Supporting Information (SI) for Publication

Tropospheric Alkene Ozonolysis Chemistry: An Extended Computational Chemistry Assessment of Structural Effects.

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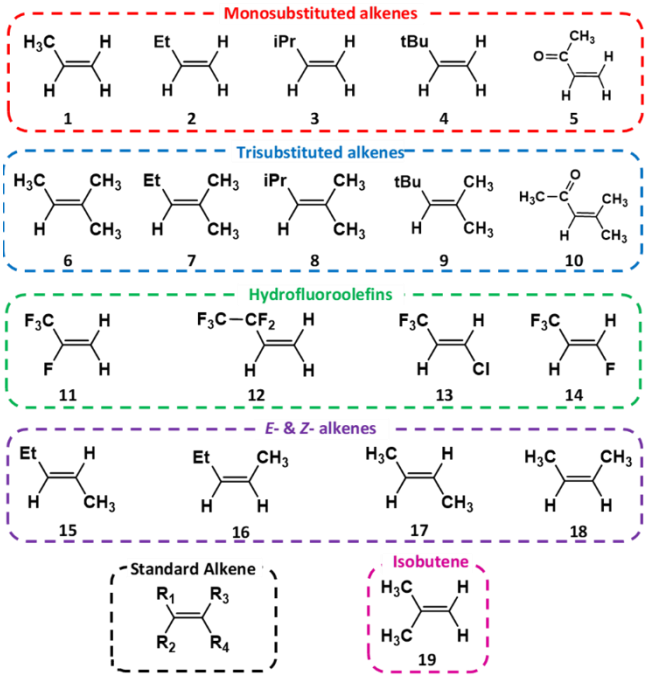

*Figure S1: Alkenes, labelled **1**-**19** and delineated by structural factors, modelled for this ozonolysis study.*

S1 Supporting Equations

S1.1 Canonical Rate Constant (k_{CAN})

To determine canonical rate constant (k_{CAN}) for a single step reaction use Equation S1:

$$k_{CAN} = \sum(k_1/k_{-1} \times k_2)$$ *Equation S1*

Both types of rate constants produced by MESMER are generated from single step reactions or from pseudo-single step simulations of multistep reactions.

S1.2 Conventional transition state theory rate constant (k_{TST})

Using either the partition functions (Q) and zero-point corrected energy (ΔZPE) values or the Gibbs free energy (ΔG) value, determined from the computational chemistry calculations, the Equations S2—S7 are used to determine the conventional transition state theory rate constant (k_{TST}):

$$k_{TST} = \sum k_{TS}$$ *Equation S2*

$$k_{TS} = K_{eq} \times k_2$$ *Equation S3*

$$K_{eq} = \frac{RT}{P_0} \frac{Q_{PRC}}{Q_{R1}Q_{R2}} e^{-(\Delta ZPE_{PRC})/RT}$$ *Equation S4*

$$K_{eq} = \frac{RT}{P_0} e^{-(\Delta G_{PRC})/RT}$$ *Equation S5*

$$k_2 = \boldsymbol{\kappa} \frac{k_B T}{h} \frac{Q_{TS}}{Q_{PRC}} e^{-(\Delta ZPE_{TS} - \Delta ZPE_{PRC})/RT}$$ *Equation S6*

$$k_2 = \boldsymbol{\kappa} \frac{k_B T}{h} e^{-(\Delta G_{TS} - \Delta G_{PRC})/RT}$$ *Equation S7*

The factors in these equations are: $\boldsymbol{\kappa}$ is the tunneling constant (see section 2.6); k_B is Boltzmann constant; T is temperature; h is Planck's constant; R is the gas constant; P_0 is the pressure of the system; Q_{TS}, Q_{PRC}, Q_{R1} and Q_{R2} are the partition functions for transition state, pre-reaction complex, reactant 1 and reactant 2; ΔG_{TS} and ΔG_{PRC} are the relative molar Gibbs free energy for the transition state and pre-reaction complex, at 298 K.

S1.3 Structure activity relationships rate constant (k_{SAR})

To the author's knowledge there are no k_{EXP} values for the O_3 + 2,4-dimethyl-2-pentene reaction in the literature, so to assess the k_{THEO} values determined here a rate constant derived from the structure activity relationship, SAR, models (k_{SAR}) is used as a comparative tool. This model was designed mainly by McGillen *et al.* in a 2008 study, which incorporates both the inductive and steric inputs of the alkene used into one combined factor that is then used to calculate the rate constant.[1] The inputs in the SAR Equation incorporate: a factor that corresponds to the increase in reactivity of the >C=C< bond provided by each extra alkyl substituent group attached; and a steric hinderance factor for the reaction, which is gradually reduced as the bulkiness moves away from the >C=C< bond.

In order of greatest intrusion, the alkyl groups can cause steric interference by being placed within disubstituted olefin alkene, on the α-C of a substituent, or on a ß-C of a substituent. These types of steric interference are identified in the structures of Figure S2 but beyond the ß-C, the steric interference, caused by extra alkyl groups, is experimentally shown to be negligible. This method has been fitted to the experimental rate constants in the literature and the theoretical results have the potential to be fitted too. It has been shown to provide a strong linear relationship (0.90—0.94) between $\log_{10}$ (k_{EXP}) and that combined factor.[1,2] The three different types of steric factors (s_0, s_1, s_2), identified in Figure S2: disubstituted alkyl groups (s_0), α-alkyl groups (s_1) and ß-alkyl groups (s_2)

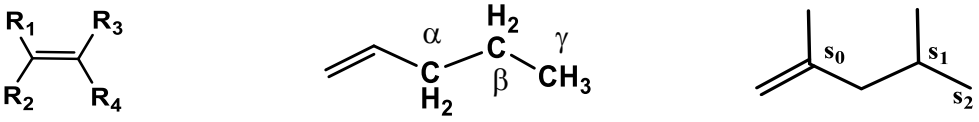

Figure S2: Alkenes R_1—R_4 substituent positions and the positions of hydrogen analogues on a substituent carbon chain labelled using Greek letters (α, ß, γ …), and the structure of 2,4-dimethyl-1-pentene labelled s_0, s_1 & s_2 according to which alkyl segment(s) causes the s_0, s_1 & s_2 steric effect in the SAR model.

To determine structure—activity relationship rate constant (k_{SAR}), use Equations S8-S10, which involves using the number of alkyl groups attached to the >C=C< bond, which ranges from 0-4, to produce the total inductive factor (I). Then the total steric factor (S) is calculated, which increases depending on the number of steric interferences in those substituent groups.

$$S = \sum s_n \qquad \textit{Equation S8}$$

$$x = (yS) + I \qquad \textit{Equation S9}$$

The steric effect (S) depends on three factors: the clash between two alkyl groups at the end of an olefin bond (s_0 = 0.20); the steric interference of extra α-alkyl groups (s_1 = 0.033); and the steric interference of extra ß-alkyl groups (s_2 = 0.020). The final SAR equation (Equation S10), then uses these factors to produce the structure activity relationship rate constant.

$$\log k_{SAR}(298\ K) = (1.28\ \pm\ 0.05)x - (18.14\ \pm\ 0.07) \qquad \textit{Equation S10}$$

S1.4 Effective Rate Constant (k_{EFF})

Equation S11 uses the concentration of the co-reactant and the rate constant of the reaction to determine the effective Rate Constant (k_{EFF}), a tool that can be used to determine, the rough atmospheric impact of a reaction. For more results relating to the effective rate constant, see Section S7.

$$k_{EFF} = k_{ME}\ [\text{co-reactant}] \qquad \textit{Equation S11}$$

S2 Computational Rates and Product Branching Ratios Data

S2.1 Master Equation Rate Constants (k_{ME})

The grainsize used to determine the master Equation Rate constants and the master Equation Rate constants at various temperatures are categorised in this section.

*Table S1: Calculated Master Equation Rate Constants (k_{ME}) at Standard Pressure over a variety of Temperatures for the Ozonolysis of Alkenes **1**—**12**.*

O_3 + Alkene 1		O_3 + Alkene 2		O_3 + Alkene 3	
Grainsize: 10		Grainsize: 20		Grainsize: 20	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	2.63E-18	200	9.13E-18	200	5.98E-18
275	2.04E-17	275	6.58E-17	275	3.94E-17
298	3.24E-17	298	1.03E-16	298	6.06E-17
325	5.23E-17	325	1.63E-16	325	9.50E-17
400	1.53E-16	400	4.59E-16	400	2.64E-16
O_3 + Alkene 4		O_3 + Alkene 5		O_3 + Alkene 6	
Grainsize: 10		Grainsize: 20		Grainsize: 10	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	2.26E-18	200	1.14E-17	200	3.90E-15
275	1.47E-17	275	4.90E-17	275	4.12E-15
298	2.25E-17	298	6.90E-17	298	4.34E-15
325	3.50E-17	325	9.92E-17	325	4.66E-15
400	9.50E-17	400	2.32E-16	400	5.86E-15
O_3 + Alkene 7		O_3 + Alkene 8		O_3 + Alkene 9	
Grainsize: 10		Grainsize: 15		Grainsize: 10	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	4.78E-15	200	8.86E-17	200	7.64E-17
275	4.89E-15	275	1.99E-16	275	1.95E-16
298	5.12E-15	298	2.459E-16	298	2.456E-16
325	5.46E-15	325	3.10E-16	325	3.15E-16
400	6.81E-15	400	5.54E-16	400	5.66E-16
O_3 + Alkene 10		O_3 + Alkene 11		O_3 + Alkene 12	
Grainsize: 15		Grainsize: 10		Grainsize: 25	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	4.84E-19	200	3.84E-23	200	1.20E-22
275	1.26E-18	275	4.15E-21	275	1.12E-20
298	1.57E-18	298	1.14E-20	298	2.99E-20
325	2.24E-18	325	3.15E-20	325	8.07E-20
400	6.17E-18	400	2.83E-19	400	6.97E-19

*Table S2: Calculated Master Equation Rate Constants (k_{ME}) at Standard Pressure over a variety of Temperatures for the Ozonolysis of Alkenes **13**—**19**.*

O_3 + Alkene 13		O_3 + Alkene 14		O_3 + Alkene 15	
Grainsize:	10	Grainsize:	10	Grainsize:	25
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	8.75E-23	200	2.07E-23	200	7.31E-16
275	7.18E-21	275	2.84E-21	275	1.34E-15
298	1.85E-20	298	8.11E-21	298	1.13E-15
325	4.82E-20	325	2.34E-20	325	9.64E-16
400	3.79E-19	400	2.25E-19	400	4.46E-15
O_3 + Alkene 16		O_3 + Alkene 17		O_3 + Alkene 18	
Grainsize:	15	Grainsize:	10	Grainsize:	10
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	1.31E-15	200	3.68E-17	200	4.41E-16
275	2.15E-15	275	1.34E-16	275	9.62E-16
298	2.48E-15	298	1.81E-16	298	1.18E-15
325	2.93E-15	325	2.48E-16	325	1.46E-15
400	4.54E-15	400	5.15E-16	400	2.50E-15
O_3 + Alkene 19					
Grainsize:	10				
T (K)	k_{ME} (cm^3 s^{-1})				
200	1.04E-18				
275	9.29E-18				
298	1.51E-17				
325	2.49E-17				
400	7.60E-17				

*Table S3: Calculated Master Equation Rate Constants (k_{ME}) at non-standard pressure over a select range of Temperatures for the Ozonolysis of Alkenes **4** & **5**.*

O_3 + Alkene 4		O_3 + Alkene 5	
Grainsize:	10	Grainsize:	20
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
210	3.08E-18	281	9.20E-17
218	3.88E-18	284	9.55E-17
226	4.83E-18	287	9.90E-17
235	6.08E-18	289	1.01E-16
245	7.74E-18	292	1.05E-16
255	9.71E-18	295	1.09E-16
288	1.88E-17	-	-
301	2.37E-17	-	-

S2.2 Canonical Rate Constants (k_{CAN})

Canonical Rate constants produced by MESMER are displayed in this section.

*Table S4: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **20** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

Alkene #	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	TS_{OZO} 1			TS_{OZO} 2		
			k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	2.63E-18	1.01E-10	1.37E+12	3.31E+04	1.01E-10	6.63E+11	1.26E+03
	275	2.04E-17	1.01E-10	1.04E+13	1.82E+06	1.01E-10	4.89E+12	1.38E+05
	298	3.24E-17	1.01E-10	1.52E+13	4.11E+06	1.01E-10	7.09E+12	3.60E+05
	325	5.23E-17	1.01E-10	2.16E+13	9.24E+06	1.01E-10	1.01E+13	9.32E+05
	400	1.53E-16	1.00E-10	4.15E+13	4.89E+07	1.00E-10	1.91E+13	6.61E+06
4	200	2.26E-18	1.01E-10	1.01E+12	2.23E+04	1.01E-10	2.03E+11	6.44E+01
	275	1.47E-17	1.00E-10	4.77E+12	6.69E+05	1.00E-10	1.41E+12	8.68E+03
	298	2.25E-17	1.00E-10	6.30E+12	1.34E+06	1.00E-10	2.02E+12	2.36E+04
	325	3.50E-17	1.00E-10	8.14E+12	2.65E+06	1.00E-10	2.82E+12	6.37E+04
	400	9.50E-17	1.00E-10	1.27E+13	1.09E+07	1.00E-10	5.19E+12	4.90E+05
6	200	3.90E-15	9.99E-11	3.90E+13	1.44E+09	1.01E-10	1.21E+10	2.49E+04
	275	4.12E-15	9.99E-11	1.21E+14	4.54E+09	1.00E-10	2.89E+11	1.06E+06
	298	4.34E-15	9.99E-11	1.46E+14	5.73E+09	1.00E-10	5.33E+11	2.28E+06
	325	4.66E-15	9.99E-11	1.74E+14	7.21E+09	1.00E-10	9.59E+11	4.88E+06
	400	5.86E-15	9.99E-11	2.28E+14	1.16E+10	1.00E-10	2.97E+12	2.34E+07
9	200	7.62E-17	1.01E-10	2.79E+10	1.81E+04	1.00E-10	7.46E+10	8.01E+03
	275	1.95E-16	1.00E-10	5.32E+11	8.37E+05	1.00E-10	1.27E+12	4.63E+05
	298	2.456E-16	1.00E-10	9.35E+11	1.83E+06	1.00E-10	2.17E+12	1.06E+06
	325	3.15E-16	1.00E-10	1.60E+12	3.98E+06	1.00E-10	3.65E+12	2.41E+06
	400	5.66E-16	9.97E-11	4.50E+12	1.96E+07	9.97E-11	9.75E+12	1.30E+07
11	200	3.84E-23	1.01E-10	4.72E+07	1.79E-06	1.01E-10	4.72E+07	1.62E-05
	275	4.15E-21	1.01E-10	4.35E+08	3.03E-03	1.01E-10	4.35E+08	1.49E-02
	298	1.14E-20	1.01E-10	6.57E+08	1.39E-02	1.01E-10	6.57E+08	6.02E-02
	325	3.15E-20	1.01E-10	9.70E+08	6.29E-02	1.01E-10	9.70E+08	2.40E-01
	400	2.83E-19	1.01E-10	2.00E+09	1.42E+00	1.01E-10	2.00E+09	4.20E+00
13	200	8.75E-23	1.01E-10	2.45E+11	1.73E-01	1.00E-10	4.51E+11	7.27E-02
	275	7.18E-21	1.01E-10	8.49E+11	4.51E+01	1.00E-10	1.58E+12	2.89E+01
	298	1.85E-20	1.01E-10	1.05E+12	1.40E+02	1.00E-10	1.95E+12	9.83E+01
	325	4.82E-20	1.01E-10	1.27E+12	4.32E+02	1.00E-10	2.37E+12	3.30E+02
	400	3.79E-19	1.00E-10	1.73E+12	4.38E+03	1.00E-10	3.24E+12	4.02E+03
14	200	2.07E-23	1.00E-10	2.37E+11	2.23E-02	1.01E-10	5.51E+11	6.18E-02
	275	2.84E-21	1.00E-10	4.91E+11	6.45E+00	1.00E-10	1.55E+12	2.36E+01
	298	8.11E-21	1.00E-10	5.46E+11	2.05E+01	1.00E-10	1.83E+12	7.93E+01
	325	2.34E-20	1.00E-10	5.95E+11	6.46E+01	1.00E-10	2.12E+12	2.64E+02
	400	2.25E-19	1.00E-10	6.52E+11	6.86E+02	1.00E-10	2.64E+12	3.15E+03
17	200	3.68E-17	1.01E-10	3.48E+10	1.27E+04	Degeneracy of 2		
	275	1.34E-16	1.01E-10	9.70E+11	1.29E+06	Degeneracy of 2		
	298	1.81E-16	1.01E-10	1.85E+12	3.32E+06	Degeneracy of 2		
	325	2.48E-16	1.01E-10	3.45E+12	8.50E+06	Degeneracy of 2		
	400	5.15E-16	1.00E-10	1.15E+13	5.91E+07	Degeneracy of 2		
18	200	4.41E-16	1.01E-10	3.49E+13	1.52E+08	1.01E-10	9.08E+10	2639.8
	275	9.62E-16	1.01E-10	8.94E+13	8.37E+08	1.01E-10	6.10E+11	128231
	298	1.18E-15	1.01E-10	1.04E+14	1.18E+09	1.01E-10	8.66E+11	283266
	325	1.46E-15	1.00E-10	1.19E+14	1.67E+09	1.01E-10	1.20E+12	621017
	400	2.50E-15	1.00E-10	1.44E+14	3.39E+09	1.01E-10	2.18E+12	3.13E+06
19	200	2.08E-18	1.01E-10	9.65E+10	9.97E+02	Degeneracy of 2		

