.6620 1363.6246 1366.0936 1419.9247 1423.3959 1427.9158 1491.7727 1505.2222 1529.5639 1540.1067 3051.6991 3054.3623 3059.1109 3112.0068 3118.3630 3128.2831 3166.1776 3844.7741 3845.4356

TS_{51}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-2.89845900	-0.64733700	0.80205900
O	-2.83437500	-0.55832100	-0.58929100
C	-1.43675200	-0.63894700	-0.81674500
H	-1.26183500	-0.37584000	-1.86507700
H	-1.06419800	-1.64781200	-0.59840300
C	-0.86873400	0.36316200	0.20347800
H	-1.81982500	0.03448700	0.96789100
C	-1.08012700	1.81142800	-0.17844700
H	-0.86131700	2.47634700	0.66189000
H	-0.42213600	2.08875500	-1.01219900
H	-2.11346600	1.96721700	-0.49966600
C	0.46035000	0.01066900	0.83090500
H	0.68060500	0.69111900	1.66024300
H	0.42147600	-1.00993800	1.22805400
O	2.76255300	-0.31782900	0.51191100

C	1.59914500	0.09207300	-0.18421100
H	1.73105700	1.11454100	-0.55424100
H	1.41575800	-0.57530400	-1.03747100
O	3.85954700	-0.16493700	-0.42397600
H	4.13646100	-1.08649900	-0.48652600

Absolute energies (Hartree): -497.174361 ZPE (Hartree): 0.162664

Harmonic Vibrational Frequencies (cm^{-1}):

-2688.2324 53.4967 74.5943 95.5609 132.7893 162.7537 189.7476 238.4626 260.6926 302.9012 323.4028 376.3774 418.3069 489.3315 670.9865 701.3664 819.4848 852.3898 917.7472 963.7840 995.2153 1024.0942 1035.8967 1059.0962 1089.4708 1137.3488 1151.9406 1203.4690 1232.9072 1277.2593 1285.0205 1307.8173 1330.7842 1344.5988 1371.8462 1380.3080 1421.4521 1430.9602 1499.2506 1507.6330 1510.1711 1520.2709 1548.3771 1846.0062 3053.4699 3058.4209 3067.1396 3084.5015 3120.0531 3143.8184 3147.3261 3150.0957 3176.6173 3844.4426

$O_2CCC•(C)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.86712400	0.17162200	0.62146200
H	-1.76767200	-0.27270900	1.62030300
H	-2.85101200	0.64580300	0.53046200
C	-0.76731100	1.13860700	0.33813200
C	-0.93582700	2.07333800	-0.81741000
H	-0.18935500	2.87308300	-0.79403600
H	-0.82881100	1.54250400	-1.77495800
H	-1.93399000	2.52358000	-0.81572800
C	0.61156200	0.84361700	0.84389300
H	0.56388300	0.30796500	1.79835100
H	1.16612100	1.77572300	1.00495100
O	2.67601200	-0.21402900	0.43739800
O	-1.76651800	-0.86295500	-0.37229400
O	-2.90867100	-1.72936500	-0.18046200
H	-2.46669600	-2.49800600	0.19889900
C	1.40208100	-0.00894200	-0.15447100
H	1.51683200	0.51638300	-1.10899300
H	0.89702200	-0.96542700	-0.33077600
O	3.46439500	-0.93904800	-0.53736900
H	3.51164600	-1.79518200	-0.09630300

Absolute energies (Hartree): -497.207826 ZPE (Hartree): 0.165546

Harmonic Vibrational Frequencies (cm^{-1}):

35.2079 48.1114 88.0844 102.4381 111.8943 132.8915 136.7775 193.4836 206.2659 217.9698 286.5894 341.0601 391.7946 460.7878 493.3374 539.0548 820.0214 829.0128 923.8617 981.8440 999.4628 1020.9195 1035.1303 1058.5761 1064.3173 1070.8228 1111.3401 1233.5489 1241.7704 1288.1283 1305.6225 1354.2594 1358.5849 1365.7079 1370.8570 1416.7637 1422.2631 1425.6918 1490.5228 1506.2029 1508.2959 1534.8380 1550.3201

3036.4070 3056.3381 3071.7922 3078.6804 3115.2531 3120.9463 3126.5023 3147.4392 3160.0022 3837.5856 3841.0508

$O_2CCCC(C)COO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.28988500	-0.02290200	0.87478800
H	0.50383400	-0.55351200	1.41077300
H	1.92223700	0.53248800	1.57335200
C	0.75895700	0.86298800	-0.24112400
H	0.36140500	0.20345500	-1.01608800
C	-0.38510700	1.74879900	0.27671800
H	-0.68470600	2.41775800	-0.54129000
H	0.00988100	2.39757900	1.07198800
C	-1.62985500	1.02125800	0.80204500
H	-2.31650700	1.77079400	1.21658300
H	-1.38132100	0.34870500	1.62747200
C	-2.41882900	0.24265800	-0.24571900
H	-2.69585000	0.89493500	-1.08220900
H	-3.33389700	-0.16554200	0.20176600
O	-1.70922800	-0.80193800	-0.89162400
O	-1.42151500	-1.79106300	0.13548200
H	-0.48825000	-1.95666800	-0.07693500
O	2.18318600	-1.04617600	0.33297300
O	1.52041200	-1.99405500	-0.23639100
C	1.88645700	1.71172300	-0.82955200
H	2.26518100	2.41747700	-0.08088100
H	2.71865100	1.08473700	-1.16259600
H	1.52744800	2.28650900	-1.68838400

Absolute energies (Hartree): -536.486723 ZPE (Hartree): 0.198484

Harmonic Vibrational Frequencies (cm^{-1}):

66.9450 89.6552 129.2698 139.8893 150.2995 176.8231 236.9079 251.2643 262.6710 299.2831 360.7939 399.3151 430.7995 466.1736 541.8575 570.9089 603.9662 806.6860 825.1114 871.4550 901.4507 916.9139 921.3183 964.3721 977.0759 1049.6158 1059.2585 1128.5041 1165.7529 1172.0785 1206.9719 1245.4871 1271.6788 1289.1879 1324.8756 1344.1450 1360.3217 1383.8233 1400.7181 1413.7559 1426.4732 1429.5772 1433.8107 1462.8275 1487.6979 1497.3996 1503.8692 1510.4025 1520.3617 1522.3880 3045.9177 3064.5037 3064.9273 3082.1444 3097.8613 3117.7146 3131.0897 3140.9334 3151.7981 3159.0246 3167.1646 3205.8409 3723.2873

TS_{52}

Cartesian Coordinates (Å)

At.	X	Y	Z
O	-3.42112700	-0.73836200	0.80535600

O	-3.36116600	-0.64713400	-0.58634400
C	-1.96138000	-0.66000200	-0.81441400
H	-1.79888800	-0.38813600	-1.86242300
H	-1.54118800	-1.65047500	-0.59734600
C	-1.44044700	0.36681300	0.20610900
H	-2.37511900	-0.00241800	0.97083100
C	-1.71513800	1.80380700	-0.17685500
H	-1.54102300	2.47700200	0.66765600
H	-1.05726000	2.11160700	-0.99983200
H	-2.74984800	1.91204800	-0.51299700
C	-0.09297600	0.07518900	0.82353600
H	0.08969100	0.77266400	1.65050500
H	-0.10366600	-0.93885500	1.24329700
C	1.05244900	0.18551700	-0.19579300
H	1.10230600	1.19968800	-0.60381100
H	0.87857300	-0.50203900	-1.03152400
O	3.36316200	-0.00247700	-0.57263400
C	2.38919100	-0.14764900	0.44722900
H	2.39389800	-1.17576000	0.83344700
H	2.60725400	0.54141200	1.27191800
O	4.64559500	-0.24256100	0.05752000
H	4.89336300	-1.05450800	-0.39978200

Absolute energies (Hartree): -536.429367 ZPE (Hartree): 0.191514

Harmonic Vibrational Frequencies (cm^{-1}):

-2658.3887 46.2293 50.7929 78.5191 111.0563 139.6159 148.1338 197.5170 206.3313 239.6823 286.1793 307.6119 354.6132 397.5499 432.2545 498.7002 671.7457 701.2897 771.3251 849.2706 888.3032 913.8259 964.4152 993.2845 1025.0343 1038.4060 1059.7832 1089.9493 1105.1766 1140.0300 1150.1850 1203.8223 1225.4891 1272.4608 1277.2799 1287.9908 1306.4835 1324.6813 1352.9808 1369.1137 1375.2101 1388.5284 1420.2181 1434.9553 1496.5137 1506.7159 1509.2658 1515.7179 1520.3150 1551.7984 1846.2978 3054.3650 3058.1612 3062.1251 3065.9925 3087.7120 3112.5860 3117.3854 3142.8486 3147.8858 3155.0517 3174.9634 3843.2974

$O_2CCCC•(C)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.38466400	0.00266500	0.63507800
H	-2.18953600	-0.43327900	1.62356500
H	-3.42793800	0.33643400	0.58594700
C	-1.44120700	1.11707300	0.32890600
C	-1.74289900	1.98287600	-0.85286100
H	-1.16593800	2.91281300	-0.82159700
H	-1.49607000	1.46862600	-1.79342200
H	-2.80817100	2.23123700	-0.89727600

C	-0.03095900	1.03397300	0.82518700
H	-0.01047000	0.54416900	1.80708100
H	0.37517300	2.04626100	0.95504600
O	-2.18082300	-0.99813400	-0.37656700
O	-3.18850200	-2.01356200	-0.15488500
H	-2.62579400	-2.72935300	0.16264000
C	0.88587100	0.25604900	-0.14233300
H	0.91519400	0.76367600	-1.11182000
H	0.47831100	-0.74583700	-0.30572500
O	3.05926700	-0.53637600	-0.56962500
C	2.29972300	0.15847100	0.40595900
H	2.31514100	-0.39032500	1.35759300
H	2.72680600	1.15585600	0.56742100
O	4.42100200	-0.57025400	-0.07305300
H	4.51054600	-1.52030100	0.06395700

Absolute energies (Hartree): -536.46171 ZPE (Hartree): 0.194231

Harmonic Vibrational Frequencies (cm^{-1}):

31.0204 39.9534 63.4314 92.2412 97.6386 118.8255 133.3814 144.1436 168.5958 190.7790 205.7953 238.4173 338.2079 353.7300 416.3829 434.7564 517.2001 551.1937 771.8022 822.6776 887.8769 913.6426 981.0166 1003.0251 1018.0159 1024.8370 1047.3023 1058.8990 1088.9621 1094.7192 1127.0939 1225.7324 1240.8740 1269.3583 1291.0599 1317.9996 1334.5101 1360.6013 1366.2468 1368.9867 1380.0320 1421.1687 1423.3606 1432.1647 1489.4394 1501.6065 1508.0305 1518.4324 1534.5474 1551.3626 3036.5378 3049.0172 3052.0249 3055.4760 3099.4054 3107.3255 3108.8080 3114.8464 3117.1364 3157.4506 3163.3737 3840.0708 3845.1954

TS_{53}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.41405800	-0.79829300	0.76263100
H	2.20623200	-0.42134800	1.41802800
H	1.15578100	-1.82818400	1.02412200
C	0.18249300	0.13051500	0.80563500
H	-0.11787500	0.23162800	1.85775200
C	0.55973500	1.47844500	0.23023000
H	1.51597300	1.13494200	-0.55324500
H	1.05468800	2.15820200	0.92475000
O	1.88235100	-0.84592500	-0.57480200
O	2.44032100	0.40019200	-0.84299800
H	-0.20522900	1.96240800	-0.37544900
C	-0.96243100	-0.51166300	0.03274700
H	-1.18576100	-1.51044700	0.42598300
H	-0.71054800	-0.59128700	-1.03151200
O	-2.08578000	0.33664100	0.21489600

O	-3.18505300	-0.29754400	-0.48044500
H	-3.29110800	0.32315300	-1.21108900

Absolute energies (Hartree): -457.929902 ZPE (Hartree): 0.133557

Harmonic Vibrational Frequencies (cm^{-1}):

-2000.5236 76.8159 100.7016 121.6576 179.6750 206.7510 290.4377 353.6040 400.7170 478.7906 494.5344 515.4997 639.6991 744.7422 868.7708 928.1921 952.5090 968.2010 977.1675 1012.9048 1087.1585 1117.3240 1152.3033 1188.4040 1208.7862 1247.6187 1266.5251 1292.5721 1301.7781 1366.8551 1376.2338 1391.9981 1435.5974 1480.3290 1496.5261 1545.9930 1615.0355 3067.1567 3073.5273 3091.3885 3129.1933 3138.3899 3170.0674 3234.8171 3837.9969

$O_2CC(C\bullet)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.27884000	0.42897300	0.67683800
H	-1.24547900	-0.05423800	1.66327800
H	-2.14004900	1.10596000	0.63980100
C	0.00957800	1.87099500	-0.92631800
H	0.73273200	2.65043800	-1.13450000
H	-0.50812300	1.40619100	-1.75336400
C	1.27972500	0.39929500	0.67673600
H	1.22254400	-0.10665700	1.65101700
H	2.15176600	1.06441900	0.67193100
O	1.40728600	-0.55042800	-0.36390400
O	2.68952700	-1.19400900	-0.13750800
H	2.38479900	-2.10559600	-0.06463300
O	-1.40716900	-0.54759500	-0.34180800
O	-2.72193300	-1.13293600	-0.15274100
H	-2.45601700	-2.04419400	0.01535700
C	0.00493000	1.21543100	0.41972100
H	0.02377900	1.99524300	1.19694900

Absolute energies (Hartree): -457.939912 ZPE (Hartree): 0.135145

Harmonic Vibrational Frequencies (cm^{-1}):

74.3316 79.7343 98.7533 125.6878 140.5274 159.5380 172.5001 194.5937 222.9464 338.8907 344.3613 418.1538 483.1179 552.9300 679.4721 858.3826 909.5671 915.3676 975.2308 994.1932 1025.0112 1036.6465 1128.7524 1174.8709 1202.1489 1263.3323 1274.9883 1329.9400 1361.2437 1373.8109 1388.6276 1410.5389 1431.2303 1489.9241 1536.6221 1545.2320 3041.5826 3045.7682 3057.0711 3108.7358 3117.2344 3208.6452 3333.2367 3847.7796 3850.4180

TS_{54}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.98000900	-0.75408500	0.76898300

H	2.77982200	-0.34532100	1.39637700
H	1.72738800	-1.77203700	1.07774800
C	0.73805900	0.16571000	0.78556400
H	0.47047000	0.30645900	1.84403000
C	1.12195600	1.49496900	0.16811300
H	2.07916400	1.12381100	-0.60296000
H	1.61424500	2.20056700	0.83885900
O	2.43162600	-0.85397500	-0.57015200
O	2.99179900	0.37749000	-0.88866400
H	0.37785100	1.96479000	-0.47488600
C	-0.42692800	-0.50313900	0.04824900
H	-0.52889800	-1.54170300	0.38206700
H	-0.21492300	-0.52271300	-1.02561900
O	-2.72647600	-0.51939200	-0.42169800
C	-1.74721700	0.20772400	0.30076200
H	-1.72361200	1.24798700	-0.04710500
H	-1.99334600	0.20088500	1.37014500
O	-3.99286000	0.12713200	-0.13929100
H	-4.21614900	0.42016100	-1.03025400