	275	1.86E-17	1.01E-10	9.03E+11	8.34E+04	Degeneracy of 2
	298	3.02E-17	1.01E-10	1.37E+12	2.06E+05	Degeneracy of 2
	325	4.99E-17	1.00E-10	2.04E+12	5.06E+05	Degeneracy of 2
	400	1.52E-16	1.00E-10	4.26E+12	3.22E+06	Degeneracy of 2

*Table S5: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **2** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 2										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	9.13E-18	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.45E+11	1.38E+04	1.01E-10	5.75E+11	1.14E+04	1.01E-10	2.05E+12	6.69E+04
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	8.45E+11	1.75E+03	1.00E-10	2.31E+12	1.15E+03	1.01E-10	1.16E+12	1.18E+04
275	6.58E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.15E+12	9.21E+05	1.01E-10	6.35E+12	7.95E+05	1.01E-10	8.63E+12	1.91E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	5.73E+12	1.64E+05	1.00E-10	1.31E+13	1.16E+05	1.00E-10	5.76E+12	5.34E+05
298	1.03E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	7.85E+12	2.17E+06	1.01E-10	1.00E+13	1.89E+06	1.01E-10	1.11E+13	3.77E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	8.16E+12	4.15E+05	1.00E-10	1.81E+13	2.98E+05	1.00E-10	7.67E+12	1.16E+06
325	1.63E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	1.17E+13	5.07E+06	1.01E-10	1.54E+13	4.47E+06	1.01E-10	1.41E+13	7.41E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	1.14E+13	1.04E+06	1.00E-10	2.43E+13	7.57E+05	1.00E-10	1.00E+13	2.50E+06
400	4.59E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	2.47E+13	2.91E+07	1.01E-10	3.49E+13	2.62E+07	1.00E-10	2.09E+13	2.98E+07
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	2.08E+13	6.90E+06	1.00E-10	4.14E+13	5.18E+06	1.00E-10	1.60E+13	1.22E+07

*Table S6: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **3** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 3										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	5.98E-18	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.01E-10	1.48E+12	4.94E+04	1.01E-10	2.13E+12	4.68E+04	1.00E-10	4.39E+12	6.98E+03
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	5.26E+12	2.43E+03	1.00E-10	1.39E+12	2.39E+03	1.00E-10	4.21E+12	6.60E+02
275	3.94E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.01E-10	1.20E+13	2.21E+06	1.00E-10	8.44E+12	1.29E+06	1.00E-10	1.51E+13	3.00E+05
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	2.38E+13	1.91E+05	1.00E-10	6.07E+12	1.41E+05	1.00E-10	1.59E+13	5.65E+04
298	6.06E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	1.77E+13	4.80E+06	1.00E-10	1.07E+13	2.53E+06	1.00E-10	1.88E+13	6.45E+05
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	3.12E+13	4.66E+05	1.00E-10	7.88E+12	3.23E+05	1.00E-10	2.00E+13	1.40E+05
325	9.50E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	2.57E+13	1.03E+07	1.00E-10	1.34E+13	4.93E+06	1.00E-10	2.28E+13	1.38E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	4.01E+13	1.13E+06	1.00E-10	1.00E+13	7.35E+05	1.00E-10	2.48E+13	3.44E+05
400	2.64E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.11E+13	5.02E+07	1.00E-10	1.95E+13	1.94E+07	1.00E-10	3.13E+13	6.57E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	6.22E+13	6.93E+06	1.00E-10	1.52E+13	3.99E+06	1.00E-10	3.55E+13	2.19E+06

*Table S7: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **7** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 7										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	4.78E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.01E-10	2.82E+13	4.19E+08	1.01E-10	2.11E+13	5.25E+04	1.01E-10	2.11E+13	5.41E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	5.15E+10	1.61E+04	1.01E-10	5.15E+10	2.02E+01	1.01E-10	5.15E+10	3.40E+05
275	4.89E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.01E-10	7.83E+13	1.32E+09	1.00E-10	7.84E+13	2.03E+06	1.00E-10	7.84E+13	1.84E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	9.45E+11	8.00E+05	1.01E-10	9.45E+11	5.03E+03	1.01E-10	9.45E+11	7.09E+06
298	5.11E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.27E+13	1.66E+09	1.00E-10	9.86E+13	4.30E+06	1.00E-10	9.86E+13	2.36E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	1.65E+12	1.78E+06	1.01E-10	1.65E+12	1.56E+04	1.01E-10	1.65E+12	1.32E+07
325	5.46E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.07E+14	2.08E+09	1.00E-10	1.22E+14	9.05E+06	1.00E-10	1.22E+14	3.02E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.82E+12	3.93E+06	1.00E-10	2.82E+12	4.78E+04	1.00E-10	2.82E+12	2.44E+07
400	6.82E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.34E+14	3.32E+09	1.00E-10	1.73E+14	4.21E+07	1.00E-10	1.73E+14	5.05E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.83E+12	2.01E+07	1.00E-10	7.83E+12	4.84E+05	1.00E-10	7.83E+12	8.71E+07

*Table S8: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **8** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 8										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	8.85E-17	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	2.07E+13	1.44E+07	1.00E-10	2.07E+13	1.43E+05	1.01E-10	4.15E+14	1.18E+05
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	2.55E+11	4.67E+04	1.01E-10	2.55E+11	1.90E+02	1.01E-10	4.15E+14	9.89E+03
275	1.98E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	7.37E+13	1.08E+08	1.00E-10	7.37E+13	3.68E+06	1.00E-10	5.14E+14	3.12E+06
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	2.37E+12	1.08E+06	1.01E-10	2.37E+12	1.90E+04	1.00E-10	5.14E+14	4.46E+05
298	2.443E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.18E+13	1.62E+08	1.00E-10	9.18E+13	7.15E+06	1.00E-10	5.15E+14	6.08E+06
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	3.60E+12	2.05E+06	1.01E-10	3.60E+12	4.85E+04	1.00E-10	5.15E+14	9.71E+05
325	3.07E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.12E+14	2.43E+08	1.00E-10	1.12E+14	1.38E+07	1.00E-10	5.06E+14	1.18E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	5.34E+12	3.86E+06	1.00E-10	5.34E+12	1.23E+05	1.00E-10	5.06E+14	2.10E+06
400	5.45E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.55E+14	5.60E+08	1.00E-10	1.55E+14	5.36E+07	1.00E-10	4.49E+14	4.60E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	1.11E+13	1.42E+07	1.00E-10	1.11E+13	8.39E+05	1.00E-10	4.49E+14	1.02E+07

*Table S9: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **12** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 12										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.20E-22	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	1.81E+12	1.27E+00	9.99E-11	1.81E+12	3.22E-03	1.00E-10	9.79E+11	3.32E-02
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	9.50E+11	4.29E-01	1.00E-10	1.11E+14	1.84E-02	1.00E-10	9.79E+11	9.67E-03
275	1.12E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	2.02E+12	1.17E+02	1.00E-10	2.02E+12	1.47E+00	1.00E-10	2.54E+12	1.95E+01
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.05E+12	8.70E+01	1.00E-10	6.83E+13	8.45E+00	1.00E-10	2.54E+12	7.62E+00
298	2.99E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.98E+12	2.95E+02	1.00E-10	1.98E+12	5.15E+00	1.00E-10	2.96E+12	7.17E+01
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.30E+12	2.57E+02	1.00E-10	5.91E+13	2.95E+01	1.00E-10	2.96E+12	2.98E+01
325	8.08E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.90E+12	7.33E+02	1.00E-10	1.90E+12	1.78E+01	1.00E-10	3.37E+12	2.60E+02
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.52E+12	7.51E+02	1.00E-10	5.02E+13	1.02E+02	1.00E-10	3.37E+12	1.15E+02
400	6.97E-19	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.60E+12	4.78E+03	1.00E-10	1.60E+12	2.28E+02	1.00E-10	4.07E+12	3.71E+03
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.82E+12	6.83E+03	1.00E-10	3.28E+13	1.31E+03	1.00E-10	4.07E+12	1.86E+03

*Table S10: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **15** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 15										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	7.31E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	4.48E+13	2.40E+08	1.00E-10	1.76E+11	1.92E+05	1.00E-10	1.19E+14	5.30E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	6.07E+13	1.07E+07	9.98E-11	7.42E+13	9.52E+06	9.99E-11	5.15E+13	5.24E+06
275	1.34E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	1.93E+14	1.59E+09	1.00E-10	2.68E+12	6.78E+06	1.00E-10	4.67E+14	5.15E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	2.41E+14	1.56E+08	9.99E-11	2.40E+14	1.22E+08	9.99E-11	2.48E+14	8.78E+07
298	1.59E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	2.50E+14	2.33E+09	1.00E-10	4.50E+12	1.40E+07	1.00E-10	5.94E+14	8.18E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	3.08E+14	2.70E+08	9.99E-11	2.92E+14	2.05E+08	9.99E-11	3.30E+14	1.56E+08
325	1.93E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	3.17E+14	3.41E+09	1.00E-10	7.38E+12	2.89E+07	1.00E-10	7.39E+14	1.29E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	3.84E+14	4.64E+08	9.99E-11	3.49E+14	3.44E+08	9.99E-11	4.28E+14	2.76E+08
400	3.15E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	4.77E+14	7.46E+09	1.00E-10	1.89E+13	1.28E+08	1.00E-10	1.07E+15	3.33E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.99E-11	5.59E+14	1.41E+09	9.99E-11	4.63E+14	9.92E+08	1.00E-10	6.78E+14	8.92E+08

*Table S11: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **16** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 16										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.31E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	3.25E+13	5.96E+07	1.01E-10	3.02E+12	2.30E+03	1.01E-10	3.02E+12	3.27E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.96E+11	9.28E+03	1.01E-10	2.56E+11	3.49E+00	1.01E-10	2.56E+11	9.81E+04
275	2.14E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	8.26E+13	3.55E+08	1.00E-10	1.11E+13	1.70E+05	1.00E-10	1.11E+13	1.76E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	4.39E+12	4.34E+05	1.01E-10	1.43E+12	7.66E+02	1.01E-10	1.43E+12	1.67E+06
298	2.48E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.61E+13	5.10E+08	1.00E-10	1.39E+13	4.07E+05	1.00E-10	1.39E+13	2.47E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	5.98E+12	9.52E+05	1.00E-10	1.96E+12	2.31E+03	1.00E-10	1.96E+12	2.98E+06
325	2.93E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.10E+14	7.30E+08	1.00E-10	1.71E+13	9.61E+05	1.00E-10	1.71E+13	3.46E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.96E+12	2.07E+06	1.00E-10	2.62E+12	6.88E+03	1.00E-10	2.62E+12	5.27E+06
400	4.54E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.32E+14	1.53E+09	1.00E-10	2.40E+13	5.55E+06	1.00E-10	2.40E+13	6.91E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	1.33E+13	1.03E+07	1.00E-10	4.41E+12	6.54E+04	1.00E-10	4.41E+12	1.71E+07

*Table S12: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkenes **5** & **10** based on a steady state treatment of individual canonical rate coefficients (k_1, k_{-1}, & k_2)*

O_3 + Alkene 5													
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 2.1**			**TS_{OZO} 2.2**		
		k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.14E-17	1.00E-10	4.45E+11	6.67E+02	1.01E-10	2.87E+12	1.02E+03	1.00E-10	6.45E+11	7.19E+04	1.01E-10	5.54E+11	1.06E+02
275	4.90E-17	1.00E-10	2.20E+12	4.53E+04	1.01E-10	1.22E+13	8.15E+04	1.00E-10	1.39E+12	6.36E+05	1.01E-10	4.69E+12	1.98E+04
298	6.90E-17	1.00E-10	2.93E+12	1.07E+05	1.00E-10	1.57E+13	1.99E+05	1.00E-10	1.56E+12	9.85E+05	1.01E-10	6.98E+12	5.79E+04
325	9.92E-17	1.00E-10	3.82E+12	2.50E+05	1.00E-10	1.99E+13	4.83E+05	1.00E-10	1.72E+12	1.52E+06	1.00E-10	1.02E+13	1.67E+05
400	2.32E-16	1.00E-10	6.08E+12	1.44E+06	1.00E-10	2.97E+13	2.99E+06	1.00E-10	1.92E+12	3.66E+06	1.00E-10	2.04E+13	1.49E+06
O_3 + Alkene 10													
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 2.1**			**TS_{OZO} 2.2**		
		k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.42E-19	9.97E-11	3.98E+12	1.21E+03	9.98E-11	2.29E+15	2.34E+03	1.00E-10	1.60E+11	1.78E+02	1.00E-10	5.77E+14	8.55E+02
275	9.33E-19	9.98E-11	1.83E+13	4.88E+04	9.98E-11	2.95E+15	1.24E+05	1.00E-10	2.73E+12	1.79E+04	1.00E-10	5.51E+14	2.68E+04
298	1.43E-18	9.98E-11	2.40E+13	1.04E+05	9.98E-11	2.98E+15	2.79E+05	1.00E-10	4.69E+12	4.60E+04	1.00E-10	5.24E+14	5.41E+04
325	2.24E-18	9.98E-11	3.08E+13	2.19E+05	9.99E-11	2.96E+15	6.23E+05	1.00E-10	7.87E+12	1.17E+05	1.00E-10	4.89E+14	1.09E+05
400	6.29E-18	9.98E-11	4.74E+13	1.02E+06	9.99E-11	2.68E+15	3.29E+06	1.00E-10	2.12E+13	8.05E+05	1.00E-10	3.91E+14	8.05E+05

S2.3 Product Branching Fractions (Γ_{THEO})

Complete product branching ratios (Γ_{THEO}) of alkene ozonolysis reactions are found herein. The branching fractions for O_3 + Alkenes **13**—**18** are displayed with new Γ_{THEO} labelling, for *anti*- & *syn*-R_1R_2COO ($\Gamma_{ANTI\text{-}R1}$ & $\Gamma_{SYN\text{-}R1}$) and *anti*- & *syn*-R_3R_4COO ($\Gamma_{ANTI\text{-}R3}$ & $\Gamma_{SYN\text{-}R3}$). One important factor is that the MESMER treatment for all other O_3 + alkene reactions went through a single POZ conformer to determine the Γ_{THEO} values.

*Table S13: Product Branching Ratios of Ozonolysis of Alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **19**.*

T (K)	O_3 + Alkene **1**				O_3 + Alkene **6**			
	Grainsize			20	Grainsize			40
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{ANTI}	Γ_{AO} (1)	Γ_{AO} (2)	Γ_{SYN}
200	0.666	0.050	0.012	0.271	0.001	0.994	0.005	<0.001
275	0.563	0.109	0.050	0.278	0.157	0.636	0.165	0.042
298	0.438	0.175	0.148	0.239	0.216	0.509	0.203	0.072
325	0.437	0.176	0.148	0.239	0.211	0.520	0.199	0.070
400	0.428	0.181	0.155	0.236	0.231	0.478	0.209	0.081
T (K)	O_3 + Alkene **4**				O_3 + Alkene **9**			
	Grainsize			20	Grainsize			15
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{ANTI}	Γ_{AO} (1)	Γ_{AO} (2)	Γ_{SYN}
200	0.112	0.618	0.220	0.050	<0.001	<0.001	1.000	<0.001
275	0.475	0.303	0.165	0.057	0.067	0.006	0.868	0.058
298	0.470	0.303	0.168	0.059	0.114	0.010	0.778	0.098
325	0.472	0.303	0.167	0.058	0.121	0.011	0.763	0.105
400	0.460	0.304	0.174	0.062	0.130	0.014	0.742	0.114
T (K)	O_3 + Alkene **11**				O_3 + Alkene **13**			
	Grainsize			40	Grainsize			40
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	$\Gamma_{ANTI\text{-}R1}$	$\Gamma_{SYN\text{-}R3}$	$\Gamma_{ANTI\text{-}R3}$	$\Gamma_{SYN\text{-}R1}$
200	<0.001	0.524	0.476	<0.001	0.592	0.093	0.110	0.204
275	<0.001	0.545	0.455	<0.001	0.605	0.091	0.107	0.196
298	<0.001	0.532	0.468	<0.001	0.604	0.091	0.108	0.197
325	<0.001	0.544	0.456	<0.001	0.571	0.103	0.120	0.207
400	<0.001	0.548	0.452	<0.001	0.556	0.108	0.125	0.211
T (K)	O_3 + Alkene **14**				O_3 + Alkene **17**			
	Grainsize			25	Grainsize			15
	$\Gamma_{ANTI\text{-}R1}$	$\Gamma_{SYN\text{-}R1}$	$\Gamma_{ANTI\text{-}R3}$	$\Gamma_{SYN\text{-}R3}$	Γ_{ANTI}		Γ_{SYN}	
200	0.475	0.456	0.046	0.024	0.216		0.784	
275	0.474	0.451	0.049	0.026	0.535		0.465	
298	0.473	0.450	0.050	0.027	0.520		0.480	
325	0.472	0.449	0.051	0.028	0.527		0.473	
400	0.469	0.445	0.055	0.031	0.540		0.460	
T (K)	O_3 + Alkene **18**				O_3 + Alkene **19**			
	Grainsize			30	Grainsize			15
	Γ_{ANTI}		Γ_{SYN}		Γ_{AO}		Γ_{FO}	
200	0.998		0.002		0.999		0.001	
275	0.879		0.121		0.828		0.172	
298	0.817		0.183		0.842		0.158	
325	0.814		0.186		0.817		0.183	
400	0.798		0.202		0.837		0.163	