Absolute energies (Hartree): -497.183524 ZPE (Hartree): 0.162321

Harmonic Vibrational Frequencies (cm^{-1}):

-2020.6941 56.7283 63.3114 88.2770 149.6091 153.1509 192.5461 253.4277 302.1797 385.8159 429.7756 470.6382 499.9216 521.4448 649.1186 751.5679 817.6786 866.4365 920.4381 956.4686 963.4589 1005.0016 1021.9790 1078.7941 1092.4191 1131.8767 1153.0361 1181.7355 1203.8007 1240.3027 1252.8969 1281.6762 1292.4587 1314.4224 1338.5972 1371.2861 1381.8382 1400.3802 1441.2732 1479.0986 1497.0367 1512.6608 1551.3509 1616.3843 3047.9279 3057.7415 3086.4263 3089.4411 3109.3970 3132.7042 3151.9473 3169.9156 3226.9307 3845.8796

$O_2CCC(C\bullet)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.85313800	0.19717000	-0.60183800
H	1.72683400	-0.15735800	-1.63396200
H	2.88711100	0.53165600	-0.46048100
C	0.99197800	1.79531000	1.12185200
H	0.50960600	2.71733100	1.42373800
H	1.42233700	1.15639900	1.88058600
C	-0.57185700	1.04500200	-0.72515400
H	-0.59578800	0.80682900	-1.79527200
H	-1.16144000	1.95736200	-0.58022500
O	-2.62251200	0.00687100	-0.30448800
O	1.57695200	-0.85427500	0.31251100
O	2.59876600	-1.85733200	0.09152900

H	2.04712400	-2.56827700	-0.25556200
C	-1.24978600	-0.06932100	0.06008700
H	-1.14137200	0.08581400	1.13882400
H	-0.84669800	-1.05323000	-0.19670600
O	-3.29880300	-1.03015000	0.44841800
H	-3.55308600	-1.60832600	-0.27974000
C	0.88585700	1.33964300	-0.30035700
H	1.21416400	2.16407000	-0.95249600

Absolute energies (Hartree): -497.196433 ZPE (Hartree): 0.164118

Harmonic Vibrational Frequencies (cm^{-1}):

43.7127 78.4051 86.0024 112.5168 123.7475 152.5132 168.5113 186.1121 193.4432 212.4642 286.7810 329.9689 404.3835 427.3515 461.2875 507.1321 670.1071 815.0285 847.1522 912.6667 921.5763 978.0626 1000.3442 1022.6844 1059.6373 1085.3065 1129.7950 1173.1950 1199.7518 1248.1330 1262.9473 1310.5834 1312.4366 1359.8055 1366.8956 1368.7960 1394.9184 1421.3056 1438.9911 1488.6362 1509.2990 1541.0744 1545.8749 3037.4356 3055.0467 3076.9338 3086.8517 3120.4402 3128.7815 3152.9747 3206.7805 3329.7416 3839.8856 3845.2400

TS_{55}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.56429100	-0.66982800	0.81219500
H	3.42010900	-0.20583100	1.31512200
H	2.30886300	-1.62244600	1.28465500
C	1.35197100	0.28716800	0.77883200
H	1.16170200	0.59018200	1.81995300
C	1.72471900	1.49751200	-0.05173000
H	2.60828600	0.98302100	-0.82694400
H	2.28792000	2.27206100	0.47092300
O	2.91267100	-0.98183500	-0.52611200
O	3.47798200	0.16904200	-1.06381600
H	0.94524300	1.90045400	-0.69837200
C	0.11671500	-0.43432500	0.22908200
H	0.01589300	-1.40241900	0.73705000
H	0.27979900	-0.65000300	-0.83366300
C	-1.17811400	0.35775400	0.41562700
H	-1.11683100	1.32516900	-0.09384800
H	-1.34175500	0.55728200	1.48077400
O	-3.50423300	0.42661800	0.07659100
C	-2.37404300	-0.40527200	-0.13067700
H	-2.51001600	-1.35484300	0.40051900
H	-2.24806300	-0.61429300	-1.20164700
O	-4.65463100	-0.33433500	-0.36608200
H	-4.89868700	0.18769700	-1.13914000

Absolute energies (Hartree): -536.438277 ZPE (Hartree): 0.191142

Harmonic Vibrational Frequencies (cm^{-1}):

-2007.3080 44.3029 51.9024 73.9829 115.7896 139.3203 144.5300 202.1782 235.8646 244.6846 364.6590 385.2824 434.0833 481.0761 512.5898 522.3701 645.9570 749.1439 773.6067 857.6633 894.0992 913.2302 953.2474 961.5899 1005.1193 1038.5709 1072.0030 1091.2702 1096.0879 1129.9837 1154.0928 1182.5377 1206.6576 1237.4363 1242.1007 1277.2773 1281.9300 1310.5677 1314.5386 1329.9190 1367.5040 1374.3912 1389.1266 1410.8796 1439.5417 1478.2346 1496.3014 1505.7061 1519.0426 1552.0145 1615.7742 3047.4791 3053.2454 3064.6294 3084.8476 3085.5994 3110.6195 3119.7363 3131.6627 3149.1942 3166.8361 3225.5997 3842.6369

$O_2CCCC(C\bullet)COO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.37571200	-0.02513800	-0.60244600
H	-2.19667800	0.29986100	-1.63685900
H	-3.44581800	-0.22146900	-0.46943300
C	-1.73461800	-1.70407400	1.14220200
H	-1.41900400	-2.69492600	1.44730100
H	-2.01633400	-0.98821900	1.90206000
C	-0.08678100	-1.19601300	-0.71269000
H	-0.04795900	-0.94559100	-1.78183200
H	0.34702500	-2.19931100	-0.60761600
O	-1.97849000	0.99328900	0.30455800
O	-2.88481300	2.10217000	0.07729000
H	-2.25253700	2.75301800	-0.24935400
C	0.76672500	-0.20439400	0.08071200
H	0.67336000	-0.40445400	1.15270900
H	0.42144000	0.81755900	-0.09077000
O	2.92552300	0.66756500	0.42731300
C	2.22868100	-0.31735200	-0.31932000
H	2.35754700	-0.13447200	-1.39538400
H	2.62638900	-1.31164900	-0.08207400
O	4.32870200	0.50546400	0.10096300
H	4.47639200	1.33863200	-0.36087600
C	-1.57130700	-1.28511900	-0.28550300
H	-2.01312800	-2.06433200	-0.92660000

Absolute energies (Hartree): -536.450206 ZPE (Hartree): 0.192898

Harmonic Vibrational Frequencies (cm^{-1}):

36.6753 50.8245 81.1012 99.5967 108.0066 135.9511 147.5973 161.6916 173.8185 189.3255 209.2959 231.3498 325.9833 361.5947 405.1408 416.3792 482.9801 522.3697 674.7649 772.0155 840.3382 884.6265 910.1022 912.8474 975.1218 999.0598 1018.7758 1080.2740 1089.8369 1102.2997 1133.5622 1177.8002 1199.6907 1237.1177 1256.2418 1293.9238 1304.3873 1325.4454 1337.5985 1365.8571 1367.2391 1397.4626 1402.6606 1424.1226 1437.5942 1487.5680 1502.1008 1517.6094 1540.8658 1551.7094 3033.6295 3045.7275 3049.7893

3056.1296 3102.7622 3105.1871 3108.2710 3117.3072 3173.2327 3205.1232 3328.3121 3841.6479 3845.1856

TS_{56}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.45912400	0.44048300	0.00099300
H	-2.79150100	0.29076700	1.03326400
H	-3.25802000	0.88118300	-0.60009000
C	-1.17181600	1.28606100	-0.04991700
H	-0.97175000	1.52749000	-1.09874500
H	-1.33785100	2.22389600	0.49372400
C	-0.01294500	0.50844500	0.54039400
H	-0.45899200	-0.68011300	0.45509100
H	0.12685900	0.63965700	1.61610200
O	-2.17199100	-0.81552300	-0.59001900
O	-1.35927100	-1.49426900	0.30752500
C	1.27440100	0.56569500	-0.23838500
H	1.67673800	1.58924400	-0.25502500
H	1.11211900	0.23546400	-1.27303100
O	2.18041500	-0.29788300	0.42472600
O	3.43082800	-0.19481800	-0.29738400
H	3.47945400	-1.09174000	-0.64858000

Absolute energies (Hartree): -457.930586 ZPE (Hartree): 0.133952

Harmonic Vibrational Frequencies (cm^{-1}):

-2003.3796 50.0726 94.6296 109.0742 147.7464 217.7571 256.4840 368.2093 413.8176 435.3116 514.5467 534.6212 643.6515 829.9207 891.7901 905.3431 942.0882 993.3831 1000.5471 1098.6259 1125.7457 1136.5064 1163.0711 1182.3446 1228.0189 1267.7432 1285.3571 1294.6171 1322.3653 1371.5436 1380.4118 1399.4544 1433.6485 1488.3205 1501.1573 1533.8129 1613.9538 3038.6666 3078.2720 3094.1770 3095.1405 3139.6501 3157.0076 3177.8823 3841.4380

$O_2CC•CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.82857700	0.34753900	-0.03179800
H	-1.72502300	0.96154600	0.86886000
H	-1.91081300	1.00726600	-0.90575600
C	0.62871100	0.14988200	-0.40113800
H	0.65040200	0.95966900	-1.12440700
O	2.88384500	0.61477200	-0.00230000
O	-2.97828000	-0.47647300	0.07058000
O	-4.09336800	0.41695700	0.30592400
H	-4.57775700	0.27997200	-0.51634100
C	1.93318200	-0.44099000	0.00509500

H	2.25816000	-1.22983000	-0.69528700
H	1.86978400	-0.88798700	1.00597500
O	4.14995000	0.00876700	0.35195300
H	4.63039200	0.16339400	-0.46933900
C	-0.64456700	-0.60037800	-0.18211500
H	-0.57225900	-1.22645600	0.71368600
H	-0.85255200	-1.27607700	-1.02690600

Absolute energies (Hartree): -457.944397 ZPE (Hartree): 0.135717

Harmonic Vibrational Frequencies (cm^{-1}):

24.4080 31.6077 75.3562 110.0351 128.7508 154.2794 194.7178 196.9266 225.9117 286.8735 397.3055 468.2391 513.7107 517.0635 806.1236 912.5606 925.4269 971.1983 1035.0132 1072.6461 1095.0511 1103.8249 1161.2462 1173.7168 1235.7964 1250.3910 1272.0504 1308.1408 1361.1802 1371.9510 1379.7451 1430.7324 1466.0626 1498.8479 1529.9760 1551.2942 2994.6708 3029.0131 3059.8859 3081.5645 3117.6521 3135.8452 3225.0236 3844.3411 3846.6547

TS_{57}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.04100800	-0.26143900	0.03135800
H	3.33340600	-0.05471900	1.06617400
H	3.89638400	-0.62467300	-0.54334200
C	1.85354300	-1.24015200	-0.02705800
H	1.69451400	-1.51703800	-1.07381700
H	2.11109400	-2.14710000	0.53438300
C	0.60330600	-0.58713700	0.52978000
H	0.92224900	0.63342300	0.41384600
H	0.50063800	-0.69163300	1.61493400
O	2.63562100	0.94588300	-0.59428200
O	1.73131700	1.54942900	0.26726700
C	-0.68620600	-0.80806100	-0.23089900
H	-0.97679600	-1.86617000	-0.17322800
H	-0.53246300	-0.56732000	-1.28849400
O	-2.96220800	-0.26627700	-0.44901400
C	-1.81501000	0.04720200	0.32286300
H	-1.57115500	1.11354400	0.22903900
H	-2.00099000	-0.18422900	1.37853900
O	-4.05096800	0.50489900	0.11265500
H	-4.18683500	1.13197800	-0.60731100

Absolute energies (Hartree): -497.186342 ZPE (Hartree): 0.162819

Harmonic Vibrational Frequencies (cm^{-1}):

-1989.5171 42.1199 65.7886 95.8533 102.7812 148.3818 215.0405 219.8149 313.8609 363.7629 409.8722 493.9330 509.0115 530.2697 634.7240 794.1610 836.8661 903.3926 917.7973 939.5849 1001.0369 1002.6419 1088.5910 1090.8387 1126.0035 1152.0295 1162.8057 1181.5967 1224.2282 1258.0011 1272.6777 1301.0233

1307.1365 1317.6057 1353.0159 1372.1037 1397.1138 1403.0522 1440.4161 1487.0471 1500.3770 1500.6422 1552.0481 1621.7699 3056.3061 3063.7404 3074.7790 3092.9463 3111.1383 3119.8892 3136.3380 3146.5536 3176.3293 3840.3000

$O_2CCC•CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.63849200	0.54406800	0.50723700
H	3.44145800	1.28502100	0.58710500
H	2.48199300	0.07344600	1.48623900
C	0.20689100	0.21959800	-0.05761200
H	0.42949300	-0.81545700	-0.30050800
O	2.98922600	-0.43948000	-0.45526400
O	4.23405500	-1.02430400	-0.00406100
H	3.91723300	-1.90324200	0.23469200
C	-1.18946800	0.71263900	-0.26056000
H	-1.35527900	0.98687600	-1.31533600
H	-1.36353900	1.62044300	0.32905000
O	-3.48862300	0.22057600	-0.16454900
C	-2.21887900	-0.33933400	0.12838900
H	-2.15130800	-0.57525200	1.19599300
H	-2.06890300	-1.26085400	-0.44974400
O	-4.46874700	-0.75046400	0.27651600
H	-4.83694400	-0.99777500	-0.57947600
C	1.35075300	1.17994800	0.00262900
H	1.10248900	2.02190300	0.66188400
H	1.54928400	1.61275100	-0.99151700

Absolute energies (Hartree): -497.201069 ZPE (Hartree): 0.164882

Harmonic Vibrational Frequencies (cm^{-1}):

30.3931 41.6825 59.7981 108.3312 116.5561 129.4702 162.6135 199.2369 205.5452 250.7805 291.3180 313.4557 425.7674 471.4053 486.2351 568.8974 794.0857 830.8030 909.0631 930.9511 949.3031 1033.5926 1078.0428 1082.6198 1101.1613 1108.0323 1163.2728 1172.1895 1235.6766 1250.7690 1258.7425 1297.3674 1307.5086 1355.7309 1372.1652 1372.9172 1421.0231 1429.5576 1458.3463 1473.1478 1499.1720 1546.4280 1552.2469 3021.0542 3024.2030 3057.9456 3062.8084 3097.5881 3105.4057 3126.3029 3128.2509 3221.1639 3840.3418 3844.5028

TS_{58}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.61798800	-0.19540600	-0.05861400
H	3.95550000	-0.00211800	0.96497300
H	4.45508300	-0.51538300	-0.68392300
C	2.46235200	-1.21318900	-0.08086200

H	2.26583400	-1.47803700	-1.12469700
H	2.77550000	-2.12036300	0.45116500
C	1.21622600	-0.61308800	0.54234500
H	1.49224700	0.61819500	0.45625900
H	1.15003300	-0.75762800	1.62581800
O	3.14093100	1.01104100	-0.63313300
O	2.26547100	1.56525400	0.28966200
C	-0.09411700	-0.83560700	-0.18157000
H	-0.32160500	-1.91283000	-0.19003300
H	0.02628300	-0.53098200	-1.22914000
C	-1.25485100	-0.06830100	0.45273800
H	-1.02200800	1.00220600	0.46197700
H	-1.39072700	-0.38829500	1.49164100
O	-3.54869700	0.44379200	0.38456400
C	-2.55281300	-0.29297500	-0.30547400
H	-2.82021300	-1.35667400	-0.31879100
H	-2.46786800	0.06348500	-1.34081200
O	-4.79563700	0.18309900	-0.30567300
H	-4.96331200	1.06433500	-0.65917300

Absolute energies (Hartree): -536.440701 ZPE (Hartree): 0.191557

Harmonic Vibrational Frequencies (cm^{-1}):

-1971.5881 34.3847 50.9941 75.4121 83.0346 129.8187 141.3274 179.7247 203.7951 281.4629 302.4009 408.1678 434.2551 479.3396 525.0873 535.4068 635.5937 763.7938 817.9994 868.1216 911.4189 913.1607 955.7985 998.1243 1011.9640 1069.5182 1087.6092 1098.9452 1132.0281 1151.8307 1164.4781 1183.7448 1221.4491 1250.8684 1256.7641 1294.1731 1297.5522 1314.4323 1329.7941 1336.4023 1368.3939 1376.3306 1397.4383 1415.2443 1441.2041 1486.7958 1493.1126 1500.8534 1518.7287 1552.4663 1620.9329 3036.9465 3053.4707 3073.6891 3085.5609 3092.6336 3098.1378 3108.3847 3122.7037 3143.2296 3148.7077 3175.1818 3843.4057

$O_2CCCC•CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.28749200	0.53380400	0.47670000
H	4.10980600	1.25690000	0.51385300
H	3.13587000	0.10684000	1.47624700
C	0.83760700	0.24824300	-0.03210800
H	1.02385600	-0.80032500	-0.24533400
O	3.59784600	-0.49590800	-0.45066000
O	4.83202500	-1.09785600	0.00742700
H	4.49313000	-1.95594000	0.28810700
C	-0.55164600	0.77177300	-0.20384600
H	-0.68993100	1.14012200	-1.23587500
H	-0.69777600	1.64644600	0.44587500

C	-1.62541700	-0.27745200	0.09772400
H	-1.52503900	-0.62174500	1.13194100
H	-1.48553400	-1.14544100	-0.55593100
C	2.00674100	1.18019900	-0.03285100
H	1.79240300	2.05535700	0.59477000
H	2.19927000	1.56624200	-1.04741100
C	-3.02448200	0.27953700	-0.10531200
H	-3.16991800	0.60582200	-1.14411200
H	-3.20734800	1.13158300	0.56054100
O	-3.92368500	-0.77282500	0.20507400
O	-5.25614200	-0.21817300	0.07584000
H	-5.56090200	-0.72439000	-0.68595900

Absolute energies (Hartree): -536.455101 ZPE (Hartree): 0.193597

Harmonic Vibrational Frequencies (cm^{-1}):

26.6449 37.5049 49.7158 87.0207 101.2500 105.7768 136.4080 149.9730 198.3627 203.9069 231.1946 257.0672 292.9260 371.3712 428.5380 448.9309 517.1813 560.5511 763.2317 818.1909 877.0606 912.2187 923.3777 953.1079 1050.1760 1062.4874 1077.6981 1095.4017 1108.5758 1115.5285 1165.6296 1170.7693 1228.3813 1245.9778 1249.1653 1288.2672 1304.9806 1322.7955 1330.2211 1368.5717 1372.7003 1390.5446 1423.8031 1438.6933 1453.4167 1473.0031 1491.9720 1519.9910 1546.2311 1552.7863 2996.7437 3021.9623 3051.8970 3062.2845 3069.8802 3089.4182 3094.6857 3108.7927 3125.1202 3151.6801 3223.1119 3840.0709 3844.1444

$O_2CC(C)CCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.47905800	0.77623900	0.39065700
H	2.18128400	1.31506200	-0.25636600
C	1.00587500	-0.50282300	-0.29903700
H	0.42566500	-0.21723400	-1.18302800
C	0.14167000	-1.38077000	0.61555500
H	0.03492800	-2.37611900	0.16693000
H	0.66011400	-1.52002800	1.57464300
C	-1.25460400	-0.86378100	0.92822300
H	-1.25965300	0.15632900	1.30649200
H	-1.77984400	-1.53572900	1.61065900
O	0.44027000	1.66018900	0.78378200
O	-0.08041500	2.24335500	-0.43334800
H	-0.87055700	1.69259500	-0.55854700
O	-2.07247100	-0.89241900	-0.28249600
O	-2.11583400	0.24242200	-0.89005400
H	1.98041700	0.53013100	1.33590400
C	2.23192600	-1.29334700	-0.76509600
H	2.85945900	-0.69064400	-1.42837100
H	2.84073600	-1.60077900	0.09327800

H	1.93149700	-2.19506000	-1.30648400

Absolute energies (Hartree): -497.232489 ZPE (Hartree): 0.16935

Harmonic Vibrational Frequencies (cm^{-1}):

74.1433 91.9540 133.9594 148.4966 184.3814 217.2984 239.1435 290.1211 320.8811 373.2513 441.5570 480.8466 532.9935 575.0680 587.3674 799.3566 830.4316 871.2744 926.8746 946.0777 968.9122 1044.7649 1054.1245 1093.0282 1140.3025 1173.4775 1199.9246 1257.4010 1279.3478 1329.1332 1341.3068 1359.7587 1393.9637 1414.2241 1423.0547 1424.5366 1438.1751 1468.0278 1475.9808 1490.6407 1516.1339 1519.4051 1521.7180 3059.8673 3062.9016 3066.9990 3108.7678 3119.0449 3131.3430 3132.6270 3152.9669 3165.7241 3224.8470 3718.3082

TS_{59}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.46833800	0.12825800	-0.43007200
H	-2.81282500	0.68886900	0.44500400
H	-3.25729200	0.07610200	-1.18433400
C	-1.17026000	0.72781200	-1.00174200
H	-0.95476200	0.21687300	-1.94600100
H	-1.32656300	1.79377700	-1.21391000
C	-0.02718200	0.54357000	-0.01734900
H	-0.46661600	-0.43103900	0.64470500
O	-2.19570700	-1.21180100	-0.05503200
O	-1.39218200	-1.14592700	1.07177300
C	0.13688800	1.66550400	0.98897300
H	0.83109300	1.38650600	1.78358300
H	0.53496900	2.55742100	0.48681800
H	-0.82692200	1.92472200	1.43675700
C	1.25092100	0.07132600	-0.67007700
H	1.66276100	0.85889700	-1.32047900
H	1.06513300	-0.82610400	-1.27465600
O	2.16550400	-0.21683000	0.37304400
O	3.39813100	-0.61544600	-0.27246800
H	3.41287400	-1.54481800	-0.01442100

Absolute energies (Hartree): -497.191448 ZPE (Hartree): 0.162342

Harmonic Vibrational Frequencies (cm^{-1}):

-1995.4519 54.1668 99.9172 113.0903 134.1392 202.4345 217.1764 222.2569 282.3812 330.9689 397.7523 411.7103 437.0861 526.9144 541.2905 666.3802 828.1555 888.7047 929.5837 954.5768 965.4225 999.6401 1014.8977 1065.7742 1109.5344 1141.5540 1170.7293 1219.9867 1232.4214 1249.9863 1261.4723 1295.4149 1346.2338 1368.4684 1374.9174 1400.3060 1410.7603 1425.3325 1481.8707 1499.8695 1502.1455 1515.2633 1530.5014 1612.6249 3029.2253 3057.5743 3067.4345 3094.0639 3094.4089 3135.9438 3146.2685 3175.1413 3187.2086 3838.6397

$O_2CC•(C)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.40216700	-0.00875400	-0.15453500
H	1.51691700	0.51636700	-1.10917400
H	0.89700400	-0.96522500	-0.33064100
C	0.61177500	0.84410000	0.84368300
H	0.56444500	0.30884200	1.79838200
H	1.16616800	1.77639100	1.00419400
C	-0.76726800	1.13858100	0.33814300
C	-1.86680200	0.17137200	0.62182300
H	-2.85079300	0.64546900	0.53144100
H	-1.76680200	-0.27315400	1.62052600
C	-0.93636300	2.07295900	-0.81759900
H	-1.93454200	2.52317000	-0.81554000
H	-0.18991400	2.87274100	-0.79488900
H	-0.82985000	1.54178600	-1.77501200
O	-1.76656200	-0.86290500	-0.37223100
O	-2.90864900	-1.72930100	-0.18038200
H	-2.46666900	-2.49806600	0.19871400
O	2.67609800	-0.21384900	0.43731800
O	3.46432100	-0.93926400	-0.53733200
H	3.51131200	-1.79531300	-0.09607300

Absolute energies (Hartree): -497.207825 ZPE (Hartree): 0.165545

Harmonic Vibrational Frequencies (cm^{-1}):

35.2416 48.0794 88.0936 102.3505 111.8750 132.8651 136.7727 193.4713 206.3127 217.8746 286.5720 341.0569 391.8264 460.7640 493.3378 539.0670 820.0413 829.0065 923.8044 981.8190 999.4490 1020.9292 1035.1451 1058.5169 1064.1502 1070.8163 1111.3512 1233.5482 1241.7776 1288.1352 1305.6202 1354.2521 1358.6079 1365.7257 1370.8597 1416.7673 1422.2557 1425.6941 1490.5214 1506.2024 1508.2997 1534.8457 1550.3242 3036.4261 3056.3053 3071.7873 3078.6709 3115.2568 3120.8982 3126.4811 3147.4254 3160.0041 3837.6141 3841.0511

$O_2CCC(C)CCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.96763400	-1.24929600	-0.41856800
H	0.81102800	-0.52663800	-1.21945600
H	0.89476000	-2.26599600	-0.80745600
C	0.06863400	-1.00029600	0.78175400
H	0.16836400	-1.84363600	1.47567600
H	0.41813500	-0.10111000	1.29077700
C	-1.41389200	-0.83316900	0.40218200
H	-1.95942100	-0.69244000	1.34623700
C	-1.69660900	0.39384100	-0.47754000

H	-2.75816800	0.36829300	-0.75960100
H	-1.13394800	0.34019000	-1.41499000
C	-1.45573400	1.75557900	0.16659600
H	-2.01143400	1.84081000	1.10774800
H	-1.78882300	2.55069800	-0.51252900
O	-0.12144600	2.01691700	0.56982100
O	0.66751900	2.06272600	-0.65146200
H	1.41483100	1.51311700	-0.36279400
O	2.37208700	-1.13761400	-0.02572100
O	2.72879100	0.09174000	0.11822000
C	-1.95857000	-2.09874500	-0.27035200
H	-1.71691800	-2.99199700	0.31577100
H	-3.04640900	-2.04477100	-0.37682900
H	-1.53638200	-2.22415500	-1.27385200

Absolute energies (Hartree): -536.484973 ZPE (Hartree): 0.198653

Harmonic Vibrational Frequencies (cm^{-1}):

67.3880 93.7411 122.0026 146.3615 149.7999 191.3990 240.8499 251.2427 280.4952 287.2949 337.4647 387.6381 436.9834 504.2367 552.7597 589.8852 612.4350 781.3494 815.7964 843.4847 900.4246 936.6069 943.1667 979.6938 1018.4091 1026.6548 1039.8888 1122.0423 1151.5144 1172.2495 1209.7079 1247.6981 1278.2149 1302.2278 1325.4210 1340.0459 1357.4770 1367.5930 1388.9323 1415.6186 1423.2439 1426.2114 1440.6716 1463.3922 1488.0572 1498.3649 1510.8671 1518.2054 1523.6546 1527.3840 3058.0078 3061.3092 3062.6108 3073.7138 3088.4664 3127.6795 3134.2865 3142.6144 3148.9719 3156.5553 3178.4872 3211.1860 3718.4962

TS_{60}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.97083200	-0.07635000	-0.35186400
H	-3.33803000	0.36959600	0.57844700
H	-3.78599500	-0.17594500	-1.07281400
C	-1.78983000	0.72266700	-0.93107100
H	-1.55647300	0.31069900	-1.91787300
H	-2.09113900	1.77177200	-1.05702600
C	-0.57862700	0.62065500	-0.01629500
H	-0.85803400	-0.44832200	0.57371200
O	-2.51544300	-1.39577600	-0.09389700
O	-1.66380600	-1.30939900	0.99462400
C	-0.55268700	1.66211000	1.08859000
H	0.13724100	1.39231200	1.89282100
H	-0.23741800	2.63218800	0.68098000
H	-1.54666400	1.78329900	1.52904100
C	0.73638300	0.39257700	-0.74065000
H	0.98040700	1.28002900	-1.34288500

H	0.62458100	-0.45049700	-1.43192200
O	2.97662800	-0.28398200	-0.62777800
C	1.89068100	0.09210000	0.20374000
H	1.62485700	-0.73150800	0.88119200
H	2.17242500	0.96808900	0.79720900
O	4.11107200	-0.47916700	0.25062000
H	4.19610700	-1.43766900	0.18586200

Absolute energies (Hartree): -536.44622 ZPE (Hartree): 0.191303

Harmonic Vibrational Frequencies (cm^{-1}):

-1970.8524 43.5233 81.9623 101.6442 111.7071 145.1481 176.5621 216.6473 224.8737 277.6214 302.7196 322.4792 391.8224 431.3066 510.3801 515.1353 534.2127 658.6340 808.5884 825.9272 888.4405 915.5752 953.6057 991.2316 1008.0190 1017.1566 1064.1669 1091.9908 1110.8229 1148.9369 1170.8137 1212.5278 1225.9360 1244.3303 1254.7530 1289.9011 1312.9103 1338.5106 1350.1131 1367.0564 1372.4835 1399.7285 1421.4386 1438.8617 1482.2256 1496.4749 1499.3540 1506.1795 1517.0647 1550.3835 1622.6577 3048.6291 3053.6127 3055.9939 3063.6945 3092.6007 3115.5936 3133.9415 3138.9473 3142.5843 3168.5831 3174.0253 3839.4755