*Table S14: Product Branching Ratios of Ozonolysis of Alkenes **2**, **3**, **7**, **8** & **12**.*

O_3 + Alkene **2**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.159	0.132	0.300	0.034	0.027	0.042	0.015	0.016	0.023	0.107	0.001	0.144
275	0.131	0.109	0.190	0.068	0.057	0.073	0.056	0.050	0.065	0.083	0.019	0.100
298	0.130	0.108	0.188	0.068	0.058	0.073	0.057	0.051	0.065	0.082	0.019	0.099
325	0.131	0.109	0.190	0.068	0.057	0.073	0.056	0.050	0.064	0.083	0.019	0.100
400	0.132	0.110	0.193	0.067	0.056	0.072	0.054	0.049	0.063	0.084	0.018	0.102
O_3 + Alkene **3**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.115	0.199	0.151	0.068	0.114	0.074	0.039	0.073	0.057	0.018	0.079	0.013
275	0.111	0.183	0.142	0.072	0.116	0.078	0.044	0.078	0.063	0.022	0.076	0.017
298	0.110	0.180	0.141	0.072	0.117	0.078	0.045	0.079	0.063	0.022	0.075	0.017
325	0.114	0.195	0.149	0.069	0.115	0.075	0.040	0.075	0.058	0.018	0.078	0.014
400	0.107	0.167	0.135	0.075	0.119	0.081	0.048	0.083	0.068	0.025	0.073	0.019
O_3 + Alkene **7**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{AO} (1.1)	Γ_{AO} (1.2)	Γ_{AO} (1.3)	Γ_{AO} (2.1)	Γ_{AO} (2.2)	Γ_{AO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.029	0.033	0.115	0.142	0.166	0.292	0.034	0.034	0.109	0.018	0.002	0.026
275	0.018	0.023	0.093	0.138	0.185	0.369	0.023	0.024	0.097	0.011	0.001	0.018
298	0.023	0.027	0.102	0.141	0.178	0.334	0.028	0.028	0.103	0.014	0.002	0.021
325	0.046	0.047	0.140	0.141	0.137	0.203	0.050	0.047	0.121	0.027	0.005	0.038
400	0.035	0.038	0.121	0.140	0.157	0.266	0.039	0.038	0.112	0.021	0.003	0.030
O_3 + Alkene **8**										Grainsize:		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{AO} (1.1)	Γ_{AO} (1.2)	Γ_{AO} (1.3)	Γ_{AO} (2.1)	Γ_{AO} (2.2)	Γ_{AO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.000	0.000	0.000	0.040	0.959	0.000	0.000	0.000	0.000	0.000	0.000	0.000
275	0.024	0.045	0.002	0.285	0.495	0.041	0.044	0.056	0.003	0.003	0.001	0.000
298	0.029	0.050	0.003	0.286	0.466	0.044	0.049	0.062	0.003	0.004	0.002	0.001
325	0.025	0.045	0.003	0.285	0.494	0.041	0.044	0.056	0.003	0.004	0.001	0.000
400	0.045	0.066	0.007	0.281	0.381	0.052	0.065	0.080	0.007	0.008	0.004	0.002
O_3 + Alkene **12**										Grainsize: 30		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.008	0.021	0.005	0.082	0.345	0.104	0.071	0.292	0.069	0.001	0.001	0.000
275	0.010	0.026	0.007	0.087	0.329	0.109	0.076	0.280	0.072	0.001	0.002	0.000
298	0.010	0.025	0.007	0.086	0.333	0.107	0.074	0.283	0.071	0.001	0.002	0.000
325	0.012	0.029	0.008	0.093	0.316	0.113	0.080	0.271	0.075	0.001	0.002	0.000
400	0.041	0.078	0.030	0.133	0.183	0.141	0.111	0.170	0.089	0.008	0.012	0.003

*Table S15: Product Branching Ratios of Ozonolysis of Alkenes **15** & **16**.*

						O_3 + Alkene **15**				Grainsize: 25		
T (K)	Γ_{ANTI} (1.1)	Γ_{ANTI} (1.2)	Γ_{ANTI} (1.3)	Γ_{SYN} (1.1)	Γ_{SYN} (1.2)	Γ_{SYN} (1.3)	Γ_{ANTI} (2.1)	Γ_{ANTI} (2.2)	Γ_{ANTI} (2.3)	Γ_{SYN} (2.1)	Γ_{SYN} (2.2)	Γ_{SYN} (2.3)
200	0.001	0.024	0.083	0.190	0.030	0.273	0.001	0.066	0.088	0.099	0.000	0.144
275	0.027	0.071	0.128	0.122	0.058	0.125	0.033	0.105	0.127	0.087	0.015	0.102
298	0.018	0.068	0.129	0.129	0.057	0.136	0.023	0.105	0.128	0.091	0.008	0.107
325	0.031	0.073	0.128	0.118	0.058	0.120	0.037	0.105	0.126	0.086	0.018	0.099
400	0.002	0.066	0.133	0.139	0.058	0.148	0.006	0.108	0.132	0.096	0.004	0.115
						O_3 + Alkene **16**				Grainsize: 25		
T (K)	Γ_{ANTI} (1.1)	Γ_{ANTI} (1.2)	Γ_{ANTI} (1.3)	Γ_{SYN} (1.1)	Γ_{SYN} (1.2)	Γ_{SYN} (1.3)	Γ_{ANTI} (2.1)	Γ_{ANTI} (2.2)	Γ_{ANTI} (2.3)	Γ_{SYN} (2.1)	Γ_{SYN} (2.2)	Γ_{SYN} (2.3)
200	0.116	0.003	0.277	0.001	0.000	0.001	0.122	0.123	0.357	0.000	0.000	0.000
275	0.142	0.036	0.221	0.019	0.006	0.026	0.157	0.148	0.217	0.009	0.001	0.019
298	0.141	0.040	0.215	0.022	0.008	0.030	0.156	0.146	0.209	0.011	0.001	0.022
325	0.141	0.039	0.215	0.022	0.009	0.030	0.156	0.146	0.209	0.011	0.001	0.022
400	0.137	0.046	0.201	0.029	0.015	0.039	0.152	0.140	0.191	0.016	0.003	0.030

*Table S16: Product Branching Ratios of Ozonolysis of Alkenes **5** & **10**.*

T (K)	O_3 + Alkene **5**							
	Grainsize				60			
	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{SYN} (1)	Γ_{SYN} (2)
200	0.008	0.028	0.011	0.597	0.028	0.314	0.001	0.014
275	0.009	0.032	0.014	0.583	0.032	0.313	0.001	0.016
298	0.012	0.035	0.017	0.571	0.036	0.310	0.002	0.018
325	0.019	0.042	0.025	0.539	0.045	0.302	0.004	0.024
400	0.038	0.066	0.048	0.438	0.076	0.283	0.011	0.041
T (K)	O_3 + Alkene **10**							
	Grainsize				60			
	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{SYN} (1)	Γ_{SYN} (2)
200	0.000	0.000	0.001	0.979	0.001	0.019	0.000	0.000
275	0.005	0.019	0.053	0.679	0.035	0.207	0.000	0.003
298	0.005	0.019	0.055	0.674	0.036	0.207	0.000	0.003
325	0.006	0.020	0.057	0.669	0.037	0.208	0.000	0.003
400	0.007	0.023	0.062	0.654	0.040	0.210	0.001	0.004

S2.4 Epoxide Related Results

Complete Rate Constants and Product Branching Ratios for Epoxide pathways simulations in Section 3.8 of the main manuscript.

*Table S17: Overall and Epoxidation Master Equation Rate Constants (k_{ME}) and Canonical Rate Constants (k_{CAN}) for O_3 + Alkene **1**. (Using B3LYP Energies)*

Rate Constants: O_3 + Alkene 1 Grainsize 20							
T (K)	k_{ME} (Total)	k_{ME} (EPO)	Total k_{CAN}	TS_{OZO} 1.1	TS_{OZO} 1.2	TS_{EPO} 1.1	TS_{EPO} 1.2
200	2.68E-16	1.56E-26	2.68E-16	2.42E-16	2.63E-17	3.59E-28	1.53E-26
275	6.00E-16	1.60E-23	6.00E-16	4.98E-16	1.02E-16	1.31E-24	1.47E-23
298	7.37E-16	7.03E-23	7.37E-16	5.97E-16	1.39E-16	7.39E-24	6.29E-23
325	9.21E-16	3.13E-22	9.21E-16	7.28E-16	1.93E-16	4.20E-23	2.71E-22
400	1.59E-15	7.71E-21	1.59E-15	1.18E-15	4.08E-16	1.66E-21	6.05E-21

*Table S18: Product Branching Ratio both all pathways including the epoxidation pathway for O_3 + Alkene **1**. (Using B3LYP Energies)*

Product Branching Ratio O_3 + Alkene 1 Grainsize 50										
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{EPO} (1.1)	Γ_{EPO} (1.2)	Γ_{EPO} (2.1)	Γ_{EPO} (2.2)	Γ_{EPO} (2.3)	Γ_{EPO} (2.4)
200	0.616	0.140	0.102	0.142	8.65E-29	1.98E-29	4.70E-18	2.00E-16	8.52E-26	2.82E-27
275	0.566	0.157	0.128	0.149	1.25E-20	1.52E-21	1.66E-10	1.86E-09	1.91E-17	5.13E-19
298	0.578	0.154	0.120	0.149	4.42E-19	7.45E-20	2.34E-09	1.99E-08	3.43E-16	1.34E-17
325	0.566	0.157	0.128	0.149	1.25E-20	1.52E-21	1.66E-10	1.86E-09	1.91E-17	5.13E-19
400	0.450	0.199	0.183	0.168	2.88E-15	8.58E-16	1.04E-06	3.79E-06	4.10E-13	4.37E-14

*Table S19: Overall and Epoxidation Master Equation Rate Constants (k_{ME}) and Canonical Rate Constants (k_{CAN}) for O_3 + Alkene **5**. (Using B3LYP Energies)*

Rate Constants: O_3 + Alkene 5 Grainsize 20											
T (K)	k_{ME} (Total)	k_{ME} (EPO)	Total k_{CAN}	TS_{OZO} 1.1	TS_{OZO} 1.2	TS_{OZO} 2.1	TS_{OZO} 2.2	TS_{EPO} 1.1	TS_{EPO} 1.2	TS_{EPO} 1.3	TS_{EPO} 1.4
200	4.09E-17	8.44E-28	3.94E-17	2.08E-18	3.65E-19	3.68E-17	1.57E-19	5.44E-30	1.59E-28	2.72E-30	6.46E-28
275	1.23E-16	2.36E-24	1.29E-16	1.39E-17	3.65E-18	1.09E-16	1.96E-18	5.62E-26	7.11E-25	2.74E-26	1.50E-24
298	1.60E-16	1.16E-23	1.72E-16	2.13E-17	6.07E-18	1.41E-16	3.41E-18	3.91E-25	4.17E-24	1.90E-25	7.69E-24
325	2.20E-16	6.42E-23	2.34E-16	3.31E-17	1.02E-17	1.85E-16	6.01E-18	2.74E-24	2.47E-23	1.32E-24	3.96E-23
400	5.20E-16	2.74E-21	4.89E-16	8.83E-17	3.23E-17	3.47E-16	2.09E-17	1.67E-22	1.05E-21	7.96E-23	1.27E-21

S3 Relative Energies, Enthalpies and Gibbs Free Energies.

S3.1 Main Computational Results

The Relative Energies, Enthalpies and Gibbs Free Energies in this section is based on the DF-LCCSD(T)-F12a molecular energy calculations, used for vast majority of analysis

*Table S20: Relative Energies of O_3 + Alkene **1** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-18.43	-14.65	-13.38	21.63
TSOzo1	5.45	11.59	8.51	56.97
POZ1	-254.53	-235.22	-240.87	-186.41
PRC2	-18.27	-14.82	-13.21	19.76
TSOzo2	9.87	15.96	12.93	61.14
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TSpoz1	-241.46	-223.97	-231.14	-172.84
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TSpoz2	-241.99	-224.36	-231.40	-173.44
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TS_{Anti} 1	-172.31	-162.77	-167.46	-114.40
C_{ANTI}	-273.71	-266.76	-267.15	-225.00
HCHO + Anti-RCHOO	-231.60	-234.74	-233.24	-233.71
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{FO} 1	-166.50	-156.71	-161.60	-108.14
$C_{FO\ 1}$	-263.60	-259.95	-258.36	-223.57
RCHO + HCHOO	-238.38	-239.30	-238.95	-241.66
POZ2	-254.91	-235.60	-241.26	-186.80
TS_{FO} 2	-164.11	-154.11	-158.96	-105.96
C_{FO} 2	-258.38	-256.17	-253.22	-227.23
	-238.38	-239.30	-238.95	-241.66
POZ2				
TS_{Syn}	-254.91	-235.70	-241.53	-186.34
C_{SYN}	-171.23	-161.14	-166.17	-112.08
HCHO + Syn-RCHOO	-275.28	-271.46	-270.32	-232.19

*Table S21: Relative Energies of O_3 + Alkene **2** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 2			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$EtCHCH_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$EtCHCH_2$ con 2 + O_3	0.28	0.64	0.34	1.35
PRC1.1	-19.79	-16.27	-14.71	19.99
TSOzo1.1	5.09	11.18	8.34	56.93
POZ1.1	-254.56	-235.71	-241.00	-185.95
PRC1.2	-20.79	-16.89	-15.71	20.57
TSOzo1.2	4.49	10.90	7.67	57.88
POZ1.2	-253.16	-234.23	-239.54	-184.52
PRC1.3	-14.74	-11.97	-9.75	20.88
TSOzo1.3	5.54	10.66	8.07	56.40
POZ1.3	-255.60	-236.90	-242.17	-187.13
PRC2.1	-17.80	-14.51	-12.66	20.10
TSOzo2.1	9.14	15.38	12.50	61.15
POZ2.1	-255.50	-236.70	-242.16	-186.33
PRC2.2	-16.74	-13.23	-11.63	22.06
TSOzo2.2	10.73	17.28	14.04	63.98
POZ2.2	-252.58	-233.64	-239.15	-183.07
PRC2.3	-15.76	-12.90	-10.73	19.93
TSOzo2.3	7.48	12.60	9.92	58.39
POZ2.3	-256.92	-238.39	-243.83	-188.04
POZ1.1	-254.56	-235.71	-241.00	-185.95
TS_{Anti} 1	-171.83	-162.54	-166.95	-113.30
C_{anti} 1	-274.18	-267.33	-267.35	-224.89
HCHO + *Anti*-EtCHOO Con 2	-230.48	-233.31	-231.68	-232.47
POZ1.2	-253.16	-234.23	-239.54	-184.52
TS_{Anti} 2	-171.97	-162.32	-166.83	-112.79
C_{anti} 2	-275.74	-269.04	-269.22	-226.30
HCHO + *Anti*-EtCHOO Con 1	-232.30	-235.39	-233.92	-233.79
POZ1.3	-255.60	-236.90	-242.17	-187.13
TS_{Anti} 3	-173.80	-164.43	-168.79	-115.45
C_{anti} 3	-272.75	-265.82	-265.83	-223.93
HCHO + *Anti*-EtCHOO Con 2	-230.48	-233.31	-231.68	-232.47
POZ1.1	-254.56	-235.71	-241.00	-185.95
TS_{FO} 1.1	-167.32	-158.01	-162.56	-108.70
C_{FO} 1.1	-262.48	-258.73	-256.68	-223.08
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ1.2	-253.16	-234.23	-239.54	-184.52
TS_{FO} 1.2	-167.10	-157.45	-162.07	-108.04
C_{FO} 1.2	-263.50	-260.77	-258.41	-226.73
HCHOO + EtCHOO Con 1	-240.75	-241.47	-241.31	-243.49
POZ1.3	-255.60	-236.90	-242.17	-187.13
TS_{FO} 1.3	-168.02	-158.53	-163.07	-109.21
C_{FO} 1.3	-267.16	-262.29	-260.89	-224.91
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ2.1	-255.50	-236.70	-242.16	-186.33
TS_{FO} 2.1	-164.73	-155.37	-159.84	-106.39
C_{FO} 2.1	-254.40	-252.39	-248.81	-229.31
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30

POZ2.2	-252.58	-233.64	-239.15	-183.07
TS_{FO} 2.2	-165.60	-155.96	-160.52	-106.68
C_{FO} 2.2	-260.15	-257.86	-254.77	-229.95
HCHOO + EtCHOO Con 1	-240.75	-241.47	-241.31	-243.49
POZ2.3	-256.92	-238.39	-243.83	-188.04
TS_{FO} 2.3	-166.18	-156.66	-161.10	-107.63
C_{FO} 2.3	-252.75	-249.15	-247.06	-213.44
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ2.1	-255.50	-236.70	-242.16	-186.33
TS_{Syn} 1	-172.05	-162.47	-167.22	-112.36
C_{syn} 1	-274.35	-271.35	-269.74	-231.98
HCHO + *Syn*-RCHOO Con2	-244.58	-247.65	-246.48	-246.05
POZ2.2	-252.58	-233.64	-239.15	-183.07
TS_{Syn} 2	-160.28	-150.66	-155.37	-100.89
C_{syn} 2	-262.65	-260.91	-257.37	-229.45
HCHO + *Syn*-RCHOO Con1	-242.24	-243.61	-242.67	-241.56
POZ2.3	-256.92	-238.39	-243.83	-188.04
TS_{Syn} 3	-173.28	-163.32	-168.02	-113.34
C_{syn} 3	-272.09	-267.42	-266.00	-227.72
HCHO + *Syn*-RCHOO Con1	-242.24	-243.61	-242.67	-241.56