$O_2CCC•(C)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.23286500	-0.02476500	-0.22304000
H	2.80939000	0.89527900	-0.36355800
H	1.91131300	-0.39887300	-1.20441100
C	1.03098500	0.19790500	0.68719200
H	0.59942100	-0.78017400	0.92995700
H	1.39355500	0.62515700	1.63760400
C	-0.02079500	1.08617200	0.08957700
C	-1.43638900	0.87777400	0.54702100
H	-2.02488400	1.79397600	0.43349300
H	-1.46241700	0.59506100	1.60901500
C	0.38008600	2.39340400	-0.52048700
H	-0.47295900	2.88160100	-0.99988000
H	0.77002400	3.08469300	0.24526600
H	1.16851900	2.27856100	-1.27168800
O	-3.39878100	-0.40848400	0.30703700
O	3.03801000	-0.99024000	0.43493500
O	4.24256900	-1.12219000	-0.35847500
H	4.11374600	-2.01841300	-0.68996000
C	-2.10880000	-0.23455700	-0.25728300
H	-1.53575300	-1.16810500	-0.18534000
H	-2.19512500	0.04882500	-1.31217200
O	-4.05873500	-1.41595700	-0.49902800
H	-4.12703700	-2.11821100	0.15803600

Absolute energies (Hartree): -536.459354 ZPE (Hartree): 0.19352

Harmonic Vibrational Frequencies (cm^{-1}):

16.9098 36.8902 77.0947 78.9255 88.8899 114.9980 121.7187 151.5415 169.0635 196.3836 203.7848 260.6226 306.8219 316.0642 376.9821 469.3632 493.3858 523.4088 804.1013 816.4791 824.5466 914.4610 924.8819 983.6768 1009.1089 1045.5607 1070.7614 1081.2372 1085.9731 1109.3524 1121.7732 1233.3009 1241.0898 1257.2553 1295.5133 1309.0118 1313.2303 1355.6145 1364.7315 1371.9492 1375.1681 1421.2738 1425.1287 1437.4510 1490.9184 1500.4549 1504.3998 1509.9590 1545.1388 1551.3298 3011.2540 3013.0954 3052.3077 3057.3069 3060.6704 3106.1581 3110.0534 3118.0608 3132.1933 3139.3372 3160.8510 3842.4501 3843.8832

$O_2CCCC(C)CCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.68666600	-1.46981400	-0.53876200
H	0.77007400	-0.65982800	-1.26280200
H	0.30050800	-2.37640400	-1.00716500
C	-0.08681600	-1.06228900	0.70312800
H	-0.01797900	-1.88149700	1.43007900
H	0.42199300	-0.20290700	1.13992600
C	-1.57849600	-0.76477000	0.44815000
H	-1.99509100	-0.42974800	1.40924900
C	-1.86050500	0.33348400	-0.59484500
H	-2.89431200	0.20091000	-0.93849100
H	-1.22930000	0.18349000	-1.47702400
C	-1.73046400	1.78784000	-0.11993900
H	-2.48345200	1.99101300	0.65199700
H	-1.94926700	2.45006800	-0.96508100
O	0.58896400	1.73317700	-0.49379300
O	2.04959500	-1.84817000	-0.16434300
O	2.77253700	-0.82645800	0.13560300
C	-0.37162600	2.15639500	0.45734800
H	-0.29134100	3.23828500	0.61779000
H	-0.19747200	1.65627100	1.41700600
O	1.88881200	1.98044300	0.10081800
H	2.22579200	1.06967300	0.09637300
C	-2.31514200	-2.05115200	0.04955000
H	-2.07554300	-2.87383600	0.73160400
H	-3.39795200	-1.89521800	0.06932600
H	-2.04761900	-2.36037000	-0.96685600

Absolute energies (Hartree): -575.7383 ZPE (Hartree): 0.227911

Harmonic Vibrational Frequencies (cm^{-1}):

45.6974 93.3931 116.6684 126.8837 160.1539 167.4963 191.2892 230.5384 237.5834 257.5523 288.8662 326.0784 345.5357 391.9819 460.1506 512.9022 537.0625 560.8464 604.2903 764.2156 792.1366 829.1032 902.4610 912.7870 935.6111 967.2643 981.9992 1016.2234 1028.8900 1052.3531 1088.2595 1134.4861

1153.6396 1179.1719 1198.4220 1238.0713 1263.8314 1278.0460 1311.1272 1321.1770 1339.7576 1353.9949 1370.6940 1387.4819 1398.6916 1408.8464 1425.9705 1432.4287 1438.6481 1472.5765 1491.7495 1507.2116 1507.6620 1518.4391 1520.5299 1525.8311 1562.8874 3053.7251 3063.2765 3067.3655 3071.3433 3078.4025 3085.2144 3113.7859 3127.0672 3135.5591 3140.1785 3151.3936 3158.5930 3186.0314 3217.2334 3724.7075

TS_{61}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-3.47356300	-0.24910100	-0.39286100
H	-3.89919900	0.22598800	0.49727800
H	-4.25782800	-0.45317000	-1.12614400
C	-2.33594200	0.59713200	-0.99135800
H	-2.04711500	0.14506300	-1.94573800
H	-2.70693400	1.61228600	-1.18905400
C	-1.14580000	0.63720800	-0.04378400
H	-1.36909400	-0.40287800	0.61441700
O	-2.93242900	-1.51260600	-0.03871900
O	-2.12629400	-1.29635500	1.06655800
C	-1.21276100	1.75491400	0.98069600
H	-0.51330500	1.59670400	1.80564300
H	-0.96739500	2.71422700	0.50446000
H	-2.21897700	1.83221400	1.40341500
C	0.20122700	0.43791700	-0.71715100
H	0.38658400	1.29115200	-1.38982800
H	0.14063400	-0.45571400	-1.35203400
C	1.36976100	0.28970400	0.25887200
H	1.12694200	-0.47491700	1.00596400
H	1.55303900	1.22964900	0.78836800
O	3.66975500	-0.13178600	0.50496600
C	2.64227200	-0.10671000	-0.47212000
H	2.88836100	0.62414700	-1.25237200
H	2.53619100	-1.09673400	-0.93533000
O	4.89170300	-0.46164700	-0.19991500
H	5.05504300	-1.33525300	0.17407700

Absolute energies (Hartree): -575.700822 ZPE (Hartree): 0.220061

Harmonic Vibrational Frequencies (cm^{-1}):

-1952.9037 35.7361 62.1654 80.1661 88.0407 130.5817 145.1196 162.5884 209.4282 210.5468 252.4383 278.9031 284.9075 388.9177 421.0142 427.6180 491.3833 531.8300 542.1934 656.9065 772.5433 819.6827 880.2731 892.2067 912.0832 949.7853 992.2419 1011.6623 1032.2681 1056.9220 1083.2342 1098.3401 1119.2057 1153.2747 1172.3532 1206.1825 1222.5855 1239.0311 1248.0039 1283.3637 1294.6732 1308.4939 1328.8667 1353.2120 1365.4142 1369.7705 1391.1569 1402.5531 1421.4677 1438.6799 1481.3103 1490.2466 1499.4400 1505.1835 1514.6344 1520.1610 1551.5944 1621.4857 3027.3185 3051.6506 3053.6150 3062.7645 3085.4259 3091.9438 3095.2858 3108.9026 3135.4314 3140.8138 3152.2077 3170.5248 3172.9247 3842.5586

$O_2CCCC•(C)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.98921700	-0.01738400	-0.25902400
H	3.38540100	1.00441800	-0.29708400
H	2.70542000	-0.32836200	-1.27145300
C	1.80202300	-0.12538700	0.68980200
H	1.54981300	-1.18589000	0.80387100
H	2.12056900	0.23075600	1.68555900
C	0.59655300	0.63910000	0.22777200
C	-0.74191800	0.28270100	0.80815900
H	-1.07465200	1.07965200	1.49450700
H	-0.65787700	-0.63366800	1.40500200
C	0.78226300	2.02762300	-0.30717200
H	-0.17388500	2.47507900	-0.59228400
H	1.24085800	2.68212800	0.45265400
H	1.43639600	2.05344500	-1.18538200
O	3.97585200	-0.89502000	0.26040800
O	5.10265000	-0.81753400	-0.64722900
H	5.74630600	-0.40626600	-0.05893300
C	-1.82345800	0.08095600	-0.26605000
H	-1.53864200	-0.75126200	-0.91806600
H	-1.90723600	0.97633100	-0.89001900
O	-4.08849500	-0.36974000	-0.71486700
C	-3.17806000	-0.20714500	0.36059000
H	-3.49999400	0.62650100	0.99653200
H	-3.14352500	-1.12179000	0.96804000
O	-5.39129300	-0.57895900	-0.11529400
H	-5.53839300	-1.49382800	-0.38156100

Absolute energies (Hartree): -575.713038 ZPE (Hartree): 0.222427

Harmonic Vibrational Frequencies (cm^{-1}):

19.1408 46.2537 48.5054 85.0015 90.6744 107.8805 133.0038 136.6475 143.0683 167.8077 198.9640 204.0205 219.8559 272.3550 306.8619 340.5665 396.6100 461.2274 517.8869 539.2192 767.0201 804.1084 825.6704 880.6043 911.2259 921.3230 981.4963 1002.3447 1049.0062 1072.6016 1079.8658 1089.1868 1108.3366 1115.4864 1129.3959 1227.1749 1236.3214 1248.6360 1282.9428 1291.1289 1308.7195 1318.9667 1350.5999 1354.7936 1368.5516 1371.8833 1392.4312 1424.3390 1433.6092 1438.8911 1488.2253 1497.6812 1501.6805 1509.2747 1518.1656 1551.7992 1552.7583 2999.3333 3011.2782 3014.1609 3051.5475 3064.3075 3093.1601 3101.4088 3107.8828 3108.3912 3109.8238 3127.6398 3154.8394 3160.6900 3843.8693 3843.9607

TS_{62}

Cartesian Coordinates (Å)

At.	X	Y	Z

C	-0.09888400	1.30211800	0.30949700
H	0.26544200	2.07739000	-0.36407600
H	-1.37496100	1.41239400	0.30941900
C	0.13904700	-0.13101700	-0.13129100
H	0.01109000	-0.20274800	-1.21735300
C	-0.86174200	-1.07337100	0.56165300
H	-0.99002700	-0.74609300	1.59860000
H	-0.46914300	-2.09718700	0.58936100
C	-2.21744900	-1.10631000	-0.15013800
H	-2.18428500	-1.77251300	-1.01774000
H	-3.01342700	-1.43048400	0.52975200
O	-2.55695900	0.15259600	-0.73171900
O	-2.53732800	1.11326600	0.27135100
H	0.16750000	1.48500400	1.35453900
C	1.56184800	-0.56875700	0.20675100
H	1.75982200	-1.57400100	-0.18490700
H	1.71233600	-0.57192200	1.29608600
O	2.43010500	0.36727100	-0.40743200
O	3.77587900	-0.10078200	-0.14269200
H	4.08515600	0.62537600	0.41142900

Absolute energies (Hartree): -497.183487 ZPE (Hartree): 0.162563

Harmonic Vibrational Frequencies (cm^{-1}):

-2150.2408 68.9873 109.8343 121.9079 157.7395 186.0096 208.7072 269.8617 310.0774 383.4551 401.9622 435.9350 486.7359 530.3563 650.9696 684.5713 834.1075 871.6425 921.6175 941.5781 991.2102 999.8493 1038.7046 1085.6728 1105.1739 1144.2787 1161.1680 1192.5910 1204.1389 1248.2422 1264.5623 1279.9359 1296.8928 1330.4056 1370.6022 1381.5339 1401.0499 1414.6137 1418.9534 1474.0425 1498.9897 1510.3140 1537.7001 1542.5626 3043.0139 3075.6693 3084.7072 3100.3004 3112.4244 3117.4666 3133.8750 3157.0692 3220.9265 3842.1181

$O_2CC(C\bullet)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.86064900	0.27432000	0.11920800
H	-2.11664300	0.77288700	1.06497100
H	-1.98012300	0.99016200	-0.70066200
C	0.63624500	1.86848400	-0.57132100
H	1.04306400	2.84690300	-0.34391000
H	0.54004300	1.58564200	-1.61279200
C	1.96603100	0.19205600	0.73442400
H	1.91826700	-0.53832400	1.55433400
H	2.70089100	0.96689300	0.98196900
O	2.33503500	-0.45296300	-0.47225600
O	3.66519800	-0.98315300	-0.25322700

H	3.46526000	-1.92504500	-0.30677300
O	-2.71128100	-0.84251200	-0.08937400
O	-4.05062000	-0.31019500	-0.23829600
H	-4.44653700	-0.65870100	0.56872800
C	0.58264800	0.81193600	0.48856700
H	0.30689500	1.28061400	1.44506800
C	-0.44653200	-0.28076500	0.16784100
H	-0.40020200	-1.06273100	0.93510200
H	-0.20402900	-0.74390200	-0.79312300

Absolute energies (Hartree): -497.197481 ZPE (Hartree): 0.164178

Harmonic Vibrational Frequencies (cm^{-1}):

59.8971 66.8290 78.0725 113.8646 134.3575 143.0531 156.0709 193.7847 198.5210 211.6882 295.8127 322.8565 370.3465 455.5435 477.2786 531.1085 671.3863 819.9176 868.0531 918.6954 930.4581 956.5141 998.9575 1018.9172 1090.2530 1092.7243 1134.0528 1182.2395 1199.7872 1251.9939 1267.5853 1289.1269 1314.2787 1343.7353 1368.4081 1376.3896 1392.0347 1410.8435 1435.6359 1490.3638 1515.9030 1542.3742 1550.2509 3045.1737 3048.4005 3057.8291 3085.3052 3116.5112 3123.6418 3155.8345 3195.3943 3312.4632 3841.8582 3843.5157

TS_{63}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.60803200	-1.24890600	0.44691600
H	0.19562900	-2.05468200	-0.16261700
H	1.87801100	-1.40593500	0.37886900
C	0.38257100	0.16714400	-0.05592600
H	0.45421700	0.16867500	-1.15132600
C	1.47033800	1.09905800	0.50920000
H	1.65443300	0.82807500	1.55451700
H	1.11761900	2.13715900	0.50018900
C	2.77636000	1.03579900	-0.28838500
H	2.71074600	1.65270500	-1.19006200
H	3.62856900	1.36422000	0.31730300
O	3.03002900	-0.26726500	-0.81638400
O	3.04420900	-1.16707300	0.24046700
H	0.39788500	-1.37157600	1.51367700
C	-1.01415900	0.67578900	0.33641900
H	-1.15914900	1.68009500	-0.07851500
H	-1.07869400	0.75560400	1.42850200
O	-3.33855200	0.46964200	0.09521000
C	-2.12976800	-0.22036500	-0.17793400
H	-2.13483100	-1.19374100	0.32775800
H	-2.02867400	-0.38308100	-1.25873000
O	-4.40483900	-0.36558700	-0.42063900

H	-4.84277800	-0.58637000	0.40946800

Absolute energies (Hartree): -536.437475 ZPE (Hartree): 0.191389

Harmonic Vibrational Frequencies (cm^{-1}):

-2161.3536 55.0929 78.4688 98.0600 128.2834 149.9105 197.3249 206.3847 242.9971 289.6481 310.1492 389.8321 428.7647 460.4319 508.3679 529.1986 643.0583 687.9606 813.3641 832.3316 878.8978 915.6592 954.3619 990.7310 1007.8171 1045.0792 1080.5084 1089.2227 1100.0518 1139.1295 1165.7087 1195.5401 1201.7293 1242.8853 1251.6931 1275.5254 1288.8269 1313.4742 1320.7007 1357.0426 1371.3392 1374.1602 1403.4806 1416.4438 1436.8186 1472.1737 1498.6213 1507.3288 1513.4383 1535.8177 1549.9097 3057.1846 3072.4601 3074.9807 3081.5465 3086.1322 3106.0593 3110.3068 3131.2346 3139.0340 3155.7706 3207.4623 3844.2816

$O_2CCC(C•)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.39570300	0.20076000	-0.09689300
H	2.74139100	0.73068300	-0.99528300
H	2.57642300	0.83467000	0.77810900
C	0.03025300	1.90577900	0.88832700
H	-0.36951700	2.91335100	0.87593700
H	0.24766200	1.45389200	1.84952000
C	-1.38469200	0.72461400	-0.83315300
H	-1.33374200	0.24691800	-1.81827700
H	-1.97143500	1.64414700	-0.93913100
O	3.09315200	-1.02648000	0.04598700
O	4.48620200	-0.67933200	0.24356000
H	4.85164500	-1.03590300	-0.57427900
C	0.04513800	1.08708100	-0.36545900
H	0.47064800	1.70450900	-1.17166000
C	0.92444500	-0.16232500	-0.21992800
H	0.78915900	-0.81507600	-1.09022700
H	0.62988300	-0.73060000	0.66934800
C	-2.10633400	-0.20316100	0.13185300
H	-1.63574800	-1.19130900	0.17020000
H	-2.12997100	0.22107800	1.14406900
O	-3.42681700	-0.32971000	-0.37414800
O	-4.09706400	-1.28840500	0.48126900
H	-4.73726200	-0.70143000	0.89985100

Absolute energies (Hartree): -536.451553 ZPE (Hartree): 0.193006

Harmonic Vibrational Frequencies (cm^{-1}):

51.9556 56.4260 73.4362 84.3336 107.4344 147.3132 155.3484 165.8608 181.6018 196.6036 197.1508 259.1476 300.7343 354.0993 424.0643 434.6645 482.4158 497.6671 634.6148 818.4549 821.6303 869.4396 912.2885 927.3962 955.6395 1021.3247 1038.2852 1088.1829 1091.4004 1097.8923 1135.3754 1185.1796 1197.9084 1253.1824 1257.1495 1270.0356 1307.2095 1322.4796 1329.7475 1362.3004 1368.6876 1372.5505 1399.3929

1434.6148 1439.3379 1488.2749 1510.7267 1516.1760 1549.7353 1550.4675 3036.5008 3052.5282 3060.7829 3080.1574 3081.0508 3117.0813 3121.9094 3144.0221 3144.7671 3190.5236 3306.2501 3843.2091 3843.9026

TS_{64}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.17678600	-1.24763800	0.45728400
H	0.75857100	-2.05989700	-0.13900700
H	2.44566900	-1.39944100	0.37682500
C	0.94032800	0.16237800	-0.05527600
H	1.00489300	0.15491600	-1.15153400
C	2.02629000	1.10383900	0.49698600
H	2.21856300	0.84039600	1.54286200
H	1.66803200	2.14037300	0.48460300
C	3.32848800	1.04397700	-0.30749900
H	3.25519700	1.65750600	-1.21101500
H	4.18256500	1.37872700	0.29223700
O	3.58580900	-0.25943400	-0.83221600
O	3.61158000	-1.15509000	0.22842800
H	0.98038800	-1.36103200	1.52788400
C	-0.45951800	0.66128000	0.33832200
H	-0.59125000	1.67283600	-0.06955500
H	-0.50672100	0.74971500	1.43253600
C	-1.59420000	-0.23703100	-0.15651400
H	-1.55738200	-1.21096700	0.34182200
H	-1.48506500	-0.41187900	-1.23352300
O	-3.92036700	-0.54934100	-0.31779900
C	-2.95127400	0.39146200	0.11495300
H	-3.06657600	1.33375300	-0.43747000
H	-3.08018100	0.59231100	1.18555100
O	-5.21204300	0.02631200	-0.00048100
H	-5.54793000	0.15350000	-0.89520000

Absolute energies (Hartree): -575.69189 ZPE (Hartree): 0.220136

Harmonic Vibrational Frequencies (cm^{-1}):

-2142.2282 42.0837 64.3771 69.9546 102.7935 139.1156 150.7234 190.4860 196.0224 208.1420 258.1951 296.6030 376.1122 397.6934 429.7056 461.9264 515.7545 532.1524 640.7350 687.6048 774.2652 827.9272 862.6786 896.1036 912.4321 961.6785 991.0039 1007.8517 1057.2054 1076.7789 1079.4467 1094.8256 1106.6973 1144.1762 1163.2148 1197.8265 1202.5310 1235.2231 1245.7350 1264.0989 1283.6176 1296.0494 1311.4013 1331.9323 1341.7201 1368.9973 1375.8987 1390.5590 1404.2299 1416.8220 1437.6866 1472.3196 1496.6440 1502.6856 1511.3792 1517.9289 1533.7602 1551.6734 3047.8900 3053.4693 3071.7090 3076.5795 3082.4064 3083.4744 3103.8571 3107.0031 3108.9653 3129.3908 3148.8078 3154.1882 3208.9425 3844.5675

$O_2CCCC(C\bullet)CCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.94720400	0.09480400	-0.07352400
H	3.35779000	0.63612000	-0.93721200
H	3.16675100	0.66370900	0.83652300
C	0.73790800	1.97234200	0.93916200
H	0.46506200	3.02152800	0.95542800
H	0.85196600	1.46049200	1.88818700
C	-0.76435000	0.97928100	-0.82277200
H	-0.73543400	0.53116700	-1.82514000
H	-1.24927400	1.95912300	-0.92274200
O	3.52838500	-1.19677600	0.01468600
O	4.94306400	-0.98887900	0.25221800
H	5.29095100	-1.33295000	-0.57849000
C	0.69065800	1.20150100	-0.34331600
H	1.17520900	1.80675300	-1.12532000
C	1.45190300	-0.12630500	-0.23746000
H	1.27731600	-0.72671300	-1.13835800
H	1.08683400	-0.70185200	0.62009100
C	-1.59737200	0.09560600	0.10712000
H	-1.18601300	-0.91794300	0.14426700
H	-1.57980500	0.50004300	1.12487700
O	-3.70368900	-0.86152100	0.53250800
C	-3.03870400	0.01003400	-0.36791600
H	-3.09252600	-0.39640100	-1.38528100
H	-3.51576300	0.99945000	-0.35710700
O	-5.06130000	-0.99171800	0.04173900
H	-5.52822800	-0.55495800	0.76331200

Absolute energies (Hartree): -575.705965 ZPE (Hartree): 0.221815

Harmonic Vibrational Frequencies (cm^{-1}):

40.8084 46.8672 60.7862 78.5863 90.0473 123.4916 140.7347 155.6042 157.0946 176.5548 194.1763 197.7173 207.9519 295.5841 344.6061 361.7842 420.9771 449.0107 489.9916 503.2438 648.1322 773.3428 820.5257 865.5968 887.6347 909.0454 926.5614 951.3404 1012.6366 1058.9790 1083.2522 1092.0390 1095.3603 1107.8162 1134.9984 1188.6693 1197.3451 1238.6401 1248.9879 1264.4889 1301.6218 1309.4561 1315.3649 1331.1360 1347.4696 1367.9049 1369.0734 1399.3038 1404.5875 1433.3751 1436.9040 1487.9675 1503.6895 1513.7634 1519.6918 1550.8440 1552.2511 3034.2087 3050.7525 3051.8648 3057.6063 3078.8428 3091.2092 3107.2970 3108.2843 3118.1452 3143.9261 3155.3261 3189.2714 3304.6456 3844.0779 3844.5051

TS_{65}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.29655400	0.41595000	0.82553700
H	0.52789100	0.28279200	1.88532500

H	-0.16241900	-0.71377500	0.47468600
C	-0.84804400	1.37745800	0.53413900
H	-1.54722000	1.38345800	1.37587100
H	-0.44338200	2.39501800	0.44489100
C	-1.59986900	1.00796100	-0.75730900
H	-0.87831900	0.71912600	-1.52579000
H	-2.14635400	1.87659300	-1.14028000
C	-2.60402500	-0.12698300	-0.54089400
H	-3.52747000	0.24935400	-0.08957800
H	-2.83963500	-0.63316800	-1.48395400
O	-2.14775600	-1.07980000	0.42124500
O	-0.91025600	-1.55207500	0.01431900
C	1.53399100	0.62717500	-0.00875500
H	2.02643400	1.57056800	0.27055700
H	1.29801000	0.66067500	-1.07973400
O	2.39231300	-0.46531100	0.26828400
O	3.59727000	-0.22715500	-0.50113400
H	3.56825700	-1.00526900	-1.07001800

Absolute energies (Hartree): -497.183671 ZPE (Hartree): 0.16286

Harmonic Vibrational Frequencies (cm^{-1}):

-2184.3826 61.0180 81.0597 98.2022 138.1030 199.6632 220.0576 261.7566 282.0940 319.5105 420.3253 466.2374 479.4911 598.2890 668.8488 809.5491 820.7520 892.5740 901.3944 919.6583 972.5726 1033.6573 1068.2817 1077.6408 1103.9364 1138.4679 1178.0179 1194.6516 1231.2430 1253.9357 1263.5144 1300.0624 1313.4014 1338.0328 1360.1505 1377.0086 1402.8883 1418.2616 1427.9030 1495.0263 1500.8842 1511.9491 1534.3313 1539.2531 3039.0967 3060.7868 3079.5302 3095.8025 3101.2990 3133.7069 3143.5535 3152.8627 3162.5479 3844.3488

$O_2CC•CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.67677400	0.66048500	0.36341300
H	3.37451800	1.49733000	0.26120800
H	2.65645900	0.33633000	1.41359200
O	3.11923000	-0.43589200	-0.44754800
O	4.43189100	-0.79621500	0.04325400
H	4.22557800	-1.65544200	0.42897300
C	-1.19009100	0.66442100	-0.04906300
H	-1.29463500	1.21322200	-0.99151600
H	-1.30934500	1.38294300	0.76802300
O	-3.51845400	0.32580100	-0.02512200
C	-2.29016300	-0.37978000	0.04433000
H	-2.23033400	-0.92767400	0.99252300
H	-2.21935100	-1.09824300	-0.78351500

O	-4.56351700	-0.66518100	0.13404300
H	-4.95565300	-0.61887100	-0.74550300
C	1.30874900	1.00978000	-0.11170500
H	1.18284200	1.85032200	-0.78646800
C	0.19798100	0.02080200	0.02140800
H	0.30995700	-0.52436700	0.96860800
H	0.28726500	-0.73790200	-0.77323600

Absolute energies (Hartree): -497.200195 ZPE (Hartree): 0.165244

Harmonic Vibrational Frequencies (cm^{-1}):

32.3881 44.5281 64.6409 99.8816 118.9300 123.8087 146.2603 198.1299 212.0273 233.4122 275.7703 315.4093 423.2390 460.3827 489.9620 602.3570 765.2395 873.6355 909.2562 941.9401 991.7947 1045.6935 1055.0968 1071.9732 1094.1207 1113.6895 1160.9677 1187.8358 1230.3008 1253.2794 1282.0502 1305.1619 1324.3217 1357.7444 1363.2371 1371.4747 1406.6428 1438.2381 1452.2654 1486.1270 1519.5163 1535.5365 1552.4256 3021.0128 3046.8843 3052.6873 3082.6530 3089.9922 3109.1233 3129.7088 3152.1015 3232.8879 3841.7074 3844.1522

TS_{66}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.28974300	0.59757700	0.84046500
H	-0.09945400	0.55899800	1.91799400
H	-0.60883900	-0.58941900	0.55753700
C	-1.53788500	1.38515300	0.46144400
H	-2.27007100	1.33849200	1.27406700
H	-1.25933400	2.44028700	0.33464700
C	-2.17604400	0.85984000	-0.83659900
H	-1.38756400	0.62623500	-1.55698400
H	-2.80610000	1.63192400	-1.29140100
C	-3.04313200	-0.37988600	-0.60070100
H	-4.02805200	-0.09984900	-0.21393700
H	-3.16563800	-0.95964600	-1.52268400
O	-2.52626600	-1.21959400	0.43446100
O	-1.22072100	-1.55332700	0.11584200
C	0.95668300	0.89371000	0.03234500
H	1.32164300	1.89996000	0.28099600
H	0.72981500	0.88405900	-1.03885000
O	3.17403100	0.29396600	-0.46063500
C	2.05971400	-0.11474500	0.31590100
H	1.74529200	-1.12638300	0.02768300
H	2.32530200	-0.11489200	1.37973900
O	4.24733000	-0.62492700	-0.14556300
H	4.29044700	-1.10859800	-0.97877600

Absolute energies (Hartree): -536.440191 ZPE (Hartree): 0.191762

Harmonic Vibrational Frequencies (cm^{-1}):

-2157.3633 42.5202 62.0742 80.9371 112.7696 142.2289 189.7950 217.0309 236.0707 267.0507 300.4766 383.1243 414.8880 436.2843 520.7615 599.3109 666.2235 777.6341 820.2583 845.1228 882.6005 919.3786 927.8716 963.9645 1038.6342 1064.5180 1083.4699 1090.9190 1108.3759 1150.8148 1176.9610 1201.1589 1227.4532 1244.9477 1261.6507 1284.6581 1304.0843 1312.6078 1324.5775 1358.6525 1371.0122 1387.3091 1403.7596 1418.4363 1438.4654 1493.3001 1495.9680 1504.7937 1513.9892 1544.7774 1551.2589 3056.9921 3060.3615 3064.9675 3079.1477 3096.5992 3113.1082 3120.7090 3133.0459 3139.3353 3144.0089 3160.9062 3839.7590

$O_2CCC•CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.15650900	0.34067100	0.09408600
H	3.32606200	1.13621900	-0.64152400
H	3.15535000	0.78379600	1.09922100
O	-4.27606100	0.42538500	0.12157100
O	4.18268400	-0.63323200	-0.00769200
O	5.43226700	0.07466100	0.18538600
H	5.70684200	-0.32203800	1.02006400
C	-3.10951900	-0.36975600	-0.01696900
H	-2.97950500	-1.01207300	0.86298000
H	-3.19448800	-1.00203500	-0.90865700
O	-5.38965800	-0.49845900	0.18294700
H	-5.66377000	-0.35108600	1.09543900
C	1.84941700	-0.38360000	-0.18170300
H	1.90095700	-0.84063800	-1.17567500
H	1.72181700	-1.19004600	0.54796100
C	0.65259600	0.56861400	-0.11097300
H	0.61726800	1.04755100	0.87773300
H	0.80368200	1.38923300	-0.83416200
C	-0.65114300	-0.11166300	-0.37965900
H	-0.64973800	-0.97419200	-1.04290500
C	-1.94581000	0.60250500	-0.15597600
H	-1.88340600	1.22590000	0.74387600
H	-2.16722300	1.28193900	-0.99486900