*Table S22: Relative Energies of O_3 + Alkene **3** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 3			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
iPrCHCH$_2$ con 1 + O_3	0.00	0.00	0.00	0.00
iPrCHCH$_2$ con 2 + O_3	1.07	1.73	1.40	2.43
PRC1.1	-19.29	-15.21	-13.84	22.00
TSOzo1.1	3.23	9.81	6.80	57.01
POZ1.1	-253.05	-234.17	-239.33	-183.57
PRC1.2	-14.45	-11.80	-9.36	20.79
TSOzo1.2	5.19	10.85	8.22	57.28
POZ1.2	-255.46	-236.81	-241.95	-186.07
PRC1.3	-13.87	-10.68	-8.56	22.12
TSOzo1.3	8.62	14.68	11.81	62.10
POZ1.3	-252.61	-233.81	-238.95	-183.32
PRC2.1	-15.71	-11.95	-10.25	23.40
TSOzo2.1	10.15	16.95	13.88	64.19
POZ2.1	-252.69	-233.69	-239.03	-182.28
PRC2.2	-15.10	-12.38	-9.95	20.00
TSOzo2.2	9.23	15.06	12.27	61.70
POZ2.2	-256.81	-238.24	-243.56	-187.01
PRC2.3	-14.49	-11.16	-9.12	22.26
TSOzo2.3	12.23	18.53	15.49	66.12
POZ2.3	-252.94	-234.11	-239.49	-182.71
POZ1.1	-253.05	-234.17	-239.33	-183.57
TS_{Anti} 1	-170.80	-161.17	-165.49	-110.94
C_{anti} 1	-275.14	-268.24	-268.15	-225.11
HCHO + *Anti*-iPrCHOO Con 2	-230.57	-233.20	-231.59	-231.76
POZ1.2	-255.46	-236.81	-241.95	-186.07
TS_{Anti} 2	-173.17	-163.77	-168.03	-113.79
C_{anti} 2	-273.60	-266.66	-266.35	-224.06
HCHO + *Anti*-iPrCHOO Con 1	-229.52	-232.22	-230.41	-231.49
POZ1.3	-252.61	-233.81	-238.95	-183.32
TS_{Anti} 3	-172.03	-162.26	-166.54	-112.28
C_{anti} 3	-274.29	-267.26	-267.13	-224.58
HCHO + *Anti*-iPrCHOO Con 2	-230.57	-233.20	-231.59	-231.76
POZ1.1	-253.05	-234.17	-239.33	-183.57
TS_{FO} 1.1	-167.02	-157.49	-161.97	-107.47
C_{FO} 1.1	-269.00	-264.29	-262.91	-225.17
HCHOO + iPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ1.2	-255.46	-236.81	-241.95	-186.07
TS_{FO} 1.2	-168.20	-158.94	-163.30	-109.52
C_{FO} 1.2	-262.24	-258.42	-256.02	-222.93

HCHOO + iPrCHO Con 1	-236.77	-236.98	-236.72	-239.42
POZ1.3	-252.61	-233.81	-238.95	-183.32
TS_{FO} 1.3	-166.88	-157.28	-161.66	-107.45
C_{FO} 1.3	-261.07	-257.99	-255.31	-224.78
HCHOO + iPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ2.1	-252.69	-233.69	-239.03	-182.28
TS_{FO} 2.1	-163.47	-153.96	-158.36	-103.84
C_{FO} 2.1	-257.09	-254.73	-251.26	-229.83
HCHOO + iPrCHO Con 2	-236.77	-236.99	-236.57	-240.13
POZ2.2	-256.81	-238.24	-243.56	-187.01
TS_{FO} 2.2	-166.41	-157.12	-161.46	-107.28
C_{FO} 2.2	-257.10	-254.42	-251.05	-226.90
HCHOO + iPrCHO Con 1	-238.76	-238.97	-238.72	-241.42
POZ2.3	-252.94	-234.11	-239.49	-182.71
TS_{FO} 2.3	-165.00	-155.49	-159.79	-105.66
C_{FO} 2.3	-257.09	-254.73	-251.26	-229.83
HCHOO + iPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ2.1	-252.69	-233.69	-239.03	-182.28
TS_{Syn} 1	-160.09	-150.47	-155.15	-100.06
C_{syn} 1	-261.06	-259.90	-256.04	-229.02
HCHO + *Syn*-iPrCHOO Con2	-241.25	-243.13	-241.95	-240.82
POZ2.2	-256.81	-238.24	-243.56	-187.01
TS_{Syn} 2	-170.93	-161.07	-165.66	-110.04
C_{syn} 2	-273.81	-269.33	-267.78	-228.79
HCHO + *Syn*-iPrCHOO Con1	-241.25	-243.13	-241.95	-240.82
$TS_{ISO\text{-}syn}$	-214.73	-216.68	-217.74	-211.43
HCHO + *Syn*-iPrCHOO Con2	-241.25	-243.13	-241.95	-240.82
POZ2.3	-252.94	-234.11	-239.49	-182.71
TS_{Syn} 3	-159.58	-149.55	-154.14	-98.74
C_{syn} 3	-258.81	-254.77	-252.52	-216.06
HCHO + *Syn*-iPrCHOO Con1	-232.50	-233.76	-232.48	-231.33

*Table S23: Relative Energies of O_3 + Alkene **4** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 4			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-15.54	-12.97	-10.45	19.48
TSOzo1	4.65	10.25	7.70	57.57
POZ1	-253.90	-235.92	-240.68	-185.31
PRC2	-17.88	-15.34	-12.78	16.62
TSOzo2	11.41	17.26	14.55	64.78
POZ2	-254.59	-236.49	-241.47	-185.03
POZ1	-253.90	-235.92	-240.68	-185.31
TS_{Anti} 1	-173.06	-164.1	-167.98	-113.91
C_{ANTI}	-276.02	-269.74	-269.06	-227.35
HCHO + Anti-RCHOO	-231.15	-234.43	-232.32	-233.83
POZ1	-253.90	-235.92	-240.68	-185.31
TS_{FO} 1	-168.56	-159.7	-163.84	-109.85
$C_{FO\ 1}$	-269.51	-265.56	-263.43	-228.42
RCHO + HCHOO	-240.54	-241.35	-240.65	-244.73
POZ2	-254.59	-236.49	-241.47	-185.03
TS_{FO} 2	-163.64	-154.9	-158.95	-104.95
C_{FO} 2	-258.84	-257.02	-253.14	-231.57
POZ2	-254.59	-236.49	-241.47	-185.03
TS_{Syn}	-160.76	-151.5	-155.88	-100.30
C_{SYN}	-258.57	-255.77	-253.11	-217.46
HCHO + Syn-RCHOO	-233.27	-235.59	-234.04	-233.33

*Table S24: Relative Energies of O_3 + Alkene **5** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
MVK con 2 + O_3	0.00	0.00	0.00	0.00
TSmvk	22.60	20.01	18.56	21.79
MVK con 1 + O_3	2.30	1.68	1.86	1.21
PRC1.1	-15.65	-13.35	-10.69	17.58
TSiso1.1	8.19	8.12	9.06	44.3
PRC1.2	-14.31	-12.10	-9.77	21.70
PRC2.1	-15.65	-13.35	-10.69	17.58
TSiso2.1	6.90	6.49	8.00	39.3
PRC2.2	-18.75	-16.01	-14.02	19.65
PRC2.1	-15.65	-13.35	-10.69	17.58
TSiso2.2	9.27	9.13	10.25	43.1
PRC2.2	-18.75	-16.01	-14.02	19.65
PRC1.1	-15.65	-13.3	-10.69	17.58
TSOzo1.1	9.92	15.2	12.46	62.0
POZ1.1	-219.69	-203.50	-208.01	-155.52
PRC1.2	-14.31	-12.10	-9.77	21.70
TSOzo1.2	11.72	17.4	14.46	64.6
POZ1.2	-236.61	-220.08	-224.82	-171.52
PRC2.1	-10.64	-9.0	-5.61	15.95
TSOzo2.1	2.29	7.8	5.01	54.9
POZ2.1	-224.38	-208.15	-212.79	-159.25
PRC2.2	-18.75	-16.01	-14.02	19.65
TSOzo2.2	12.70	18.3	15.40	65.7
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52
TSpoz1.1	-207.86	-193.10	-199.35	-141.89
POZ2.1	-224.38	-208.15	-212.79	-159.25
POZ1.2	-236.61	-220.08	-224.82	-171.52
TSpoz1.2	-219.32	-204.50	-210.52	-153.80
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.2	-236.61	-220.08	-224.82	-171.52
TSpoz1.3	-228.72	-213.61	-220.02	-161.87
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52
TSpoz2.1	-211.57	-195.09	-202.32	-141.91
POZ1.2	-236.61	-220.08	-224.82	-171.52
POZ1.1	-236.61	-220.08	-224.82	-171.52
TSpoz2.2	-217.82	-201.56	-208.48	-148.75
POZ1.2	-239.44	-222.76	-227.65	-173.95
POZ2.1	-224.38	-208.15	-212.79	-159.25
TSpoz2.3	-212.31	-195.68	-202.99	-142.43
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ2.1	-224.38	-208.15	-212.79	-159.25
TSpoz2.4	-220.97	-204.79	-211.71	-151.75
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52

TS_{Anti} 1	-140.62	-133.30	-137.01	-85.09
C_{anti} 1	-212.65	-212.56	-208.71	-186.29
HCHO + Anti-RCHOO Con 2	-191.21	-193.72	-192.92	-198.03
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{Anti} 2	-166.69	-158.76	-162.64	-110.07
C_{anti} 2	-249.38	-245.29	-244.10	-204.37
HCHO + Anti-RCHOO Con1	-213.05	-214.56	-213.99	-217.76
$TS_{ISO-ANTI}$	-188.11	-191.60	-192.68	-192.50
HCHO + Anti-RCHOO Con 2	-191.21	-193.72	-192.92	-198.03
POZ1.1	-224.38	-208.15	-212.79	-159.25
TS_{FO} 1.1	-146.22	-139.00	-142.76	-90.52
C_{FO} 1.1	-240.21	-234.56	-234.44	-190.30
HCHOO + RCHO con 1	-191.21	-193.72	-192.92	-198.03
POZ1.2	-239.44	-222.76	-227.65	-173.95
TS_{FO} 1.2	-163.33	-155.48	-159.33	-106.35
C_{FO} 1.2	-249.11	-244.23	-243.61	-201.60
HCHOO + RCHO con 2	-213.05	-214.56	-213.99	-217.76
$TS_{ISO-ALDE}$				
HCHOO + RCHO con 1	-224.38	-208.15	-212.79	-159.25
	-124.64	-118.23	-121.66	-70.22
POZ2.1	-195.65	-197.07	-192.13	-173.74
TS_{FO} 2.1	-178.76	-182.80	-181.07	-182.49
C_{FO} 2.1	-219.69	-203.50	-208.01	-155.52
HCHOO + RCHO con 1	-140.62	-133.30	-137.01	-85.09
	-212.65	-212.56	-208.71	-186.29
POZ2.2	-191.21	-193.72	-192.92	-198.03
TS_{FO} 2.2				
C_{FO} 2.2	-236.61	-220.08	-224.82	-171.52
HCHOO + RCHO con 2	-166.69	-158.76	-162.64	-110.07
	-249.38	-245.29	-244.10	-204.37
POZ2.1	-213.05	-214.56	-213.99	-217.76
TS_{Syn} 1	-188.11	-191.60	-192.68	-192.50
C_{syn} 1	-191.21	-193.72	-192.92	-198.03
HCHO + Syn-RCHOO Con2	-178.76	-182.80	-181.07	-182.49
$TS_{ISO-SYN}$	-175.10	-180.25	-180.63	-176.25
HCHO + Syn-RCHOO Con1	-202.98	-205.92	-204.89	-204.20
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{Syn} 2	-144.94	-137.01	-141.24	-88.00
C_{syn} 2	-225.90	-225.69	-222.20	-191.88

*Table S25: Relative Energies of O_3 + Alkene **6** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 6			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-12.20	-9.73	-7.64	26.04
TSOzo1	-5.62	-1.64	-3.39	44.63
POZ1	-271.15	-253.73	-259.68	-200.52
PRC2	-25.31	-22.41	-20.55	14.56
TSOzo2	-2.30	2.37	0.03	50.09
POZ2	-267.79	-250.36	-256.36	-197.69
POZ1	-271.15	-253.73	-259.68	-200.52
TSpoz1	-259.61	-244.01	-251.25	-188.39
POZ2	-267.79	-250.36	-256.36	-197.69
POZ1	-271.15	-253.73	-259.68	-200.52

TS_{Anti} 1	-189.30	-180.14	-184.97	-127.65
C_{ANTI}	-312.63	-309.87	-307.32	-275.16
$(CH_3)_2CO$ + *Anti*-CH_3CHOO	-280.30	-281.66	-280.77	-288.59
POZ1	-271.15	-253.73	-259.68	-200.52
TS_{AO} 1	-200.47	-191.43	-196.54	-138.13
C_{AO} 1	-330.72	-328.31	-326.11	-290.79
RCHO + $(CH_3)_2COO$	-296.05	-297.38	-297.35	-299.45
POZ2	-267.79	-250.36	-256.36	-197.69
TS_{AO} 2	-191.68	-182.27	-187.33	-129.23
C_{AO} 2	-326.83	-324.95	-322.60	-288.00
POZ2	-267.79	-250.36	-256.36	-197.69
TS_{Syn}	-184.69	-174.95	-180.19	-121.51
C_{SYN}	-321.21	-318.67	-315.95	-285.91
$(CH_3)_2CO$ + *Syn*-CH_3CHOO	-295.15	-295.68	-295.47	-302.28

*Table S26: Relative Energies of O_3 + Alkene **7** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 7			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$EtCHC(CH_3)_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$EtCHC(CH_3)_2$ con 2 + O_3	17.71	18.76	18.41	19.36
PRC1.1	-11.84	-9.42	-7.20	26.17
TSOzo1.1	-5.44	-0.84	-2.76	46.58
POZ1.1	-267.79	-250.50	-256.25	-195.91
PRC1.2	-12.85	-10.77	-8.46	25.04
TSOzo1.2	7.99	13.00	10.85	61.52
POZ1.2	-258.99	-241.99	-247.44	-188.94
PRC1.3	-12.85	-10.77	-8.46	25.04
TSOzo1.3	-5.83	-2.22	-4.03	45.81
POZ1.3	-270.62	-253.79	-259.37	-199.78
PRC2.1	-23.51	-20.69	-18.74	16.16
TSOzo2.1	-0.22	4.98	2.61	53.58
POZ2.1	-264.31	-247.30	-252.93	-192.89
PRC2.2	-23.51	-20.69	-18.74	16.16
TSOzo2.2	9.47	15.24	12.49	65.35
POZ2.2	-256.15	-238.92	-244.52	-185.54
PRC2.3	-23.51	-20.69	-18.74	16.16
TSOzo2.3	-4.55	-0.44	-2.69	48.56
POZ2.3	-267.99	-251.27	-256.87	-197.65
POZ1.1	-267.79	-250.50	-256.25	-195.91
TS_{Anti} 1	-180.40	-171.36	-175.98	-117.98
C_{anti} 1	-318.68	-315.65	-312.93	-278.89
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 2	-278.90	-279.79	-278.94	-287.21
POZ1.2	-258.99	-241.99	-247.44	-188.94
TS_{Anti} 2	-184.94	-175.31	-180.18	-121.25
C_{anti} 2	-310.49	-307.59	-304.76	-273.51
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 1	-280.72	-281.87	-281.18	-288.53
POZ1.3	-270.62	-253.79	-259.37	-199.78
TS_{Anti} 3	-189.88	-180.85	-185.40	-127.80
C_{anti} 3	-310.49	-307.59	-304.76	-273.51
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 2	-278.90	-279.79	-278.94	-287.21

POZ1.1	-267.79	-250.50	-256.25	-195.91
TS_{AO} 1.1	-194.63	-186.08	-190.86	-132.13
C_{AO} 1.1	-328.47	-325.89	-323.49	-289.44
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ1.2	-258.99	-241.99	-247.44	-188.94
TS_{AO} 1.2	-198.57	-189.49	-194.50	-135.08
C_{AO} 1.2	-332.78	-330.40	-328.20	-292.52
$(CH_3)_2COO$ + EtCHO Con 1	-298.14	-299.11	-299.43	-301.15
POZ1.3	-270.62	-253.79	-259.37	-199.78
TS_{AO} 1.3	-201.33	-192.45	-197.33	-138.42
C_{AO} 1.3	-325.45	-323.44	-320.75	-287.65
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.1	-264.31	-247.30	-252.93	-192.89
TS_{AO} 2.1	-183.16	-174.26	-178.99	-120.45
C_{AO} 2.1	-330.14	-327.84	-325.63	-289.76
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.2	-256.15	-238.92	-244.52	-185.54
TS_{AO} 2.2	-184.96	-175.65	-180.49	-121.51
C_{AO} 2.2	-333.69	-331.27	-329.09	-293.44
$(CH_3)_2COO$ + EtCHO Con 1	-298.14	-299.11	-299.43	-301.15
POZ2.3	-267.99	-251.27	-256.87	-197.65
TS_{AO} 2.3	-192.15	-183.30	-187.99	-129.55
C_{AO} 2.3	-328.78	-326.20	-323.86	-289.29
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.1	-264.31	-247.30	-252.93	-192.89
TS_{Syn} 1	-181.53	-172.18	-177.20	-117.61
C_{syn} 1	-321.93	-319.83	-317.03	-286.05
$(CH_3)_2CO$ + *Syn*-EtCHOO Con2	-292.99	-294.13	-293.74	-300.79
POZ2.2	-256.15	-238.92	-244.52	-185.54
TS_{Syn} 2	-168.80	-159.11	-164.27	-103.99
C_{syn} 2	-314.85	-311.53	-308.56	-279.01
$(CH_3)_2CO$ + *Syn*-EtCHOO Con1	-290.66	-290.09	-289.93	-296.31
POZ2.3	-267.99	-251.27	-256.87	-197.65
TS_{Syn} 3	-183.86	-174.15	-179.12	-119.90
C_{syn} 3	-317.73	-314.05	-311.41	-279.77
$(CH_3)_2CO$ + *Syn*-EtCHOO Con1	-290.66	-290.09	-289.93	-296.31