Absolute energies (Hartree): -537.113795 ZPE (Hartree): 0.208158

Harmonic Vibrational Frequencies (cm^{-1}):

23.6602 32.5354 52.6169 77.2444 100.1008 116.2111 128.4047 143.5808 158.7270 194.5082 197.3439 228.9328 271.1895 400.2995 432.1799 443.5376 504.3537 543.1313 763.3096 808.5302 877.4314 912.6300 915.6400 1019.5883 1050.6519 1057.5576 1087.0474 1096.8356 1109.8218 1116.0165 1162.7918 1177.4139 1229.0164 1239.6622 1250.7149 1297.8974 1301.2393 1310.3742 1324.1707 1364.1880 1369.9858 1376.4060 1423.9924 1440.4528 1456.2412 1488.5281 1500.3186 1520.0766 1552.1134 1552.8526 3000.3850 3025.5310 3052.0783 3062.7008 3071.6392 3089.8038 3103.0241 3108.7704 3125.7575 3151.1019 3199.2018 3843.9352 3844.6125

TS_{67}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.89189700	0.64316200	0.85352200
H	-0.75663800	0.64748200	1.94025800
H	-1.15668200	-0.56131800	0.59819400
C	-2.13961300	1.37969700	0.38118200
H	-2.91242500	1.34236400	1.15596200
H	-1.88407100	2.43748900	0.22852900
C	-2.69524100	0.78936200	-0.92692000
H	-1.86461800	0.55404600	-1.59775400
H	-3.32352100	1.52484500	-1.44123300
C	-3.53687300	-0.46738200	-0.68912600
H	-4.54746000	-0.20405200	-0.36112800
H	-3.59699500	-1.08142100	-1.59507800
O	-3.04814700	-1.25513900	0.39869700
O	-1.71887400	-1.55865100	0.15636300
C	0.39074500	0.94203900	0.10561400
H	0.68255200	1.98346400	0.31278400
H	0.21500100	0.87422500	-0.97503000
C	1.53199000	0.00149500	0.49891600
H	1.24855400	-1.03360200	0.27883700
H	1.71680200	0.07202500	1.57642300
O	3.79173100	-0.58092200	0.20613900
C	2.81282600	0.33983900	-0.24568000
H	3.13637300	1.36428300	-0.02409700
H	2.67297100	0.24035000	-1.33063000
O	5.02487700	-0.22022400	-0.46446200
H	5.14184400	-1.00996600	-1.00497200

Absolute energies (Hartree): -575.694351 ZPE (Hartree): 0.220459

Harmonic Vibrational Frequencies (cm^{-1}):

-2145.0292 37.0937 42.5045 68.0379 95.1677 125.2862 135.8299 160.7299 197.1595 224.6293 253.7129 284.8208 323.8985 388.1910 423.0065 458.3274 529.5983 598.5073 665.4215 759.4165 805.9795 820.9124 877.6929 885.5474 914.4247 951.3326 963.6324 1037.9413 1055.1546 1077.6304 1094.4256 1095.9846 1115.7356 1146.7408 1181.9479 1203.1607 1225.9344 1236.6606 1252.9747 1272.9120 1299.8663 1306.6463 1319.9111 1330.0773 1350.0311 1360.3920 1371.3567 1401.9262 1406.8448 1419.5551 1440.2695 1490.3535 1493.2304 1502.8791 1513.2424 1518.2099 1540.1132 1552.0285 3036.8017 3051.9000 3058.1440 3077.9718 3086.3290 3094.7400 3103.1135 3107.1723 3121.8348 3132.3117 3141.5239 3149.1191 3159.7752 3844.6023

$O_2CCCC•CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z

C	3.91605400	0.58512300	0.45993600
H	4.65688400	1.39053200	0.40297200
H	3.88914400	0.19877900	1.48827700
O	4.27340900	-0.45488100	-0.43872500
O	5.60845900	-0.87383300	-0.06604600
H	5.40813500	-1.75868600	0.26047100
C	-2.41955900	0.42698200	-0.17069100
H	-2.47359400	0.80064900	-1.19923500
H	-2.44262300	1.29313200	0.49820900
O	-4.77198700	0.37157700	-0.10815200
C	-3.63238900	-0.44560300	0.10628400
H	-3.62590100	-0.80805500	1.14136500
H	-3.65605900	-1.31064200	-0.57040300
O	-5.92324000	-0.44448100	0.22154000
H	-6.31499900	-0.52013800	-0.65608700
C	0.10346900	0.47958500	-0.24887700
H	0.03287700	1.25132300	-1.01288600
C	1.46219100	-0.01122900	0.13486200
H	1.75182600	-0.86664300	-0.49616600
H	1.43595000	-0.39469900	1.16559600
C	2.54185800	1.06893000	0.02639900
H	2.27007400	1.92313800	0.65734600
H	2.60383500	1.43061700	-1.00616400
C	-1.11237000	-0.34536800	0.02918500
H	-1.06529800	-0.72986500	1.05784600
H	-1.11891000	-1.23703500	-0.62266800

Absolute energies (Hartree): -575.70929 ZPE (Hartree): 0.22231

Harmonic Vibrational Frequencies (cm^{-1}):

20.2297 25.2783 46.3306 74.1772 93.1164 96.9308 109.3161 122.8899 148.1080 180.5887 197.1624 199.0169 235.2945 292.7124 327.7045 388.5573 418.0355 459.6735 515.0775 569.7975 747.8715 770.5873 870.4933 897.5116 911.0940 927.5264 959.5675 1039.0875 1060.3881 1062.4195 1094.0214 1109.3908 1115.0639 1120.0621 1163.7286 1174.8499 1223.4445 1234.0479 1240.9839 1274.1635 1299.1636 1309.7022 1322.5363 1330.0420 1361.6861 1370.9050 1372.8454 1407.0333 1427.8271 1438.4491 1451.0768 1485.6508 1493.7264 1498.8943 1520.0917 1546.4451 1552.8950 2995.8754 3023.5720 3051.6836 3052.0823 3068.3883 3071.6855 3081.6284 3088.9055 3108.6253 3118.2180 3141.2956 3151.3804 3197.0105 3842.1402 3844.4197

TS_{68}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.25895600	0.69824600	0.09992000
H	0.20339100	-0.11660300	-0.73046800
C	0.85873100	0.82036900	1.13486400
H	1.53500200	1.63123700	0.84178500

H	0.41582500	1.10685700	2.09957900
C	1.65915500	-0.48257100	1.29545000
H	0.96969500	-1.33110100	1.30575100
H	2.19307500	-0.48866000	2.25212700
C	2.68559000	-0.66698600	0.17616800
H	3.56984400	-0.04590700	0.35086700
H	2.98822500	-1.71612800	0.08247500
O	2.20130100	-0.18827100	-1.08132000
O	1.00508400	-0.82444700	-1.35498800
C	-0.53633400	1.95798400	-0.69211600
H	-1.33411000	1.79896500	-1.41997200
H	-0.84302200	2.76340000	-0.00985900
H	0.36939800	2.27928500	-1.21483800
C	-1.48923000	0.02318600	0.66337800
H	-2.02898500	0.71917200	1.32453900
H	-1.22544600	-0.87438800	1.23738200
O	-2.30991000	-0.32790600	-0.43755700
O	-3.50898000	-0.91240500	0.12953600
H	-3.42659900	-1.80326600	-0.23071900

Absolute energies (Hartree): -536.445905 ZPE (Hartree): 0.19123

Harmonic Vibrational Frequencies (cm^{-1}):

-2135.4285 58.3498 90.5839 97.6148 108.2330 182.3396 200.2732 219.5031 246.0865 269.4091 305.9831 341.7983 370.7975 423.7973 450.4654 500.3767 600.9868 637.4032 814.0929 864.0195 894.4947 922.6221 935.9063 958.0127 985.7021 1016.5794 1079.2472 1095.6979 1110.8986 1140.0515 1191.6375 1199.8420 1222.5240 1240.0310 1264.6075 1282.6287 1306.8750 1326.4484 1364.3093 1372.9579 1403.3943 1404.7607 1417.9274 1422.3463 1492.8732 1499.3590 1500.9777 1511.1433 1514.8891 1531.6881 1548.5978 3030.3033 3049.5304 3053.1043 3079.4244 3093.2651 3097.6765 3121.3283 3141.9534 3142.3677 3160.0547 3187.6689 3842.2365

$O_2CC•(C)CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.49757800	-0.00847800	0.70854800
H	3.20624500	0.70175700	1.14941500
H	2.33857200	-0.84311900	1.40406500
O	3.04728500	-0.51190300	-0.51865400
O	4.33211700	-1.08861900	-0.18700400
H	4.12058100	-2.02260400	-0.29985600
C	-1.32611600	0.47199500	0.14973900
H	-1.40784400	1.22132200	-0.64386900
H	-1.42570800	0.99012000	1.10944600
O	-3.66276900	0.23576700	0.01320300
C	-2.46468700	-0.52331000	0.00058700

H	-2.47129600	-1.24021600	0.83039600
H	-2.37718600	-1.07724900	-0.94416100
O	-4.74902800	-0.72114300	-0.05001000
H	-5.09483200	-0.50492000	-0.92362800
C	1.21118000	0.65249400	0.33991400
C	0.03100300	-0.23566000	0.07792200
H	0.04488300	-1.06856500	0.79344500
H	0.14318400	-0.69153400	-0.92162000
C	1.27057000	2.00221000	-0.30377600
H	0.40497400	2.61915700	-0.04147000
H	2.17713400	2.53731900	-0.00924300
H	1.28329300	1.91021300	-1.40081500

Absolute energies (Hartree): -536.460548 ZPE (Hartree): 0.194156

Harmonic Vibrational Frequencies (cm^{-1}):

34.9922 36.5357 59.7274 100.0582 103.6876 116.6650 132.9808 143.5121 181.8997 198.2706 219.2358 247.7044 292.7577 364.5198 386.3708 443.3674 490.1107 608.5859 765.2680 819.3989 875.2007 913.6557 979.6625 993.6663 1009.4658 1034.5535 1064.7429 1078.6124 1094.8267 1107.4682 1128.3285 1230.2760 1240.1817 1252.4756 1297.1817 1320.1550 1326.4422 1350.8452 1363.9114 1369.1432 1397.9865 1420.3636 1425.2103 1439.2097 1484.5442 1497.7193 1507.4777 1520.6266 1536.0275 1551.9504 3002.2293 3031.0680 3051.0956 3054.7435 3084.8436 3092.0713 3109.3339 3117.5435 3120.4735 3154.0784 3166.3814 3839.6247 3843.8035

$O_2CCC(C)CCCOO$•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.20175300	-1.38701400	-0.42993900
H	0.96356200	-0.65743600	-1.20309700
H	1.02234300	-2.40495900	-0.78422100
C	0.49429600	-1.09687300	0.88056600
H	0.87086900	-1.79879700	1.63436100
H	0.77740000	-0.09586300	1.20369900
C	-1.03087100	-1.26359100	0.77720400
H	-1.47620100	-1.04247100	1.75717500
H	-1.23073900	-2.32768100	0.58986200
C	-1.77737000	-0.45362100	-0.29976000
H	-1.18970400	-0.45827700	-1.22457400
C	-2.03836100	1.01314500	0.07872000
H	-2.75640100	1.04565200	0.90993700
H	-2.51340000	1.51020600	-0.77528600
O	0.14955500	1.61803800	-0.52643200
O	2.65016200	-1.34243000	-0.23654000
O	3.07902900	-0.13609300	-0.09897200
C	-0.81233900	1.81111700	0.49564200
H	-1.05051700	2.87743200	0.59161400

H	-0.41728000	1.46275000	1.45642700
O	1.36280500	2.27407900	-0.07325600
H	1.96326200	1.51174100	-0.11284500
C	-3.12111900	-1.12873600	-0.59618000
H	-3.71698600	-1.20602400	0.32101900
H	-3.69739000	-0.55267800	-1.32724600
H	-2.97716500	-2.13891300	-0.99274400

Absolute energies (Hartree): -575.739511 ZPE (Hartree): 0.227739

Harmonic Vibrational Frequencies (cm^{-1}):

59.7963 90.9967 116.7742 130.9919 145.4408 167.1281 193.4145 238.5677 247.6434 265.9201 291.2466 322.8625 339.4892 367.1308 422.0147 487.7611 535.3993 579.4413 616.5979 746.1061 800.8367 839.0742 868.3103 915.0409 933.8536 954.5801 997.2145 1030.1149 1045.4245 1067.3781 1100.1436 1125.5505 1158.9791 1174.8019 1204.2283 1241.7391 1268.8655 1271.7059 1306.1285 1322.3212 1329.1750 1350.1080 1374.2033 1381.9040 1408.5436 1412.7540 1422.4810 1428.5922 1435.0743 1472.2594 1485.9437 1497.1596 1513.4250 1519.2105 1519.9041 1522.4297 1564.1303 3048.2026 3058.9005 3061.2609 3072.2249 3091.1132 3093.4160 3103.7377 3114.3276 3126.9349 3130.3062 3148.8359 3157.0667 3193.2298 3213.5600 3724.3171

TS_{69}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.31135900	0.86954100	-0.03011700
H	0.58784700	-0.15684000	-0.67678700
C	1.51045400	1.00505700	0.91005200
H	2.30167200	1.58231900	0.41781800
H	1.19387300	1.57779400	1.79321900
C	2.06942800	-0.35975600	1.34405000
H	1.23885200	-1.03698400	1.56179700
H	2.65358800	-0.26066600	2.26563900
C	2.97199500	-0.97848600	0.27433400
H	3.96530400	-0.51878600	0.28769100
H	3.06860200	-2.06142400	0.41225900
O	2.50999600	-0.69925700	-1.05066700
O	1.20260900	-1.13246400	-1.15541200
C	0.21835600	1.97037900	-1.06781100
H	-0.59573800	1.80376900	-1.77764400
H	0.04675400	2.93580900	-0.57100500
H	1.15493000	2.03716400	-1.62946900
C	-0.98321200	0.54488900	0.69838600
H	-1.33904200	1.44659900	1.21786300
H	-0.79657000	-0.21794800	1.46269500
O	-3.13603000	-0.37809600	0.63424400
C	-2.08044000	0.02963400	-0.22274900
H	-1.71835100	-0.82299200	-0.81354300

H	-2.44311100	0.80726700	-0.90230000
O	-4.22968100	-0.77443600	-0.22755500
H	-4.20140400	-1.72860900	-0.08998500

Absolute energies (Hartree): -575.701226 ZPE (Hartree): 0.220049

Harmonic Vibrational Frequencies (cm^{-1}):