*Table S27: Relative Energies of O_3 + Alkene **8** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 8			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
iPrCHC$(CH_3)_2$ con 1 + O_3	**0.00**	**0.00**	**0.00**	**0.00**
TS_{ISOiPR}	21.71	20.69	18.30	25.03
iPrCHC$(CH_3)_2$ con 3 + O_3	18.00	19.45	19.00	19.82
iPrCHC$(CH_3)_2$ con 2 + O_3	13.39	14.17	14.01	15.65
PRC1.1	-13.44	-10.81	-8.67	26.09
TS_{ISO}	7.06	10.05	9.85	50.1
PRC1.3	4.50	8.45	10.18	45.39
PRC1.1	-13.44	-10.81	-8.67	26.09
TSOzo1.1	-1.44	3.18	1.06	52.32
POZ1.1	-267.16	-249.83	-255.59	-194.08
PRC1.2	-13.44	-10.81	-8.67	26.09
TSOzo1.2	5.96	10.86	8.65	60.07
POZ1.2	-258.98	-241.86	-247.38	-187.83
PRC1.3	4.50	8.45	10.18	45.39
TSOzo1.3	11.66	17.02	15.10	64.70
POZ1.3	-258.98	-241.01	-246.79	-185.70
PRC2.1	-19.47	-16.91	-14.56	18.09
TSOzo2.1	-0.68	4.76	2.05	55.13
POZ2.1	-258.98	-242.09	-247.64	-186.87
PRC2.2	-19.47	-16.91	-14.56	18.09
TSOzo2.2	8.12	13.79	10.99	64.45
POZ2.2	-256.16	-239.10	-244.60	-186.41
PRC2.3	-8.13	-4.61	-2.51	33.10
TSOzo2.3	14.77	20.66	18.40	69.21
POZ2.3	-252.45	-234.55	-240.32	-179.01
POZ1.1	-267.16	-249.83	-255.59	-194.08
TS_{Anti} 1	-179.85	-170.34	-175.01	-116.25
C_{anti} 1	-319.05	-315.64	-312.83	-279.01
$(CH_3)_2CO$ + *Anti*-iPrCHOO Con 2	-277.90	-278.44	-277.61	-286.25
POZ1.2	-258.98	-241.86	-247.38	-187.83
TS_{Anti} 2	-184.69	-174.86	-179.70	-120.49
C_{anti} 2	-311.14	-307.96	-305.17	-273.80
$(CH_3)_2CO$ + *Anti*-iPrCHOO Con 1	-278.95	-279.42	-278.80	-286.52
POZ1.3	-258.98	-241.01	-246.79	-185.70
TS_{Anti} 3	-170.55	-160.37	-165.34	-105.39
C_{anti} 3	-321.13	-317.73	-315.16	-280.47
$(CH_3)_2CO$ + *Anti*-iPrCHOO Con 2	-278.95	-279.42	-278.80	-286.52
POZ1.1	-267.16	-249.83	-255.59	-194.08
TS_{AO} 1.1	-193.44	-184.77	-189.54	-130.69
C_{AO} 1.1	-330.15	-327.21	-324.92	-290.14
$(CH_3)_2COO$ + iPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ1.2	-258.98	-241.86	-247.38	-187.83
TS_{AO} 1.2	-199.95	-190.65	-195.62	-135.72
C_{AO} 1.2	-330.15	-327.21	-324.92	-290.14
$(CH_3)_2COO$ + iPrCHO Con 1	-294.11	-294.36	-294.79	-297.09
POZ1.3	-258.98	-241.01	-246.79	-185.70
TS_{AO} 1.3	-187.62	-178.02	-183.19	-122.26
C_{AO} 1.3	-316.09	-312.93	-310.61	-278.63

$(CH_3)_2COO$ + iPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.1	-258.98	-242.09	-247.64	-186.87
TS_{AO} 2.1	-183.76	-174.87	-179.61	-120.29
C_{AO} 2.1	-328.56	-325.74	-323.35	-289.16
$(CH_3)_2COO$ + iPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.2	-256.16	-239.10	-244.60	-186.41
TS_{AO} 2.2	-184.91	-175.72	-180.36	-121.40
C_{AO} 2.2	-321.01	-319.33	-316.29	-288.10
$(CH_3)_2COO$ + iPrCHO Con 1	-294.11	-294.38	-294.64	-297.81
POZ2.3	-252.45	-234.55	-240.32	-179.01
TS_{AO} 2.3	-170.14	-160.60	-165.51	-105.56
C_{AO} 2.3	-325.14	-322.87	-319.93	-290.30
$(CH_3)_2COO$ + iPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.1	-258.98	-242.09	-247.64	-186.87
TS_{Syn} 1	-173.99	-163.87	-169.05	-108.17
C_{syn} 1	-318.31	-315.03	-312.23	-281.56
$(CH_3)_2CO$ + *Syn*-iPrCHOO Con2	-289.63	-289.34	-289.15	-295.58
POZ2.2	-256.16	-239.10	-244.60	-186.41
TS_{Syn} 2	-168.61	-158.48	-163.65	-102.69
C_{syn} 2	-305.52	-301.70	-298.70	-268.15
$(CH_3)_2CO$ + *Syn*-iPrCHOO Con1	-289.63	-289.34	-289.15	-295.58
POZ2.3	-258.98	-241.01	-246.79	-185.70
TS_{Syn} 3	-159.57	-150.24	-154.97	-95.77
C_{syn} 3	-312.92	-310.07	-306.91	-278.46
$(CH_3)_2CO$ + *Syn*-iPrCHOO Con1	-280.88	-279.97	-279.69	-286.09

*Table S28: Relative Energies of O_3 + Alkene **9** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 9			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-23.80	-21.19	-18.93	14.70
TSOzo1	-0.72	3.73	1.94	52.00
POZ1	-265.48	-248.24	-253.74	-193.92
PRC2	-23.22	-20.41	-18.23	16.77
TSOzo2	1.08	6.34	4.01	55.51
POZ2	-265.57	-248.45	-253.93	-193.99
POZ1	-265.48	-248.24	-253.74	-193.92
TS_{Anti} 1	-184.71	-175.09	-179.75	-121.45
C_{ANTI}	-334.98	-332.20	-329.08	-297.29
$(CH_3)_2CO$ + *Anti*-tBuCHOO	-293.11	-294.15	-293.11	-303.48
POZ1	-265.48	-248.24	-253.74	-193.92
TS_{AO} 1	-200.90	-191.88	-196.89	-137.50
$C_{AO\ 1}$	-339.76	-338.02	-334.65	-307.46
tBuCHO + $(CH_3)_2COO$	-311.47	-312.25	-312.31	-317.30
POZ2	-265.57	-248.45	-253.93	-193.99
TS_{AO} 2	-183.05	-174.16	-178.82	-120.51
C_{AO} 2	-339.76	-338.02	-334.65	-307.46
POZ2	-265.57	-248.45	-253.93	-193.99
TS_{Syn}	-169.22	-159.80	-164.50	-105.60
C_{SYN}	-320.02	-317.27	-313.99	-285.40
$(CH_3)_2CO$ + *Syn*-tBuCHOO	-295.23	-295.32	-294.84	-302.99

*Table S29: Relative Energies of O_3 + Alkene **10** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 10			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
Mes Oxy Con 2 + O_3	0.00	0.00	0.00	0.00
$TS_{MES-OXY}$	16.30	14.95	12.56	24.50
Mes Oxy Con 1 + O_3	9.26	11.12	10.32	16.32
PRC1.1	-14.80	-12.92	-10.23	22.85
TS_{PRC}1.1	-3.67	-2.37	-2.52	44.19
PRC1.2	-8.30	-4.50	-2.52	34.74
PRC1.1	-14.80	-12.92	-10.23	22.85
TSOzo1.1	7.69	12.77	9.90	67.34
POZ1.1	-238.08	-222.39	-228.17	-163.01
PRC1.2	-8.30	-4.50	-2.52	34.74
TSOzo1.2	16.42	22.20	19.24	76.83
POZ1.2	-252.19	-236.22	-242.17	-176.60
PRC2.1	-23.18	-20.60	-18.24	18.76
TSOzo2.1	4.90	10.38	7.41	65.33
POZ2.1	-237.89	-222.33	-228.10	-162.51
PRC2.2	-7.06	-3.08	-0.71	30.52
TSOzo2.2	14.67	21.02	17.79	76.57
POZ2.2	-252.78	-236.77	-242.72	-177.13
POZ1.1	-238.08	-222.39	-228.17	-163.01
TS_{Anti} 1	-150.50	-142.57	-147.17	-84.56
C_{anti} 1	-274.60	-271.57	-269.49	-230.17
$(CH_3)_2CO$ + Anti-RCHOO Con 1	-256.49	-256.79	-256.80	-257.97
POZ1.2	-252.19	-236.22	-242.17	-176.60
TS_{Anti} 2	-166.05	-157.48	-162.46	-98.13
C_{anti} 2	-284.11	-281.23	-278.92	-240.87
$(CH_3)_2CO$ + Anti-RCHOO Con 2	-241.83	-242.72	-242.55	-244.16
POZ1.1	-238.08	-222.39	-228.17	-163.01
TS_{FO} 1.1	-171.70	-163.75	-168.53	-104.90
C_{FO} 1.1	-299.10	-295.41	-294.57	-247.29
HCHOO + RCHO con 1	-245.05	-246.58	-247.08	-245.14
POZ1.2	-252.19	-236.22	-242.17	-176.60
TS_{FO} 1.2	-198.49	-189.68	-194.87	-129.68
C_{FO} 1.2	-309.06	-305.44	-304.47	-257.88
HCHOO + RCHO con 2	-266.88	-267.41	-268.15	-264.87
POZ2.1	-237.89	-222.33	-228.10	-162.51
TS_{FO} 2.1	-171.05	-162.99	-167.89	-103.43
C_{FO} 2.1	-300.77	-296.69	-296.29	-246.51
POZ2.2	-252.78	-236.77	-242.72	-177.13
TS_{FO} 2.2	-190.41	-181.46	-186.74	-120.96
C_{FO} 2.2	-307.42	-303.64	-302.64	-256.27
POZ2.1	-237.89	-222.33	-228.10	-162.51
TS_{Syn} 1	-129.70	-122.32	-126.91	-64.62
C_{syn} 1	-256.92	-254.45	-252.06	-214.15
$(CH_3)_2CO$ + Syn-RCHOO Con2	-223.63	-224.49	-224.37	-226.68
POZ2.2	-252.78	-236.77	-242.72	-177.13
TS_{Syn} 2	-157.90	-148.92	-154.39	-88.25
C_{syn} 2	-274.99	-271.85	-269.85	-231.48
$(CH_3)_2CO$ + Syn-RCHOO Con1	-247.85	-247.60	-248.19	-248.40

*Table S30: Relative Energies of O_3 + Alkene **11** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 11			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-19.53	-18.53	-14.43	-3.57
TSOzo1	26.25	31.29	28.58	80.53
POZ1	-263.99	-248.04	-252.89	-195.46
PRC2	-19.53	-18.53	-14.43	-3.57
TSOzo2	22.50	27.49	24.78	76.83
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TSpoz1	-224.01	-210.05	-215.68	-157.22
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TSpoz2	-240.38	-225.97	-231.85	-172.67
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TS_{Anti} 1	-126.84	-120.93	-124.11	-70.70
C_{ANTI}	-210.73	-209.97	-206.04	-174.53
HCHO + *anti*-CF_3CFOO	-178.03	-181.17	-179.23	-180.35
POZ1	-263.99	-248.04	-252.89	-195.46
TS_{FO} 1	-196.69	-188.06	-192.16	-136.32
$C_{FO\ 1}$	-304.64	-297.76	-297.17	-253.94
HCHOO + CF_3CFO	-269.01	-267.38	-267.17	-270.58
POZ2	-256.62	-241.08	-245.67	-189.02
TS_{FO} 2	-195.69	-187.10	-191.14	-135.30
C_{FO} 2	-306.34	-299.06	-298.85	-254.31
POZ2	-256.62	-241.08	-245.67	-189.02
TS_{Syn}	-118.03	-112.80	-115.94	-62.60
C_{SYN}	-173.67	-175.83	-170.45	-149.89
HCHO + *Syn*-CF_3CFOO	-164.32	-168.17	-166.29	-166.18

*Table S31: Relative Energies of O_3 + Alkene **12** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 12			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$CF_3CF_2CHCH_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$CF_3CF_2CHCH_2$ con 2 + O_3	7.39	7.28	7.31	7.67
PRC1.1	-6.68	-5.40	-1.55	16.59
TSOzo1.1	20.77	26.53	23.53	75.59
POZ1.1	-226.86	-209.25	-214.02	-158.17
PRC1.2	0.61	1.85	5.68	25.05
TSOzo1.2	30.58	36.43	33.33	85.67
POZ1.2	-224.92	-207.60	-212.41	-156.91
PRC1.3	-6.68	-5.40	-1.55	16.59
TSOzo1.3	26.89	32.44	29.60	80.17
POZ1.3	-230.33	-212.87	-217.59	-161.83
PRC2.1	-10.66	-9.02	-5.60	17.00
TSOzo2.1	21.54	27.30	24.30	76.34
POZ2.1	-230.37	-212.67	-217.54	-161.02
PRC2.2	-2.89	-1.37	2.10	24.91
TSOzo2.2	34.22	40.22	37.04	89.77
POZ2.2	-227.75	-210.09	-215.11	-157.78

PRC2.3	-11.78	-10.11	-6.73	17.62
TSOzo2.3	28.77	34.26	31.44	82.30
POZ2.3	-233.19	-215.65	-220.43	-164.45
POZ1.1	-226.86	-209.25	-214.02	-158.17
TS_{Anti} 1	-120.54	-113.37	-116.88	-63.63
C_{anti} 1	-205.32	-202.11	-200.70	-160.59
HCHO + *Anti*-CF_3CF_2CHOO Con 2	-171.96	-176.50	-174.47	-175.39
POZ1.2	-224.92	-207.60	-212.41	-156.91
TS_{Anti} 2	-119.33	-112.12	-115.66	-62.00
C_{anti} 2	-194.90	-194.60	-191.29	-157.90
HCHO + *Anti*-CF_3CF_2CHOO Con 1	-171.96	-176.50	-174.47	-175.39
POZ1.3	-230.33	-212.87	-217.59	-161.83
TS_{Anti} 3	-126.06	-118.99	-122.38	-69.54
C_{anti} 3	-205.18	-201.93	-200.50	-161.01
HCHO + *Anti*-CF_3CF_2CHOO Con 2	-174.99	-179.32	-177.35	-178.73
POZ1.1	-226.86	-209.25	-214.02	-158.17
TS_{FO} 1.1	-138.19	-129.89	-133.74	-79.93
C_{FO} 1.1	-215.03	-214.07	-210.05	-190.12
HCHOO + CF_3CF_2CHO Con 2	-195.30	-196.45	-195.88	-199.17
POZ1.2	-224.92	-207.60	-212.41	-156.91
TS_{FO} 1.2	-140.15	-132.01	-135.98	-81.89
C_{FO} 1.2	-214.89	-213.82	-209.87	-188.75
HCHOO + EtCHOO Con 1	-195.30	-196.45	-195.88	-199.17
POZ1.3	-230.33	-212.87	-217.59	-161.83
TS_{FO} 1.3	-149.29	-141.02	-144.87	-90.70
C_{FO} 1.3	-214.28	-213.46	-209.41	-189.91
HCHOO + CF_3CF_2CHO Con 2	-195.78	-196.79	-196.25	-200.27
POZ2.1	-230.37	-212.67	-217.54	-161.02
TS_{FO} 2.1	-138.80	-130.45	-134.38	-79.94
C_{FO} 2.1	-211.17	-209.42	-206.10	-180.91
HCHOO + CF_3CF_2CHO Con 2	-195.30	-196.45	-195.88	-199.17
POZ2.2	-227.75	-210.09	-215.11	-157.78
TS_{FO} 2.2	-140.94	-132.63	-136.65	-81.34
C_{FO} 2.2	-216.06	-214.45	-211.33	-179.76
HCHOO + CF_3CF_2CHO Con 1	-195.30	-196.45	-195.88	-199.17
POZ2.3	-233.19	-215.65	-220.43	-164.45
TS_{FO} 2.3	-148.71	-140.27	-144.16	-89.72
C_{FO} 2.3	-219.72	-217.85	-214.89	-183.42
HCHOO + CF_3CF_2CHO Con 2	-195.78	-196.79	-196.25	-200.27
POZ2.1	-230.37	-212.67	-217.54	-161.02
TS_{Syn} 1	-109.89	-102.78	-106.53	-51.82
C_{syn} 1	-190.39	-189.36	-186.43	-150.41
HCHO + *Syn*-CF_3CF_2CHOO Con2	-166.87	-170.25	-168.75	-167.97
POZ2.2	-227.75	-210.09	-215.11	-157.78
TS_{Syn} 2	-100.18	-93.61	-97.26	-42.60
C_{syn} 2	-184.71	-185.70	-181.17	-160.08
HCHO + *Syn*-CF_3CF_2CHOO Con1	-165.85	-169.57	-168.03	-168.40
POZ2.3	-233.19	-215.65	-220.43	-164.45
TS_{Syn} 3	-112.26	-105.54	-109.12	-54.81
C_{syn} 3	-187.93	-188.49	-184.47	-155.40
HCHO + *Syn*-CF_3CF_2CHOO Con1	-165.85	-169.57	-168.03	-168.40

*Table S32: Relative Energies of O_3 + Alkene **13** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 13			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-13.43	-12.02	-8.49	15.06
TSOzo1	20.86	26.17	23.07	75.97
POZ1	-240.10	-223.91	-228.77	-172.10
PRC2	-13.46	-12.00	-8.54	16.44
TSOzo2	23.52	28.60	25.58	78.39
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TSpoz1	-225.51	-211.11	-217.19	-157.62
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TSpoz2	-207.29	-192.88	-198.81	-139.72
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TS_{Anti} 1	-155.35	-148.12	-152.03	-97.72
C_{ANTI} 1	-257.15	-253.27	-251.49	-216.77
ClCHO + *Anti*-CF_3CHOO	-229.39	-229.48	-229.39	-233.22
POZ1	-240.10	-223.91	-228.77	-172.10
TS_{Syn} 1	-143.58	-136.39	-140.38	-85.43
C_{SYN} 1	-243.20	-238.42	-237.49	-197.24
CF_3CHO + *syn*-ClCHOO	-210.34	-209.63	-210.26	-213.55
POZ2	-233.71	-217.82	-222.55	-166.38
TS_{Anti} 1	-144.41	-137.35	-141.37	-86.45
C_{ANTI} 1	-226.39	-223.95	-221.46	-189.16
CF_3CHO + *Anti*-ClCHOO	-198.03	-199.02	-198.93	-202.71
POZ2	-233.71	-217.82	-222.55	-166.38
TS_{Syn} 2	-148.03	-141.04	-144.88	-90.29
C_{SYN} 2	-248.31	-245.43	-242.72	-213.71
ClCHO + *syn*-CF_3CHOO	-226.84	-226.10	-226.55	-228.09

*Table S33: Relative Energies of O_3 + Alkene **14** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-10.3	-9.03	-5.33	13.27
TSOzo1	25.4	30.68	27.65	79.94
POZ1	-261.9	-245.40	-250.48	-193.42
PRC2	-12.2	-10.65	-7.20	16.43
TSOzo2	24.4	29.62	26.62	78.71
POZ2	-250.4	-234.99	-239.50	-183.99
POZ1	-261.9	-245.40	-250.48	-193.42
TSpoz2	-246.7	-231.97	-238.24	-178.68
POZ2	-250.4	-234.99	-239.50	-183.99
POZ1	-261.9	-245.40	-250.48	-193.42
TS_{Anti} 1	-181.2	-173.54	-177.81	-122.87
C_{ANTI} 1	-295.0	-289.86	-288.41	-251.51
FCHO + *Anti*-CF_3CHOO	-266.8	-266.43	-266.10	-269.64
POZ1	-261.9	-245.40	-250.48	-193.42
TS_{Syn} 1	-151.2	-144.07	-147.97	-93.51
C_{SYN} 1	-237.4	-234.07	-231.81	-199.06
CF_3CHO + *syn*-FCHOO	-211.9	-211.35	-211.57	-215.26
POZ2	-250.4	-234.99	-239.50	-183.99
TS_{Anti} 1	-150.9	-143.86	-147.82	-93.28
C_{ANTI} 1	-238.5	-235.73	-233.23	-200.49
CF_3CHO + *Anti*-FCHOO	-206.6	-207.63	-207.27	-211.34
POZ2	-250.4	-234.99	-239.50	-183.99
TS_{Syn} 2	-173.7	-166.33	-170.49	-115.58
C_{SYN} 2	-286.6	-283.10	-280.36	-250.29
FCHO + *syn*-CF_3CHOO	-264.2	-263.04	-263.25	-264.51

*Table S34: Relative Energies of O_3 + Alkene **15** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 15			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
E-$EtCHCHCH_3$ con 1 + O_3	0.00	0.00	0.00	0.00
E-$EtCHCHCH_3$ con 2 + O_3	1.20	1.65	1.37	2.40
PRC1.1	-14.16	-10.58	-9.24	28.19
TSOzo1.1	-3.01	2.09	-0.20	47.81
POZ1.1	-264.53	-246.43	-251.97	-194.80
PRC1.2	-21.81	-18.70	-16.93	18.26
TSOzo1.2	-0.07	5.35	2.69	52.58
POZ1.2	-262.12	-244.07	-249.49	-192.84
PRC1.3	-13.70	-9.70	-8.70	30.32
TSOzo1.3	3.40	7.70	5.56	53.82
POZ1.3	-265.08	-247.24	-252.67	-195.93
PRC2.1	-13.71	-10.04	-8.75	28.69
TSOzo2.1	2.15	7.56	5.10	53.60
POZ2.1	-264.29	-246.06	-251.63	-194.26
PRC2.2	-12.23	-9.06	-7.44	28.56
TSOzo2.2	1.95	7.68	4.81	55.25
POZ2.2	-262.27	-244.11	-249.57	-192.52

PRC2.3	-14.98	-10.99	-9.95	28.86
TSOzo2.3	1.05	5.48	3.18	51.83
POZ2.3	-265.99	-248.17	-253.61	-196.75
POZ1.1	-264.53	-246.43	-251.97	-194.80
TS_{Anti} 1.1	-173.78	-164.51	-169.09	-113.92
C_{anti} 1.1	-295.78	-291.16	-289.70	-251.99
CH_3CHOO + *Anti*-EtCHOO Con 2	-256.77	-257.68	-257.19	-261.09
POZ1.2	-262.12	-244.07	-249.49	-192.84
TS_{Anti} 1.2	-180.34	-170.84	-175.49	-120.06
C_{anti} 1.2	-298.32	-293.64	-292.54	-253.36
CH_3CHOO + *Anti*-EtCHOO Con 1	-258.59	-259.76	-259.44	-262.41
POZ1.3	-265.08	-247.24	-252.67	-195.93
TS_{Anti} 1.3	-181.94	-172.59	-177.07	-122.47
C_{anti} 1.3	-286.48	-284.05	-280.86	-252.22
CH_3CHOO + *Anti*-EtCHOO Con 2	-256.77	-257.68	-257.19	-261.09
POZ1.1	-264.29	-246.06	-251.63	-194.26
TS_{SYN} 2.1	-182.80	-173.62	-178.37	-122.27
C_{SYN} 1.1	-297.33	-294.89	-292.58	-258.83
syn-CH_3CHOO + EtCHO Con 2	-270.87	-272.02	-272.00	-274.67
POZ1.2	-262.27	-244.11	-249.57	-192.52
TS_{SYN} 2.2	-172.06	-162.66	-167.40	-111.46
C_{SYN} 1.1	-290.57	-287.53	-284.47	-257.44
syn-CH_3CHOO + EtCHO Con 1	-268.53	-267.98	-268.19	-270.19
POZ1.3	-262.27	-244.11	-249.57	-192.52
TS_{SYN} 2.3	-183.74	-174.22	-178.92	-122.98
C_{SYN} 2.3	-300.51	-296.49	-294.34	-260.19
syn-CH_3CHOO + EtCHO Con 2	-268.53	-267.98	-268.19	-270.19
POZ2.1	-264.29	-246.06	-251.63	-194.26
TS_{Anti} 2.1	-174.25	-165.26	-169.77	-114.76
C_{anti} 2.1	-288.01	-285.05	-282.64	-249.26
Anti-CH_3CHOO + EtCHOO Con 2	-256.33	-257.17	-256.78	-260.98
POZ2.2	-262.27	-244.11	-249.57	-192.52
TS_{Anti} 2.2	-181.69	-172.47	-176.99	-121.89
C_{anti} 2.2	-288.43	-286.18	-283.60	-252.55
Anti-CH_3CHOO + EtCHOO Con 1	-260.26	-261.28	-261.11	-264.17
POZ2.3	-262.27	-244.11	-249.57	-192.52
TS_{Anti} 2.3	-181.95	-172.83	-177.26	-122.54
C_{anti} 2.3	-293.82	-289.22	-287.71	-251.74
Anti-CH_3CHOO + EtCHOO Con 2	-256.33	-257.17	-256.78	-260.98
POZ2.1	-264.53	-246.43	-251.97	-194.80
TS_{SYN} 1.1	-183.55	-174.44	-179.09	-123.53
C_{SYN} 1.1	-297.35	-294.56	-291.99	-261.11
CH_3CHOO + *syn*-EtCHO Con 2	-271.18	-271.19	-271.47	-274.67
POZ2.2	-262.12	-244.07	-249.49	-192.84
TS_{SYN} 1.2	-181.45	-171.69	-176.56	-120.22
C_{SYN} 1.2	-298.66	-296.45	-293.90	-264.20
CH_3CHOO + *syn*-EtCHO Con 1	-275.11	-275.30	-275.81	-277.86
POZ2.3	-265.08	-247.24	-252.67	-195.93
TS_{SYN} 1.3	-184.57	-175.23	-179.92	-124.15
C_{SYN} 1.3	-300.36	-297.11	-294.89	-261.99
CH_3CHOO + *syn*-EtCHO Con 2	-271.18	-271.19	-271.47	-274.67

*Table S35: Relative Energies of O_3 + Alkene **16** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 16			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
Z-EtCHCHCH$_3$ con 1 + O_3	0.00	0.00	0.00	0.00
Z-EtCHCHCH$_3$ con 2 + O_3	15.00	15.85	15.59	16.46
PRC1.1	-11.83	-8.60	-6.70	26.26
TSOzo1.1	-1.34	3.71	1.62	49.57
POZ1.1	-260.48	-242.5	-247.92	-190.5
PRC1.2	-13.46	-11.32	-8.89	21.44
TSOzo1.2	11.88	16.94	14.97	62.29
POZ1.2	-257.04	-239.32	-244.63	-186.90
PRC1.3	-13.46	-11.32	-8.89	21.44
TSOzo1.3	-3.22	0.57	-1.25	46.58
POZ1.3	-264.13	-246.36	-251.75	-194.58
PRC2.1	-16.09	-13.78	-11.35	19.34
TSOzo2.1	6.52	11.87	9.54	58.31
POZ2.1	-258.23	-240.58	-246.08	-188.18
PRC2.2	-16.09	-13.78	-11.35	19.34
TSOzo2.2	15.53	21.77	18.92	70.53
POZ2.2	-252.06	-234.07	-239.71	-181.18
PRC2.3	-16.58	-13.99	-11.48	16.53
TSOzo2.3	1.23	5.55	3.26	52.70
POZ2.3	-262.42	-244.92	-250.46	-192.94
POZ1.1	-260.48	-242.46	-247.92	-190.47
TS_{Anti} 1.1	-186.65	-177.9	-182.50	-125.5
C_{anti} 1.1	-289.58	-287.94	-285.23	-253.06
CH_3CHOO + *Anti*-EtCHOO Con 2	-261.45	-263.04	-262.51	-265.35
POZ1.2	-257.04	-239.32	-244.63	-186.90
TS_{Anti} 1.2	-181.46	-171.84	-176.74	-118.88
C_{anti} 1.2	-295.09	-293.06	-290.84	-254.98
CH_3CHOO + *Anti*-EtCHOO Con 1	-263.26	-265.12	-264.75	-266.67
POZ1.3	-264.13	-246.36	-251.75	-194.58
TS_{Anti} 1.3	-187.87	-179.02	-183.54	-127.14
C_{anti} 1.3	-292.36	-290.06	-287.68	-252.80
CH_3CHOO + *Anti*-EtCHOO Con 2	-261.45	-263.04	-262.51	-265.35
POZ2.1				
TS_{Anti} 2.1	-260.48	-242.46	-247.92	-190.47
C_{anti} 2.1	-182.06	-173.41	-178.00	-121.30
Anti-CH_3CHOO + EtCHOO Con 2	-298.86	-294.53	-293.24	-254.64
	-261.00	-262.53	-262.09	-265.23
POZ2.2				
TS_{Anti} 2.2	-257.04	-239.32	-244.63	-186.90
C_{anti} 2.2	-186.99	-177.86	-182.57	-125.68
Anti-CH_3CHOO + EtCHOO Con 1	-303.28	-299.46	-298.23	-258.47
	-264.94	-266.64	-266.42	-268.42
POZ2.3				
TS_{Anti} 2.3	-264.13	-246.36	-251.75	-194.58
C_{anti} 2.3	-188.49	-179.58	-184.20	-127.56
Anti-CH_3CHOO + EtCHOO Con 2	-298.50	-294.58	-293.02	-256.00
	-261.00	-262.53	-262.09	-265.23
POZ2.1				
TS_{SYN} 1.1	-258.23	-240.58	-246.08	-188.18
C_{SYN} 1.1	-174.21	-164.50	-169.54	-111.34
CH_3CHO + *syn*-EtCHOO Con 2	-296.40	-294.82	-292.33	-259.12
	-275.54	-277.38	-277.31	-278.93

POZ2.2				
TS_{SYN} 1.2	-252.06	-234.07	-239.71	-181.18
C_{SYN} 1.2	-161.66	-151.87	-156.96	-98.21
CH_3CHO + *syn*-EtCHOO Con 1	-295.24	-292.89	-289.78	-261.70
	-273.20	-273.34	-273.50	-274.44
POZ2.3				
TS_{SYN} 1.3	-262.42	-244.92	-250.46	-192.94
C_{SYN} 1.3	-177.70	-167.78	-172.70	-115.02
CH_3CHO + *syn*-EtCHOO Con 2	-292.52	-289.91	-287.06	-258.15
	-273.20	-273.34	-273.50	-274.44
POZ2.1				
TS_{SYN} 2.1	-258.23	-240.58	-246.08	-188.18
C_{SYN} 1.1	-178.17	-168.70	-173.64	-115.56
syn-CH_3CHOO + EtCHO Con 2	-306.12	-303.78	-301.69	-266.10
	-275.85	-276.55	-276.79	-278.93
POZ2.2				
TS_{SYN} 2.2	-252.06	-234.07	-239.71	-181.18
C_{SYN} 1.1	-171.49	-161.85	-166.69	-109.03
syn-CH_3CHOO + EtCHO Con 1	-308.42	-305.95	-303.95	-268.37
	-279.79	-280.66	-281.12	-282.12
POZ2.3				
TS_{SYN} 2.3	-262.42	-244.92	-250.46	-192.94
C_{SYN} 2.3	-178.51	-169.13	-173.92	-116.44
syn-CH_3CHOO + EtCHO Con 2	-305.23	-302.50	-300.39	-265.57

*Table S36: Relative Energies of O_3 + Alkene **17** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-26.22	-22.45	-21.34	16.40
TSOzo1	1.80	6.81	4.40	52.30
POZ1	-264.18	-245.81	-251.55	-195.30
POZ1	-264.18	-245.81	-251.55	-195.30
TS_{Anti} 1	-180.38	-170.94	-175.64	-121.33
C_{ANTI} 1	-288.19	-285.95	-283.02	-253.55
CH_3CHO + *Anti*-CH_3CHOO	-258.06	-259.47	-258.96	-262.48
POZ1	-264.18	-245.81	-251.55	-195.30
TS_{Syn} 1	-183.17	-173.65	-178.57	-123.19
C_{SYN} 1	-298.71	-296.17	-293.89	-261.60
CH_3CHO + *syn*-CH_3CHOO	-272.91	-273.49	-273.65	-276.18

*Table S37: Relative Energies of O_3 + Alkene **18** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-11.79	-8.50	-6.75	26.44
TSOzo1	-1.40	3.05	1.13	47.67
POZ1	-263.59	-245.13	-250.94	-194.21
PRC1	-17.61	-15.00	-12.59	14.73
TSOzo1	5.96	10.93	8.54	56.50
POZ1	-261.12	-242.86	-248.83	-191.86
PRC2	-263.59	-245.13	-250.94	-194.21
TSOzo2	-254.01	-237.46	-244.64	-183.50
POZ2	-261.12	-242.86	-248.83	-191.86
POZ1	-263.59	-245.13	-250.94	-194.21
TS_{Anti} 1	-187.21	-178.13	-183.01	-126.86
C_{ANTI} 1	-294.48	-292.19	-290.18	-254.43
CH_3CHO + *Anti*-CH_3CHOO	-262.58	-264.51	-264.04	-266.41
POZ1	-261.12	-242.86	-248.83	-191.86
TS_{Syn} 1	-177.65	-167.59	-172.83	-115.70
C_{SYN} 1	-307.47	-304.77	-302.95	-267.08
CH_3CHO + *syn*-CH_3CHOO	-277.44	-278.52	-278.74	-280.11

*Table S38: Relative Energies of O_3 + Alkene **19** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 19			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-19.59	-16.8	-14.60	15.70
TSOzo1	7.09	12.3	9.91	58.44
POZ1	-258.76	-241.1	-246.53	-189.89
POZ1	-258.76	-241.1	-246.53	-189.89
TS_{Anti} 1	-181.66	-172.8	-177.24	-121.97
C_{ANTI} 1	-296.33	-293.1	-291.46	-252.61
CH_3CHO + *Anti*-CH_3CHOO	-262.49	-275.6	-275.50	-274.23
POZ1	-258.76	-241.1	-246.53	-189.89
TS_{Syn} 1	-167.63	-158.4	-162.78	-108.02
C_{SYN} 1	-279.14	-275.9	-274.27	-235.42
CH_3CHO + *syn*-CH_3CHOO	-253.52	-254.7	-253.43	-261.33

S3.2 Epoxide Results

The Relative Energies, Enthalpies and Gibbs Free Energies in this section is based on the B3LYP molecular energy calculations, used only for epoxide pathway calculations.