-2087.9517 29.4965 49.2744 84.7547 93.7401 133.5277 153.3560 203.0096 215.8130 226.0726 259.8442 300.5508 313.5172 347.3665 383.9710 444.5868 460.3965 515.4816 601.1699 632.3969 804.8528 818.1915 854.0152 894.2061 919.5290 933.3001 973.9720 1002.5918 1015.7923 1074.6735 1085.1130 1099.1401 1109.8996 1151.9629 1191.3176 1202.5640 1221.6730 1232.3842 1261.9110 1268.1451 1301.9607 1316.4269 1320.5042 1340.1138 1367.0143 1371.0821 1403.7529 1416.8050 1417.4265 1436.4135 1489.2846 1493.2471 1501.6607 1504.3556 1512.9265 1514.7870 1550.4509 1555.5026 3048.1791 3050.9711 3054.8933 3059.2942 3079.2854 3093.9562 3117.4854 3119.3080 3135.9852 3140.3764 3141.8398 3159.1439 3173.8251 3838.5453

$O_2CCC•(C)CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.08514200	-0.02466000	0.70508400
H	3.79599200	0.67793100	1.15499100
H	2.91630700	-0.86282600	1.39393900
O	3.63957000	-0.52322900	-0.52200800
O	4.91789000	-1.11196300	-0.18617200
H	4.69919500	-2.04359300	-0.30470500
C	-0.73885800	0.48154100	0.15817600
H	-0.80427600	1.25494400	-0.61626700
H	-0.81443800	0.99019400	1.12774200
C	-1.90568000	-0.49396700	-0.00180300
H	-1.87883200	-1.24157200	0.79873800
H	-1.81363000	-1.02829000	-0.95444900
C	1.80521200	0.64671000	0.33270000
C	-3.24505100	0.22274500	0.04161700
H	-3.32839200	0.94840000	-0.77882000
H	-3.37520200	0.75070700	0.99397800
O	-4.24028400	-0.77958500	-0.09156000
O	-5.51611400	-0.10127600	0.01750600
H	-5.83624600	-0.22864600	-0.88293000
C	0.61592000	-0.22811400	0.06808600
H	0.62533300	-1.07099300	0.77185600
H	0.71429100	-0.67212600	-0.93856100
C	1.88063800	1.99646600	-0.31009200
H	1.02492600	2.62544800	-0.04346700
H	2.79570900	2.51922800	-0.01952700
H	1.88683700	1.90528600	-1.40726300

Absolute energies (Hartree): -575.714706 ZPE (Hartree): 0.22291

Harmonic Vibrational Frequencies (cm^{-1}):

26.5313 33.6074 52.0920 78.5638 82.1762 113.7142 121.3609 129.1955 144.6420 178.0516 199.6413 215.9687 221.1322 256.5331 328.7168 386.0477 405.1765 438.0270 510.3394 604.7796 748.4556 808.0259 821.3029 912.3311 925.6740 982.1809 995.0806 1009.7186 1034.2164 1061.8481 1065.8289 1083.4935 1096.5099 1113.9058 1139.0169 1224.3596 1237.8027 1242.5755 1280.0641 1298.4522 1321.7805 1337.5753 1350.4415 1360.3604 1364.5683 1371.2128 1409.8970 1421.8644 1424.8129 1438.8596 1482.9418 1497.0215 1506.9828 1511.0421 1521.9924 1535.9795 1552.4156 2999.8269 3030.7915 3052.0182 3054.5351 3066.1040 3081.9748 3085.6344 3108.5451 3115.3480 3118.6176 3120.5825 3146.7942 3165.0942 3839.5443 3843.9427

TS_{70}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.20234200	-1.19168100	-0.09742600
H	-0.20287100	-1.45050200	0.96572100
H	1.03633700	-1.39289100	-0.35854300
C	-0.56708000	0.25283000	-0.36204600
H	-0.64357700	0.41773200	-1.44427600
C	1.79738100	1.24262400	-0.55202000
H	1.67602600	0.73617900	-1.51404400
H	2.11216700	2.26831500	-0.77575300
C	2.94221000	0.58235400	0.20660700
H	3.83234700	0.51091200	-0.42939800
H	3.18868700	1.14367200	1.11381300
O	2.61268500	-0.71102700	0.71076700
O	2.22792200	-1.51206500	-0.35596300
C	0.45604000	1.25014600	0.20748400
H	0.01480200	2.25245400	0.16096000
H	0.62118100	1.02286300	1.26872300
H	-0.73447700	-1.92340900	-0.70594500
C	-1.94025200	0.55479900	0.24181300
H	-2.25339100	1.57569400	-0.00816500
H	-1.90885000	0.44500100	1.33549400
O	-2.84915700	-0.37638200	-0.32081800
O	-4.15764200	-0.02039300	0.18901200
H	-4.32458000	-0.79351500	0.74095700

Absolute energies (Hartree): -536.438548 ZPE (Hartree): 0.191395

Harmonic Vibrational Frequencies (cm^{-1}):

-2102.9525 61.6037 94.7203 110.5570 135.0893 151.2551 200.2748 211.0883 248.2313 297.3893 332.4956 367.7386 404.1399 443.9493 556.0869 575.9645 615.8284 652.4732 775.2940 877.6418 908.4218 920.5552 929.5950 954.2648 1004.6138 1031.8159 1081.8998 1085.4145 1117.3156 1141.2504 1168.5162 1177.4827 1188.6292 1249.0859 1254.4842 1275.3369 1290.3571 1314.3587 1321.0425 1369.0693 1377.6178 1396.2365 1406.5585 1414.1475 1421.0748 1472.1300 1500.0500 1504.1906 1509.9057 1518.3659 1541.9551 3043.5544 3065.1679 3076.5114 3085.9064 3089.8935 3110.1211 3112.7692 3124.7425 3138.8531 3153.7361 3214.3111

3839.7179

$O_2CC(C•)CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	2.55369100	0.14643900	0.70790200
H	3.37112700	0.85616500	0.87663700
H	2.46925300	-0.52421500	1.57454400
O	2.81274500	-0.60830200	-0.46640800
O	4.11692000	-1.21018300	-0.28475200
H	3.85125600	-2.13323400	-0.19777400
C	-1.28599200	0.53869300	0.17553900
H	-1.33301900	1.22197900	-0.67841500
H	-1.46069200	1.12772900	1.08358800
O	-3.60900100	0.22892800	-0.04170300
C	-2.39162100	-0.49527200	0.04084700
H	-2.41572200	-1.16131600	0.91177900
H	-2.24994400	-1.10181200	-0.86397500
O	-4.66673000	-0.75979500	-0.09697800
H	-4.96949500	-0.61215600	-1.00035000
C	1.23609300	0.88259300	0.46580100
H	1.01501600	1.42707700	1.39521800
C	0.08817700	-0.12690300	0.24122200
H	0.10195700	-0.85387400	1.06555100
H	0.28032200	-0.68171500	-0.68341600
C	1.36472700	1.86411800	-0.65751800
H	0.76865100	2.76741100	-0.67664100
H	1.94937000	1.60476700	-1.53077600

Absolute energies (Hartree): -536.452103 ZPE (Hartree): 0.193076

Harmonic Vibrational Frequencies (cm^{-1}):

49.6782 53.2199 62.3339 108.1122 124.9762 139.0856 146.9198 165.0337 199.2692 202.6308 208.9122 247.4302 298.1716 344.7356 409.2776 428.5277 488.6575 532.2708 621.7551 776.7551 861.6028 886.2746 913.0984 915.1540 976.4861 1006.2871 1032.0467 1077.8646 1096.0545 1111.1303 1144.6860 1166.7734 1194.4444 1233.7844 1259.2617 1284.3154 1302.8578 1327.2689 1343.5673 1367.9935 1369.0604 1378.3615 1399.7582 1416.1520 1437.3562 1489.8330 1505.0333 1520.3130 1542.4219 1551.9880 3047.5508 3051.5381 3057.5009 3064.5160 3083.5600 3108.8045 3121.8312 3126.5715 3151.3176 3208.1859 3327.8671 3839.2275 3843.3135

TS_{71}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.27222800	-1.14774500	0.05758300
H	-0.25648400	-1.40535000	-1.00599100

H	-1.50504600	-1.39575200	0.31476900
C	0.05155700	0.30640300	0.32923200
H	0.13755200	0.45513600	1.41492500
C	-2.35598700	1.17974800	0.60179500
H	-2.19226300	0.64465500	1.54212600
H	-2.70091700	2.18463000	0.87112800
C	-3.49614800	0.50451000	-0.15049400
H	-4.36703000	0.37707700	0.50314900
H	-3.78542200	1.08584300	-1.03201200
O	-3.13037900	-0.75837100	-0.70618000
O	-2.68673300	-1.57693200	0.32237100
C	-1.03629700	1.26189000	-0.19051000
H	-0.63693100	2.28109500	-0.13811900
H	-1.21660300	1.04493800	-1.25181300
H	0.26426500	-1.87601000	0.66954300
C	1.40815800	0.67374600	-0.30208200
H	1.64729100	1.71302100	-0.04742800
H	1.32936600	0.60901300	-1.39411100
O	3.73715900	0.39771900	-0.29777500
C	2.54802200	-0.20863700	0.18295700
H	2.46812700	-1.22996800	-0.20826400
H	2.56763900	-0.24933600	1.27989600
O	4.83127200	-0.42499500	0.17884600
H	5.15344200	-0.75785400	-0.66677300

Absolute energies (Hartree): -575.692304 ZPE (Hartree): 0.220235

Harmonic Vibrational Frequencies (cm^{-1}):

-2121.3375 49.4734 69.2118 96.0554 118.0090 122.1586 169.1194 201.2935 208.8757 228.6910 289.9499 298.4445 308.9093 391.0830 431.4349 490.6482 539.2490 575.2123 610.1174 659.2795 773.6719 812.9507 883.7481 903.5400 916.2367 929.5057 988.7283 1004.1237 1032.4225 1075.5156 1084.2769 1096.4984 1117.4183 1136.1409 1170.7382 1172.4088 1188.6666 1241.1749 1255.5976 1270.7294 1281.2721 1300.6155 1316.4768 1320.4094 1347.8673 1369.9331 1378.0684 1393.2634 1405.2835 1419.7234 1435.6262 1470.2935 1498.4363 1502.9281 1509.1233 1512.3113 1517.5620 1550.3620 3056.4980 3060.0113 3066.4314 3075.2025 3076.5922 3088.7656 3102.1402 3110.2798 3122.0130 3137.3005 3139.0526 3153.2508 3199.7506 3843.7085

$O_2CCC(C•)CCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.27597900	0.67894700	0.01261300
H	4.00496900	1.38589200	-0.39956800
H	3.44873900	0.57680300	1.09116800
O	3.42177300	-0.58241000	-0.62392400
O	4.79748800	-0.98536300	-0.41573000
H	4.65121200	-1.74267600	0.16286800

C	-0.61881100	0.69760900	-0.14493100
H	-0.63103800	0.96414700	-1.21020300
H	-0.78529900	1.62644600	0.41925300
C	-1.74936700	-0.29012500	0.14582800
H	-1.77602800	-0.52779700	1.21400600
H	-1.56718200	-1.22565400	-0.39573400
C	1.85466100	1.13336700	-0.27783700
H	1.70366100	2.10524600	0.20964300
H	1.74223100	1.28168600	-1.35846700
C	-3.09879800	0.27306200	-0.26802800
H	-3.12713500	0.47364000	-1.34776000
H	-3.31512200	1.20460800	0.26911500
O	-4.06422900	-0.71051200	0.06953400
O	-5.35508500	-0.14564800	-0.26920800
H	-5.59240400	-0.72935400	-0.99889300
C	0.77015500	0.14701000	0.21115600
H	0.91653800	-0.79418700	-0.33250400
C	0.88928000	-0.11844000	1.67847000
H	1.45772400	-0.95724100	2.06012700
H	0.53096600	0.62132400	2.38793600

Absolute energies (Hartree): -575.707353 ZPE (Hartree): 0.221665

Harmonic Vibrational Frequencies (cm^{-1}):

31.0140 48.1459 63.9897 66.9403 105.3424 105.5876 134.6544 141.8770 151.2639 192.6134 201.2181 230.0518 242.3228 266.4127 320.7944 385.7443 395.0919 443.1614 488.0325 539.1990 591.7304 772.3169 810.7306 872.7595 880.4719 910.8048 928.8330 960.1840 1010.2121 1045.3123 1066.9045 1090.4759 1096.3734 1116.7576 1129.1826 1178.2375 1196.1415 1231.5505 1260.8889 1263.0056 1288.8626 1308.9358 1327.8850 1335.6638 1367.5523 1370.6412 1378.8519 1390.0184 1399.4377 1427.3098 1436.9836 1481.0668 1489.0089 1508.9655 1519.0025 1548.7881 1552.0464 3046.8224 3051.8114 3063.7917 3069.3480 3084.5918 3090.0749 3104.4704 3107.6777 3120.3877 3133.4648 3149.7753 3187.3783 3306.2748 3842.6921 3843.7749

TS_{72}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	0.56281400	0.54801700	-0.38998600
H	0.56747900	0.31362700	-1.45969200
H	0.06310800	-0.53256600	0.05383200
C	-0.34474200	1.70803100	-0.03972300
H	-0.21165500	1.97760900	1.01619400
H	-0.01712600	2.57774800	-0.62897000
C	-2.46147500	0.44606100	0.67736100
H	-1.81379300	0.32991600	1.55189000
H	-3.42287500	0.82036400	1.04794600
C	-2.72774400	-0.93088300	0.08105100

H	-3.06361500	-1.62609200	0.85949800
H	-3.48505500	-0.87748300	-0.70782900
O	-1.60109600	-1.48584500	-0.59627700
O	-0.54095500	-1.55326500	0.29172400
C	-1.83654900	1.45693300	-0.30434300
H	-2.35931300	2.41579100	-0.22406200
H	-1.96520300	1.11024800	-1.33709900
C	1.95294700	0.64059100	0.18441900
H	2.43248000	1.58264600	-0.12221400
H	1.92799900	0.60577100	1.28205400
O	2.68009900	-0.46038900	-0.32896200
O	4.01604900	-0.34355700	0.22007400
H	4.04329200	-1.16563000	0.72331100

Absolute energies (Hartree): -536.438899 ZPE (Hartree): 0.191566

Harmonic Vibrational Frequencies (cm^{-1}):

-2157.3633 42.5202 62.0742 80.9371 112.7696 142.2289 189.7950 217.0309 236.0707 267.0507 300.4766 383.1243 414.8880 436.2843 520.7615 599.3109 666.2235 777.6341 820.2583 845.1228 882.6005 919.3786 927.8716 963.9645 1038.6342 1064.5180 1083.4699 1090.9190 1108.3759 1150.8148 1176.9610 1201.1589 1227.4532 1244.9477 1261.6507 1284.6581 1304.0843 1312.6078 1324.5775 1358.6525 1371.0122 1387.3091 1403.7596 1418.4363 1438.4654 1493.3001 1495.9680 1504.7937 1513.9892 1544.7774 1551.2589 3056.9921 3060.3615 3064.9675 3079.1477 3096.5992 3113.1082 3120.7090 3133.0459 3139.3353 3144.0089 3160.9062 3839.7590