*Table S39: Relative Energies of O_3 + Alkene **1** using B3LYP molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-7.07	-3.29	-2.02	32.99
TSOzo1	-2.21	3.93	0.85	49.31
POZ1	-237.29	-217.98	-223.63	-169.17
PRC2	-6.03	-2.58	-0.97	32.00
TSOzo2	1.68	7.77	4.73	52.94
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TSpoz1	-223.55	-206.06	-213.23	-154.93
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TSpoz2	-225.79	-208.17	-215.21	-157.25
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TS_{Anti} 1	-164.54	-155.00	-159.69	-106.63
C_{ANTI}	-282.66	-275.72	-276.11	-233.95
HCHO + Anti-RCHOO	-247.32	-250.46	-248.95	-249.43
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{FO} 1	-156.79	-147.01	-151.90	-98.43
$C_{FO\ 1}$	-272.72	-269.07	-267.47	-232.68
RCHO + HCHOO	-250.66	-251.58	-251.23	-253.94
POZ2	-236.89	-217.58	-223.23	-168.78
TS_{FO} 2	-154.23	-144.24	-149.08	-96.08
C_{FO} 2	-267.39	-265.18	-262.23	-236.23
POZ2	-236.89	-217.68	-223.51	-168.32
TS_{Syn}	-158.67	-148.57	-153.60	-99.51
C_{SYN}	-281.04	-277.22	-276.08	-237.95
HCHO + Syn-RCHOO	-259.26	-261.57	-260.74	-260.21
PRC1	-7.07	-3.29	-2.02	32.99
TS_{epox} 1.1	46.88	49.99	47.30	94.73
C_{epox} 1.1	-135.72	-126.87	-127.08	-87.21
PRC2	-6.03	-2.58	-0.97	32.00
TS_{epox} 1.2	38.74	42.62	39.06	89.37
C_{epox} 1.2	-132.96	-124.19	-124.22	-84.92
O2 + epoxide	-126.58	-120.8	-121.53	-113.48
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{epox} 2_1	64.20	68.04	64.86	114.97
C_{epox} 1.1	-135.72	-126.87	-127.08	-87.21
POZ2	-236.89	-217.68	-223.51	-168.32
TS_{epox} 2_2	70.90	74.06	71.13	120.52
C_{epox} 1.2	-132.96	-124.19	-124.22	-84.92
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{epox} 2_3	45.43	48.86	46.12	94.74
C_{epox} 2.3	-135.49	-126.59	-126.75	-87.12
POZ2	-236.89	-217.68	-223.51	-168.32
TS_{epox} 2_4	57.32	59.78	57.08	104.88
C_{epox} 2.4	-132.34	-124.55	-123.49	-91.75

*Table S40: Relative Energies of O_3 + Alkene **5** using B3LYP molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1.1	-2.76	-0.45	2.21	30.48
TSOzo1.1	5.56	10.86	8.10	57.61
POZ1.1	-202.73	-186.54	-191.05	-138.56
PRC1.2	-1.11	1.09	3.42	34.89
TSOzo1.2	7.85	13.52	10.59	60.76
POZ1.2	-219.24	-202.70	-207.45	-154.15
PRC2.1	-2.15	-0.47	2.88	24.44
TSOzo2.1	0.27	5.79	2.99	52.88
POZ2.1	-205.35	-189.12	-193.77	-140.23
PRC2.2	-4.42	-1.67	0.31	33.98
TSOzo2.2	9.21	14.78	11.91	62.17
POZ2.2	-221.62	-204.94	-209.83	-156.13
POZ1.1	-202.73	-186.54	-191.05	-138.56
TS_{Anti} 1	-130.81	-123.57	-127.23	-75.46
C_{anti} 1	-238.71	-235.23	-234.05	-194.35
HCHO + Anti-RCHOO Con 2	-212.89	-216.96	-215.18	-215.90
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{Anti} 2	-142.25	-134.52	-138.36	-85.65
C_{anti} 2	-240.93	-240.43	-237.09	-204.96
HCHO + Anti-RCHOO Con1	-228.11	-231.59	-229.99	-230.26
POZ1.1	-202.73	-186.54	-191.05	-138.56
TS_{FO} 1.1	-133.13	-125.81	-129.52	-77.60
C_{FO} 1.1	-220.00	-219.91	-216.05	-193.63
HCHOO + RCHO con 1	-201.98	-204.49	-203.69	-208.80
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{FO} 1.2	-156.17	-148.24	-152.12	-99.55
C_{FO} 1.2	-250.85	-246.76	-245.57	-205.85
HCHOO + RCHO con 2	-223.20	-224.72	-224.15	-227.92
POZ2.1	-205.35	-189.12	-193.77	-140.23
TS_{FO} 2.1	-141.03	-133.81	-137.57	-85.33
C_{FO} 2.1	-244.38	-238.74	-238.61	-194.47
HCHOO + RCHO con 1	-201.98	-204.49	-203.69	-208.80
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{FO} 2.2	-156.06	-148.20	-152.06	-99.08
C_{FO} 2.2	-251.90	-247.03	-246.40	-204.39
HCHOO + RCHO con 2	-223.20	-224.72	-224.15	-227.92
POZ2.1	-205.35	-189.12	-193.77	-140.23
TS_{Syn} 1	-116.44	-110.02	-113.45	-62.02
C_{syn} 1	-206.38	-207.81	-202.86	-184.48
HCHO + Syn-RCHOO Con2	-192.37	-196.41	-194.68	-196.10
C_{syn} 1	-222.13	-216.96	-216.92	-173.31
HOZ2.1	-411.77	-391.87	-396.88	-342.58
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{Syn} 2	-135.75	-127.82	-132.05	-78.81
C_{syn} 2	-230.25	-230.04	-226.55	-196.23
HCHO + Syn-RCHOO Con1	-217.59	-220.53	-219.50	-218.81

PRC2.1	-2.15	-0.47	2.88	24.44
TS_{epox} 1.1	52.36	56.03	53.49	101.94
C_{epox} 2_5	-120.48	-114.34	-113.07	-77.69
PRC2.2	-4.42	-1.67	0.31	33.98
TS_{epox} 1.2	47.33	50.72	48.40	96.02
C_{epox} 2_6	-115.05	-108.63	-107.72	-70.34
PRC1.1	-2.76	-0.45	2.21	30.48
TS_{epox} 1.3	52.21	56.28	53.35	103.76
C_{epox} 1_3	-119.48	-114.13	-111.75	-85.53
PRC1.2	-1.11	1.09	3.42	34.89
TS_{epox} 1.4	42.96	47.19	44.31	94.52
C_{epox} 1_4	-113.42	-107.94	-105.80	-75.35
O2 + epoxide	-108.76	-104.92	-104.94	-98.05
O2 + epoxide	-116.19	-112.09	-112.22	-104.58
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_1	56.53	60.34	57.76	106.46
C_{epox} 2_1	-114.50	-108.78	-106.88	-77.22
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_2	64.75	67.88	65.60	113.87
C_{epox} 2_2	-120.92	-115.21	-113.23	-83.94
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_3	66.20	69.71	67.08	116.94
C_{epox} 1_3	-119.48	-114.13	-111.75	-85.53
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_5	81.58	81.95	80.22	127.14
C_{epox} 2_5	-120.48	-114.34	-113.07	-77.69
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_7	104.81	105.51	103.12	153.07
C_{epox} 2_7	-118.72	-113.57	-110.94	-86.75
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_8	76.04	76.45	74.43	123.74
C_{epox} 2_2	-120.92	-115.21	-113.23	-83.94

*Table S41: Relative Energies of O_3 + Alkene **1** epoxide pathways using DF-LCCSD-F12a molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-18.43	-14.65	-13.38	21.63
TS_{epox} 1.1	47.41	50.52	47.83	95.26
C_{epox} 1.1	-162.46	-153.61	-153.82	-113.95
PRC2	-18.27	-14.82	-13.21	19.76
TS_{epox} 1.2	39.25	43.21	39.64	89.99
C_{epox} 1.2	-165.37	-156.60	-156.63	-117.32
O2 + epoxide	-157.37	-151.64	-152.33	-144.28
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{epox} 2_1	98.09	101.93	98.76	148.86
C_{epox} 1.1	-162.46	-153.61	-153.82	-113.95
POZ2	-254.91	-235.70	-241.53	-186.34
TS_{epox} 2_2	106.67	109.82	106.89	156.28
C_{epox} 1.2	-165.37	-156.60	-156.63	-117.32
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{epox} 2_3	91.11	94.54	91.80	140.42
C_{epox} 2.3	-162.57	-153.67	-153.83	-114.21
POZ2	-254.91	-235.70	-241.53	-186.34
TS_{epox} 2_4	98.78	101.24	98.54	146.34
C_{epox} 2.4	-165.37	-157.58	-156.52	-124.77

*Table S42: Relative Energies of O_3 + Alkene **5** epoxide pathways using DF-LCCSD-F12a molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC2.1	-10.64	-8.96	-5.61	15.95
TS_{epox} 1.1	59.08	62.74	60.20	108.65
C_{epox} 2_5	-151.60	-145.46	-144.19	-108.81
PRC2.2	-18.75	-16.01	-14.02	19.65
TS_{epox} 1.2	59.17	62.56	60.23	107.86
C_{epox} 2_6	-143.07	-136.65	-135.74	-98.36
PRC1.1	-15.65	-13.35	-10.69	17.58
TS_{epox} 1.3	55.07	59.14	56.21	106.62
C_{epox} 1_3	-155.22	-149.87	-147.49	-121.28
PRC1.2	-14.31	-12.10	-9.77	21.70
TS_{epox} 1.4	49.34	53.57	50.68	100.89
C_{epox} 1_4	-148.10	-142.62	-140.48	-110.03
O2 + epoxide	-138.13	-134.29	-134.31	-127.42
O2 + epoxide	-146.69	-142.58	-142.72	-135.08
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_1	-70.49	-66.68	-69.26	-20.56
C_{epox} 2_1	-144.26	-138.54	-136.64	-106.98
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_2	-156.24	-153.10	-155.38	-107.11
C_{epox} 2_2	-153.63	-147.92	-145.94	-116.65
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_3	-155.67	-152.17	-154.80	-104.93
C_{epox} 1_3	-155.22	-149.87	-147.49	-121.28
POZ2.1	-224.38	-208.15	-212.79	-159.25
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_5	103.04	103.41	101.68	148.59
C_{epox} 2_5	-151.60	-145.46	-144.19	-108.81
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_7	129.22	129.91	127.52	177.47
C_{epox} 2_7	-154.30	-149.15	-146.52	-122.33
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_8	90.83	91.25	89.23	138.54
C_{epox} 2_2	-153.63	-147.92	-145.94	-116.65

S4 Previous Literature Experimental Data

The literature data found in Table 2-4 in the main manuscript found in greater detail in this supporting information section. Tables S43-S45 contains the rate constants and OH yields for these alkene ozonolysis reactions are found here:

*Table S43: Literature Rate Constants (k_{EXP}) and OH yields of the Ozonolysis of Alkenes **1**, 2, **5**, **6** & **19**.*

Alkene	k_{EXP} (~298K) (10^{-18} cm^3 s^{-1})	ref	OH yield	ref
Propene	10.1 ± 2.5	3	0.33 ± 0.16	4
$CH_3CH=CH_2$	9.9	5	0.18 ± 0.04	6,7
(Alkene **1**)	11.1	8	0.30 ± 0.08	9
	10.0	10	0.39 ± 0.08	11
	9.6 ± 0.4	12	0.34 ± 0.03	13
	11.5 ± 1.1	14	0.33 ± 0.04	15
	10.6 ± 1.2	9		
Average	*10.4*		*0.34*	
Range	*9.6 - 11.5*	3,5,12,16–19	*0.30 - 0.39*	4,6,7,9,11,13
Range (± included)	*7.6 - 12.6*		*0.17 - 0.49*	
1-Butene	9.65 ± 2.5	3	0.41 ± 0.20	4
$CH_3CH_2CH=CH_2$	9.7 ± 1.9	20	0.30 ± 0.09	9
(Alkene **2**)	10.9 ± 0.8	5	0.29 ± 0.05	21
	8.8 ± 0.6	12	0.23 ± 0.04	15
	11.0 ± 3.3	17	-	
	12.4 ± 3.8	14	-	
Average	*10.4*		*0.31*	
Range	*8.8 - 12.4*	3–6,12	*0.23 - 0.41*	4,9,21
Range (± included)	*7.2 - 16.2*		*0.19 - 0.61*	
Methyl Vinyl Ketone	5.84 ± 0.39	22	0.13 ± 0.04	23
$CH_3C(O)CH=CH_2$	4.72 ± 0.09	24	0.16 ± 0.08	25
(Alkene **5**)	4.22 ± 0.85	12	0.16 ± 0.05	26
	4.77 ± 0.57	27	-	-
	4.5 ± 0.1	23	-	-
	5.1 ± 0.1	23	-	-
Average	*4.86*		*0.15*	
Range	*4.22 -5.84*	3,5,28	*0.13 - 0.16*	23,25,26
Range (± included)	*3.37 -6.23*		*0.08 - 0.24*	
2-methyl-2-butene	403 ± 141	3	0.98 ± 0.24	29
$CH_3CH=C(CH_3)_2$	410 ± 50	30	0.89 ± 0.37	4
(Alkene **6**)	410	31	0.93 ± 0.14	32
	396 ± 139	33	0.81 ± 0.16	34
	-	-	0.89 ± 0.22	35
	-	-	0.47 ± 0.04	30
Average	405		0.90	
Range	396 - 410	3,5,12,16–19	0.81 - 0.98	4,29,32,34,35
Range (± included)	257 - 544		0.52 - 1.26	
2-methylpropene	11.3 ± 3.0	3	0.84 ± 0.42	4
$(CH_3)_2C=CH_2$	11.1 ± 2.8	20	0.80 ± 0.10	9
(Alkene **19**)	10.8 ± 1.0	5	0.72 ± 0.12	21
	12.9	28	0.60 ± 0.06	13
Average	*11.5*	3,5,28	*0.74*	4,9,13,21
Range	*10.8 - 12.9*		*0.6 - 0.84*	
Range (± included)	*8.3 - 14.3*		*0.42 - 1.26*	

*Table S44: Literature Rate Constants (k_{EXP}) and OH yields of the Ozonolysis of Alkenes **17**, **18**, **15** & **16**.*

Alkene	k_{EXP} (10^{16} cm^3 s^{-1})	ref	OH yield	ref
***E*-2-butene**	1.90 ± 0.67	3	0.64 ± 0.12	29
(Alkene **17**)	1.82 ± 0.011	5	0.64 ± 0.26	4
	2.17	16	0.24 ± 0.02	6,7
	1.81 ± 0.006	12	0.54 ± 0.11	34
	2.00 ± 0.80	17	0.19	19
	1.98	14	0.68 ± 0.09	18
	-	-	0.60 ± 0.12	9
	-	-	0.75 ± 0.19	35
	-	-	0.52 ± 0.04	36
Average	1.94	3,5,12,16–19	0.58 (0.53)	18,19
Range	1.81 – 2.17		0.52 – 0.75 (0.19 – 0.75)	
Range (± included)	1.20 – 2.80		0.43 – 0.94 (0.19 – 0.94)	
***Z*-2-butene**	1.25 ± 0.31	3	0.33 ± 0.05	29
(Alkene **18**)	1.27	5	0.41 ± 0.17	4
	1.23 ± 0.18	12	0.17 ± 0.02	6,7
	1.30 ± 0.39	17	0.33 ± 0.07	34
	1.19 (± 0.12)	14	0.39	37
	-	-	0.40	19
	-	-	0.40 ± 0.05	9
Average	1.26	3–6,12	0.38 (0.35)	3–6,12,17
Range	1.23 – 1.30		0.33 – 0.41 (0.17 – 0.41)	
Range (± included)	0.91 – 1.69		0.24 – 0.58 (0.15 – 0.58)	
***E*-2-pentene**	3.15 ± 0.95	3	0.46 ± 0.08	29
(Alkene **15**)	1.62 ± 0.06	5	-	-
	3.15	28	-	-
Average	2.39	3,5,28	0.46	29
Range	1.62 – 3.15		0.46	
Range (± included)	1.62 – 4.10		0.38 – 0.54	
***Z*-2-pentene**	3.15 ± 0.95	3	0.27 ± 0.07	29
(Alkene **16**)	1.32 ± 0.04	5	0.29 ± 0.06	29
	2.09	28	-	-
Average	1.71	3,5,28	0.28	29
Range	1.32 – 2.09		0.27 – 0.29	
Range (± included)	0.94 – 2.09		0.20 – 0.35	