$O_2CC•CCCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.31052300	0.64290300	0.37135600
H	4.01118700	1.47942900	0.28689900
H	3.28055700	0.30372500	1.41648900
O	3.75797600	-0.44244700	-0.45170000
O	5.06552700	-0.81291900	0.04532700
H	4.85338500	-1.67677200	0.41729800
C	-0.55804400	0.67253700	-0.05704100
H	-0.64514700	1.22200800	-1.00326700
H	-0.65282500	1.40957400	0.74982400
C	-1.68877800	-0.35126500	0.04715600
H	-1.61302700	-0.89433900	0.99577000
H	-1.59949200	-1.08618000	-0.76101400
C	1.94689100	1.00156100	-0.10996300
H	1.83279300	1.84282000	-0.78637000
C	-3.05423300	0.31135800	-0.03032900
H	-3.18030400	0.83866700	-0.98568100
H	-3.18842200	1.02829700	0.78851900

O	-4.01144700	-0.72980400	0.08188900
O	-5.31064700	-0.08822600	0.07870000
H	-5.64329600	-0.41688300	-0.76440800
C	0.82655700	0.02274600	0.01678900
H	0.92727300	-0.52629500	0.96331400
H	0.90854300	-0.73592800	-0.77890300

Absolute energies (Hartree): -536.454466 ZPE (Hartree): 0.194036

Harmonic Vibrational Frequencies (cm^{-1}):

23.6602 32.5354 52.6169 77.2444 100.1008 116.2111 128.4047 143.5808 158.7270 194.5082 197.3439 228.9328 271.1895 400.2995 432.1799 443.5376 504.3537 543.1313 763.3096 808.5302 877.4314 912.6300 915.6400 1019.5883 1050.6519 1057.5576 1087.0474 1096.8356 1109.8218 1116.0165 1162.7918 1177.4139 1229.0164 1239.6622 1250.7149 1297.8974 1301.2393 1310.3742 1324.1707 1364.1880 1369.9858 1376.4060 1423.9924 1440.4528 1456.2412 1488.5281 1500.3186 1520.0766 1552.1134 1552.8526 3000.3850 3025.5310 3052.0783 3062.7008 3071.6392 3089.8038 3103.0241 3108.7704 3125.7575 3151.1019 3199.2018 3843.9352 3844.6125

TS_{73}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.00827800	0.74677600	-0.36916300
H	-0.02221700	0.48120900	-1.43367200
H	-0.35274200	-0.36525600	0.10963600
C	-1.07415500	1.76389100	-0.02427300
H	-0.98950100	2.04105400	1.03457100
H	-0.86598600	2.67576600	-0.60490800
C	-2.99574400	0.19854000	0.65081200
H	-2.36534800	0.18410300	1.54549100
H	-4.01484900	0.41580800	0.99186400
C	-3.03201200	-1.20402500	0.05439100
H	-3.28793400	-1.93835000	0.82731800
H	-3.76196600	-1.26564500	-0.75927400
O	-1.81423600	-1.59340300	-0.58170200
O	-0.78371600	-1.49014300	0.33506600
C	-2.51057800	1.30163200	-0.31099600
H	-3.16988600	2.17209400	-0.22731700
H	-2.57676000	0.95330500	-1.34949100
C	1.38493900	1.01798800	0.15780900
H	1.74663000	1.98088900	-0.22923000
H	1.36092300	1.09551800	1.25091800
O	3.60206600	0.25927600	0.34195900
C	2.35758900	-0.07868300	-0.25010200
H	2.46221800	-0.11967900	-1.34069500
H	2.01303200	-1.05638100	0.10933500
O	4.55050200	-0.73770600	-0.10636000

H	4.65687000	-1.23534100	0.71287900

Absolute energies (Hartree): -575.696039 ZPE (Hartree): 0.220584

Harmonic Vibrational Frequencies (cm^{-1}):

-2088.8957 44.3445 51.4524 63.1682 97.9372 132.5830 182.1314 201.3678 221.8906 226.8478 245.4630 264.5278 316.7013 394.0567 425.4094 467.0456 524.6165 591.6503 609.7428 767.9262 793.1770 805.0203 883.6149 902.3250 920.5392 964.5032 1001.9312 1029.4287 1057.4005 1084.3350 1089.2684 1119.0031 1132.0840 1144.5187 1177.9375 1190.6221 1220.2982 1237.8373 1249.8169 1284.2327 1288.0449 1298.9431 1319.0730 1321.2112 1359.0809 1370.0415 1371.7938 1406.9997 1414.8172 1422.8653 1440.5711 1489.6977 1500.2258 1502.9455 1505.2977 1509.2559 1534.2661 1555.1160 3037.6217 3058.4847 3066.0749 3071.8896 3075.2194 3086.0580 3093.7912 3106.3770 3114.2109 3128.9262 3133.9059 3135.2303 3152.0301 3838.2763

$O_2CCC•CCCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.89667300	0.41114600	0.56127100
H	4.73694000	1.11350800	0.60031800
H	3.79112700	-0.07314000	1.54193300
O	4.14077300	-0.56761300	-0.43845900
O	5.39914300	-1.19578900	-0.09496900
H	5.07579900	-2.07301300	0.14102300
C	-2.47511600	0.54948800	-0.35918700
H	-2.70886900	0.82603500	-1.40045200
H	-2.56310700	1.46597600	0.23543100
O	-4.78121300	0.15660600	-0.09664800
C	-3.51819300	-0.45387300	0.11417100
H	-3.38568200	-0.68216500	1.17726300
H	-3.44854100	-1.38679300	-0.46120500
O	-5.76789800	-0.76670500	0.42529200
H	-6.20377700	-1.00927600	-0.39968200
C	0.09935700	0.90249000	-0.21670100
H	0.22724900	1.40127400	-1.19407300
H	-0.08087400	1.71083600	0.50656600
C	1.39885700	0.17619500	0.13735600
H	1.57552500	-0.62603900	-0.58689900
H	1.28762400	-0.29772100	1.12132000
C	2.60756400	1.11150900	0.16195300
H	2.43251300	1.92414400	0.87819700
H	2.74635100	1.57079800	-0.82373500
C	-1.08902400	-0.00308200	-0.25715600
H	-0.92942300	-1.03965200	-0.54796400

Absolute energies (Hartree): -575.709289 ZPE (Hartree): 0.222311

Harmonic Vibrational Frequencies (cm^{-1}):

22.4437 26.6471 45.0026 78.8998 87.6403 94.4488 124.8546 134.2523 141.1242 184.6910 198.6663 203.0579

238.8499 285.2905 329.2822 389.3360 440.7148 462.0654 514.5583 567.1444 740.5530 796.6374 824.7081 912.3377 917.8795 929.1243 978.2764 1021.2355 1061.5620 1064.1908 1089.8865 1108.0330 1116.6087 1121.4789 1162.6246 1171.7738 1216.1508 1235.8044 1245.6095 1275.4986 1297.3371 1304.1605 1317.8252 1340.9678 1361.1535 1371.5713 1373.1233 1411.8121 1426.2416 1430.6095 1454.4210 1486.3286 1492.4784 1500.6009 1516.7773 1547.0673 1551.9423 2995.2764 3020.3548 3052.0739 3056.8436 3067.3113 3069.0899 3075.7282 3108.9373 3116.3915 3123.8303 3129.2121 3143.2955 3195.2548 3841.5498 3844.5395

$O_2CC(C)CCCCOO•$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.72637900	-1.08386100	0.48222000
H	-1.38656700	-0.37164000	1.23318600
H	-1.94487800	-2.05435100	0.93416100
C	-0.76955700	-1.19584700	-0.68988500
H	-1.23310600	-1.83898600	-1.44759100
H	-0.65568000	-0.20616600	-1.13199700
C	0.58467300	-1.80486300	-0.29122200
H	1.19881000	-1.90034800	-1.19400800
H	0.39646200	-2.83185400	0.04867500
C	1.38276000	-1.08612400	0.81180000
H	2.10811200	-1.80382500	1.21690100
H	0.71939400	-0.82556000	1.64230500
C	2.18120700	0.16589400	0.40303500
H	2.59071000	0.59250000	1.32809600
O	0.19743900	1.43747700	0.58427700
O	-3.03395100	-0.62201800	0.01880300
O	-3.02377000	0.62994500	-0.28118100
C	1.32270600	1.24135400	-0.25149400
H	1.88389900	2.17920700	-0.35202300
H	1.00259000	0.92630000	-1.25300200
O	-0.65956300	2.38593000	-0.10465000
H	-1.46642100	1.84692000	-0.14856900
C	3.35426400	-0.16987600	-0.52184600
H	3.93444700	0.72806700	-0.75747200
H	4.02494200	-0.89130700	-0.04513600
H	3.00801000	-0.59969700	-1.46716900

Absolute energies (Hartree): -575.738912 ZPE (Hartree): 0.227803

Harmonic Vibrational Frequencies (cm^{-1}):

43.4918 102.8881 118.1054 130.5961 158.2216 168.5789 200.3531 205.7680 220.7255 256.4930 284.7272 307.1556 357.4636 419.6706 442.0711 472.1468 534.2441 563.6768 594.6555 739.8086 808.6178 854.2664 887.3500 917.4061 926.6420 956.4979 973.1950 993.3137 1054.5997 1078.5116 1099.4542 1123.5181 1155.6620 1168.7025 1223.5238 1245.2014 1255.7014 1269.5889 1312.4226 1320.9060 1348.8210 1354.9864 1376.9417 1387.4326 1398.2025 1413.2073 1425.4745 1433.9132 1437.0527 1473.5976 1497.2911 1504.4156 1513.4058

1518.1452 1521.1940 1524.8776 1557.2821 3056.8510 3061.9447 3067.8709 3071.8732 3079.2692 3091.8794 3109.5059 3117.6514 3126.5153 3136.5680 3156.8925 3161.0817 3188.0968 3213.7797 3721.8943

TS_{74}

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.53302000	0.82946100	0.12717300
H	0.04325900	-0.11082000	0.73419700
C	-0.04252400	0.83984100	-1.31270700
H	-0.59069600	0.08633600	-1.88711900
H	-0.30314500	1.82307000	-1.73676000
C	1.88449900	-0.83672200	-1.11605100
H	0.99976100	-1.47800300	-1.05085400
H	2.52742800	-1.26654200	-1.89309500
C	2.65628400	-0.93169600	0.19429200
H	2.83233100	-1.97950200	0.46383700
H	3.61486700	-0.40695200	0.12615900
O	2.00580700	-0.26951700	1.28117000
O	0.75103100	-0.82225500	1.44448100
C	1.46330400	0.59680700	-1.49732400
H	1.70276900	0.78283300	-2.54983100
H	2.03739400	1.32672700	-0.91444300
C	-1.99932300	0.48933300	0.27635600
H	-2.29727800	0.50523300	1.33297100
H	-2.61991300	1.20789200	-0.28079300
C	-0.12767100	2.04180800	0.94098900
H	-0.58621800	2.94851800	0.52350600
H	-0.44372400	1.93801300	1.98285400
H	0.95769800	2.16779200	0.93116200
O	-2.17408000	-0.81296300	-0.26154600
O	-3.59416100	-1.08884300	-0.20612400
H	-3.59260700	-1.76897200	0.47799800

Absolute energies (Hartree): -575.702285 ZPE (Hartree): 0.220207

Harmonic Vibrational Frequencies (cm^{-1}):

-2046.8334 44.4959 68.9826 91.1438 142.8228 156.6346 173.6480 207.3569 223.5753 234.5877 258.2794 280.4015 321.2604 344.7146 411.3018 435.3351 444.8412 541.7222 596.9391 618.3455 753.5345 832.1490 846.4508 921.8692 935.4131 945.6081 971.8392 1001.2411 1030.6789 1048.4161 1069.9807 1108.5123 1120.3557 1152.7181 1167.1949 1200.0264 1224.5413 1238.4529 1266.5675 1273.3053 1297.3943 1311.7988 1320.6306 1363.8709 1373.0167 1392.8252 1406.8036 1411.9494 1419.0111 1420.4578 1489.1461 1500.7846 1501.9454 1504.8712 1509.4449 1516.2134 1517.0005 1531.0654 3030.2708 3033.7480 3054.4477 3076.6180 3079.0506 3086.9296 3095.7019 3123.2807 3136.4869 3137.3179 3145.8780 3152.8158 3176.6834 3837.1592

$O_2CC•(C)CCCCOO$

Cartesian Coordinates (Å)

At.	X	Y	Z
C	3.08514200	-0.02466000	0.70508400
H	3.79599200	0.67793100	1.15499100
H	2.91630700	-0.86282600	1.39393900
O	3.63957000	-0.52322900	-0.52200800
O	4.91789000	-1.11196300	-0.18617200
H	4.69919500	-2.04359300	-0.30470500
C	-0.73885800	0.48154100	0.15817600
H	-0.80427600	1.25494400	-0.61626700
H	-0.81443800	0.99019400	1.12774200
C	-1.90568000	-0.49396700	-0.00180300
H	-1.87883200	-1.24157200	0.79873800
H	-1.81363000	-1.02829000	-0.95444900
C	1.80521200	0.64671000	0.33270000
C	-3.24505100	0.22274500	0.04161700
H	-3.32839200	0.94840000	-0.77882000
H	-3.37520200	0.75070700	0.99397800
O	-4.24028400	-0.77958500	-0.09156000
O	-5.51611400	-0.10127600	0.01750600
H	-5.83624600	-0.22864600	-0.88293000
C	0.61592000	-0.22811400	0.06808600
H	0.62533300	-1.07099300	0.77185600
H	0.71429100	-0.67212600	-0.93856100
C	1.88063800	1.99646600	-0.31009200
H	1.02492600	2.62544800	-0.04346700
H	2.79570900	2.51922800	-0.01952700
H	1.88683700	1.90528600	-1.40726300

Absolute energies (Hartree): -575.714706 ZPE (Hartree): 0.22291

Harmonic Vibrational Frequencies (cm^{-1}):

26.5313 33.6074 52.0920 78.5638 82.1762 113.7142 121.3609 129.1955 144.6420 178.0516 199.6413 215.9687 221.1322 256.5331 328.7168 386.0477 405.1765 438.0270 510.3394 604.7796 748.4556 808.0259 821.3029 912.3311 925.6740 982.1809 995.0806 1009.7186 1034.2164 1061.848 1065.8289 1083.4935 1096.5099 1113.9058 1139.0169 1224.3596 1237.8027 1242.5755 1280.0641 1298.4522 1321.7805 1337.5753 1350.4415 1360.3604 1364.5683 1371.2128 1409.8970 1421.8644 1424.8129 1438.8596 1482.9418 1497.0215 1506.9828 1511.0421 1521.9924 1535.9795 1552.4156 2999.8269 3030.7915 3052.0182 3054.5351 3066.1040 3081.9748 3085.6344 3108.5451 3115.3480 3118.6176 3120.5825 3146.7942 3165.0942 3839.5443 3843.9427