*Table S45: Literature Experimental Rate Constants (k_{EXP}) range of the Ozonolysis of Alkenes **3**, **4**, **7**, **8**, **9**, **10**, **11**, **12**, **13** & **14**.*

Alkene	Alkene No	k_{EXP} (10^{-18} cm^3 s^{-1})	ref
3-methyl-1-butene	**3**	0.95 ± 0.29	3
$(CH_3)_2CHCH=CH_2$		0.73 ± 0.27	20
Average		*0.84*	3,5,28
Range		*0.73 - 0.95*	
Range (± included)		*0.46 - 1.24*	
3,3-dimethyl-1-butene	**4**	0.39 ± 0.12	3
$(CH_3)_3CCH=CH_2$		0.38 ± 0.08	20
Average		*0.385*	3,5,28
Range		*0.38 - 0.39*	
Range (± included)		*0.27 - 0.51*	
2-methyl-2-pentene	**7**	0.39 ± 0.12	3
$CH_3CH_2CH=C(CH_3)_2$		0.38 ± 0.08	2
Average		*0.385*	3,5,28
Range		*0.38 - 0.39*	
Range (± included)		*0.27 - 0.51*	
2,4-dimethyl-2-pentene $[(CH_3)_2CHCH=C(CH_3)_2]$	**8**	*223* *	1
2,4,4-trimethyl-2-pentene	**9**	1.39 ± 0.42	3
$(CH_3)_3CCH=C(CH_3)_2$		1.25 ± 0.10	28,38
Average		*1.32*	3,5,28
Range		*1.25 - 1.39*	
Range (± included)		*0.97 - 1.81*	
Mesityl Oxide $(CH_3C(O)CH=C(CH_3)_2)$	**10**	0.081 ± 0.011	39
2,3,3,3-tetrafluoro-1-propene $(CF_3CF=CH_2)$	**11**	$(2.77 \pm 0.21) \times 10^{-3}$	40
3,3,4,4,4-pentafluoro-1-butene	**12**	0.211 ± 0.035	41
$CF_3CF_2CH=CH_2$		0.20 ± 0.04	42
Average		0.21	41
Range		0.20 - 0.21	
Range (± included)		0.16 - 0.25	
***E*-1-chloro-3,3,3-trifluoro-1-propene** (*E*-$CF_3CH=CHCl$)	**13**	$(1.46 \pm 0.12) \times 10^{-3}$	43
***E*-1,3,3,3-tetrafluoro-1-propene** (*E*-$CF_3CH=CHF$)	**14**	$(2.81 \pm 0.21) \times 10^{-3}$	44

The product branching fraction literature averages and ranges are in the following table:

*Table S46: The literature experimental product branching fractions of the Ozonolysis of Alkenes **1**, **2**, **3**, **4**, **5**, **6**, **8**, **9**, **12**, **13** & **19**.*

Alkene + O_3	R_1		Product Branching Ratio (Γ_{EXP})		Ref
		#	R_1CHOO+HCHO	R_1CHO+HCHOO	
Propene *	CH_3	**1**	0.60	0.40	[45]
Range			0.517 – 0.643	0.357 – 0.483	[45–47]
1-butene	Et	**2**	0.64 ± 0.04	0.36 ± 0.04	[45]
3-methyl-1-butene	iPr	**3**	0.49 ± 0.05	0.51 ± 0.05	[45]
3,3-dimethyl-1-butene	tBu	**4**	0.32 ± 0.01	0.68 ± 0.01	[45]
methyl vinyl ketone *	$CH_3C(O)$	**5**	0.22 ± 0.17	0.78 ± 0.17	[23,25]
3,3,4,4,4-pentafluoro-1-butene	CF_3CF_2-	**12**	0.739 ± 0.017	0.261 ± 0.017	[41]
Alkene + O_3		**#**	**R_1CHOO+$(CH_3)_2CO$**	**R_1CHO+$(CH_3)_2COO$**	**Ref**
2-methyl-2-butene *	CH_3	**6**	0.321	0.679	[45–47]
			0.289 – 0.387	0.613 – 0.711	[45–47]
2,4-dimethyl-2-pentene	iPr	**8**	0.82 ± 0.04	0.18 ± 0.04	[45]
2,4,4-dimethyl-2-pentene	tBu	**9**	0.82 ± 0.05	0.18 ± 0.05	[45]
	R_1	**#**	**CF_3CHOO+ClCHO**	**CF_3CHO+ClCHOO**	
***E*-1-chloro-3,3,3-trifluoro-1-propene**	CF_3	**13**	0.63 ± 0.09	0.33 ± 0.03	[48]
	R_1	**#**	**EtCHOO+CH_3CHO**	**CH_3CHOO+EtCHO**	
***E*-2-pentene**	Et	**15**	0.59 ± 0.01	0.54 ± 0.01	[49]
***Z*-2-pentene**	Et	**16**	0.68 ± 0.01	0.52 ± 0.04	[49]
			$(CH_3)_2COO$ + HCHO	**HCHOO+$(CH_3)_2CO$**	
2-methylpropene *	$(CH_3)_2C$	**19**	0.70	0.30	[46,50–54]
Range			0.53 – 0.77	0.23 – 0.47	

S5 Reactant Atmospheric Abundance

The abundance and boiling points of the different atmospheric alkenes in analysed in this study are found in the following tables

*Table S47: Atmospheric concentrations of Alkenes **1-19** (if known) under various conditions.*

Co-reactant Environment	Abundance (Original units)	Study	Ref
Ozone (O_3)			
summertime conditions - Houston	40–60 ppbv	Ryerson *et al.*	55
Can exceed	200 ppbv	Ryerson *et al.*	55
O_3 – Boreal Forest	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	56
O_3 – Tropical Forest/Rainforest	7.3×10^{11} cm^3 s^{-1}	Vereecken *et al.*	56
O_3 – Mega city	1.9×10^{12} cm^3 s^{-1}	Vereecken *et al.*	56
O_3 – Rural Europe	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	56
Propene (Alkene 1) [General Average]			
– Mega city	1.1×10^{11} cm^3 s^{-1}	Vereecken *et al.*	57
– Rural Europe	1.5×10^{9} cm^3 s^{-1}	Vereecken *et al.*	57
High ponderosapine forest	176 ppt	Rhew *et al.*	58
Low ponderosapine forest	182 ppt	Rhew *et al.*	58
Taipei Urban - Summer Daytime	0.56 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.81 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.53 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.53 ppbv	Wang *et al.*	59
Mexico City - Urban	5.93 ppb	Percival *et al.*	60
Mexico City - Industrial	10.96 ppb	Percival *et al.*	60
Chinese Max	8.2 ppb	Percival *et al.*	60
Karthmandu, Nepal	12.8 ppb	Percival *et al.*	60
Porto Alegre, Brazil	28.3 ppb	Percival *et al.*	60
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(4.7 \pm 3.7) \times 10^{8}$	Novelli *et al.*	61
1-Butene (Alkene 2) [General Average]			
– Mega city	5.7×10^{10} cm^3 s^{-1}	Vereecken *et al.*	57
– Rural Europe	5.7×10^{8} cm^3 s^{-1}	Vereecken *et al.*	57
Taipei Urban - Summer Daytime	0.14 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.18 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.12 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.13 ppbv	Wang *et al.*	59
Taipei, Taiwan	0.90 ppb	Percival *et al.*	60
Chinese Max	2.4 ppb	Percival *et al.*	60
Karachi	1.1 ppb	Percival *et al.*	60
Dallas	0.32 ppb	Percival *et al.*	60
Porto Alegre	7.8 ppb	Percival *et al.*	60
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(1.4 \pm 4.2) \times 10^{8}$	Novelli *et al.*	61
Butene (unknown)			
High ponderosapine forest	52 ppt	Rhew *et al.*	58
Low ponderosapine forest	51 ppt	Rhew *et al.*	58
3-methyl-1-butene (Alkene 3) [General Average]			
Taipei Urban - Summer Daytime	0.03 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.04 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.02 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.02 ppbv	Wang *et al.*	59
C5	0.030 ppb	Percival *et al.*	60
3,3-dimethyl-1-butene (Alkene 4) [General Average]			
c6 alkenes	0.052	Percival *et al.*	60
Methyl vinyl ketone (Alkene 5) [General Average]			

Rainforest		2.4×10^{10} cm^3 s^{-1}	Vereecken *et al.*	57
Temperate Forest		2.5×10^{9} cm^3 s^{-1}	Vereecken *et al.*	57
Borneo		0.45 ppb	Percival *et al.*	60
2-methyl-2-butene (Alkene 6) [General Average]				
Taipei Urban - Summer Daytime		0.13 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time		0.21 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime		0.12 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time		0.12 ppbv	Wang *et al.*	59
Mexico City- Urban		1.69 ppbv	Percival *et al.*	60
Mexico City- Industrial		0.89 ppbv	Percival *et al.*	60
Porto Alegre Brazil		17 ppbv	Percival *et al.*	60
Seoul		1 ppbv	Percival *et al.*	60
2-methyl-2-pentene (Alkene 7) [General Average]				
Porto Alegre Brazil		4 ppbv	Percival *et al.*	60
Porto Alegre Brazil		0.017 ppbv	Percival *et al.*	60
Boston		17 ppbv	Percival *et al.*	60
C-6 alkene - Boston		0.052 ppbv	Percival *et al.*	60
2,4-dimethyl-2-pentene (Alkene 8) [General Average]				
C-7 alkene - Boston		0.007 ppbv	Percival *et al.*	60
C-7 alkene - Boston		0.003 ppbv	Percival *et al.*	60
2,4,4-trimethyl-2-pentene (Alkene 9) [General Average]				
C 8 alkene - Boston		0.019 ppbv	Percival *et al.*	60
C 8 alkene - Boston		0.004 ppbv	Percival *et al.*	60
2,3,3,3-tetrafluoro-1-propene (Alkene 11) [General Average] HFO-1234yf				
Jungfraujoch, Switzerland		3 ppq	Vollmer *et al.*	62
Dubendorf, Switzerland		136 ppq	Vollmer *et al.*	62
Global future scenario - annual	Average	0.34 pptv	Wang *et al.*	63
	Maximum	30.96 pptv	Wang *et al.*	63
China future scenario- annual	Average	2.62 pptv	Wang *et al.*	63
	Maximum	30.96 pptv	Wang *et al.*	63
USA future scenario - annual	Average	2.20 pptv	Wang *et al.*	63
	Maximum	19.44 pptv	Wang *et al.*	63
USA future scenario - summer	Average	4.19 pptv	Wang *et al.*	63
	Maximum	40.95 pptv	Wang *et al.*	63
USA future scenario - summer	Average	7.40 pptv	Luecken *et al.*	63,64
	Maximum	300.00 pptv	Luecken *et al.*	63,64
EU future scenario - annual	Average	2.73 pptv	Wang *et al.*	63
	Maximum	19.08 pptv	Wang *et al.*	63
EU future *STOCHEM* scenario - annual	Average	2.60 pptv	Henne *et al.*	63,65
	Maximum	18.00 pptv	Henne *et al.*	63,65
EU future *FLEXPART* scenario - annual	Average	1.50 pptv	Henne *et al.*	63,65
	Maximum	3.70 pptv	Henne *et al.*	63,65
North pole future scenario - annual	Average	0.40 pptv	Wang *et al.*	63
	Maximum	1.19 pptv	Wang *et al.*	63
(*E*)-1-chloro-3,3,3-trifluoro-1-propene (Alkene 13) [General Average] (HCFO-1233zd(E))				
Jungfraujoch, Switzerland		8 ppqv	Vollmer *et al.*	62
Dubendorf, Switzerland		12 ppqv	Vollmer *et al.*	62
Beijing, China		~20 ppqv	Sulbaek Andersen *et al.*	66
(*E*)-1,3,3,3-tetrafluoro-1-propene (Alkene 14) [General Average] (HFO-1234ze(E))				
Jungfraujoch, Switzerland		41 ppqv	Vollmer *et al.*	62
Dubendorf, Switzerland		928 ppqv	Vollmer *et al.*	62
(*E*)-2-pentene (Alkene 15) [General Average]				
- Mega city		1.4×10^{10} cm^3 s^{-1}	Vereecken *et al.*	57
- Rural Europe		2.0×10^{7} cm^3 s^{-1}	Vereecken *et al.*	57
Taipei Urban - Summer Daytime		0.12 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time		0.21 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime		0.11 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time		0.13 ppbv	Wang *et al.*	59
Mexico City - Urban		0.74 ppbv	Percival *et al.*	60
Mexico City - Industrial		1.36 ppbv	Percival *et al.*	60

Chinese Max	5.3 ppbv	Percival *et al.*	60
(*Z*)-2-pentene (Alkene 16) [General Average]			
– Mega city	6.9×10^9 cm^3 s^{-1}	Vereecken *et al.*	57
– Rural Europe	1.7×10^7 cm^3 s^{-1}	Vereecken *et al.*	57
Taipei Urban - Summer Daytime	0.05 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.09 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.04 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.05 ppbv	Wang *et al.*	59
Mexico City - Urban	0.37 ppb	Percival *et al.*	60
Mexico City - Industrial	0.7 ppb	Percival *et al.*	60
Chinese Max	9.4 ppb	Percival *et al.*	60
(*E*)-2-butene (Alkene 17) [General Average]			
– Mega city	2.0×10^{10} cm^3 s^{-1}	Vereecken *et al.*	57
– Rural Europe	2.0×10^8 cm^3 s^{-1}	Vereecken *et al.*	57
Taipei Urban - Summer Daytime	0.10 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.16 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.08 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.09 ppbv	Wang *et al.*	59
Mexico City - Urban	1.05 ppb	Percival *et al.*	60
Mexico City - Industrial	2.48 ppb	Percival *et al.*	60
Chinese Max	3.4 ppb	Percival *et al.*	60
Karachi	0.3 ppb	Percival *et al.*	60
Dallas	0.47 ppb	Percival *et al.*	60
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(6.1 \pm 3.0) \times 10^7$	Novelli *et al.*	61
(*Z*)-2-butene (Alkene 18) [General Average]			
– Mega city	1.5×10^{10} cm^3 s^{-1}	Vereecken *et al.*	57
– Rural Europe	1.3×10^8 cm^3 s^{-1}	Vereecken *et al.*	57
Taipei Urban - Summer Daytime	0.09 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.12 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.08 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.08 ppbv	Wang *et al.*	59
Mexico City - Urban	0.83 ppb	Percival *et al.*	60
Mexico City - Industrial	1.31 ppb	Percival *et al.*	60
Chinese Max	2.7 ppb	Percival *et al.*	60
Karachi	0.2 ppb	Percival *et al.*	60
Dallas	0.24 ppb	Percival *et al.*	60
2-methylpropene or Isobutene (Alkene 19) [General Average]			
Taipei Urban - Summer Daytime	0.37 ppbv	Wang *et al.*	59
Taipei Urban - Summer Night-time	0.51 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Daytime	0.41 ppbv	Wang *et al.*	59
Taipei Urban - Autumn Night-time	0.38 ppbv	Wang *et al.*	59
Mexico City - Urban	3.04 ppb	Percival *et al.*	60
Mexico City - Industrial	5.28 ppb	Percival *et al.*	60
Chinese Max	4 ppb	Percival *et al.*	60
Porto Alegre	16.5 ppb	Percival *et al.*	60
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(4.2 \pm 2.5) \times 10^8$	Novelli *et al.*	61

*Table S48: Boiling Points of Alkenes **1—19***

No	Alkene	Boiling point (^{O}C)	Ref
1	1-propene	-47.7	[67]
2	1-butene	-6	[68]
3	3-methyl-1-butene	20.1	[69]
4	3,3-dimethyl-1-butene	41.2	[69]
5	Methyl Vinyl Ketone (MVK)	81	[70]
6	2-methyl-2-butene	37.5-38.5	[71]
7	2-methyl-2-pentene	67.3	[69]
8	2,4-dimethyl-2-pentene	83.4	[69]
9	2,4,4-trimethyl-2-pentene	104.9	[72]
10	4-Methylpent-3-en-2-one (Mesityl Oxide)	130	[73]
11	2,3,3,3-tetrafluoro-1-propene (HFO-1234yf)	-28	[74]
12	3,3,4,4,4-pentafluoro-1-butene (HFO-1345fz)	3-6	[75]
13	(*E*)-1-chloro-3,3,3-trifluoro-1-propene (HCFO-1233zd(E))	18.3	[76]
14	(*E*)-1,3,3,3-tetrafluoro-1-propene (HFO-1234ze(E))	−19	[74]
15	(*E*)-2-pentene	36.3	[69]
16	(*Z*)-2-pentene	36.9	[69]
17	(*E*)-2-butene	0.9	[77]
18	(*Z*)-2-butene	4.0	[78]
19	2-methylpropene (isobutene)	-6.9	[79]

S6 Additional Analysis

S6.1 The Impact of Alkene Interconversion on Ozonolysis Chemistry

The analysis in the main body of this manuscript involves the ozonolysis of many different alkenes with various types and sizes of substituents. These alkenes can be broadly divided into conformationally—restricted alkenes, meaning they only have one conformer (Alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **19**); and conformationally—flexible alkenes, which due to their size and mobility produce multiple conformers (Alkenes **2**, **3**, **5**, **7**, **8**, **10**, **12**, **15** & **16**). An example these multiple conformers interconverting over an isomerisation barrier (TS_{ISO}) is seen for Alkene **10**, in Figure S3.

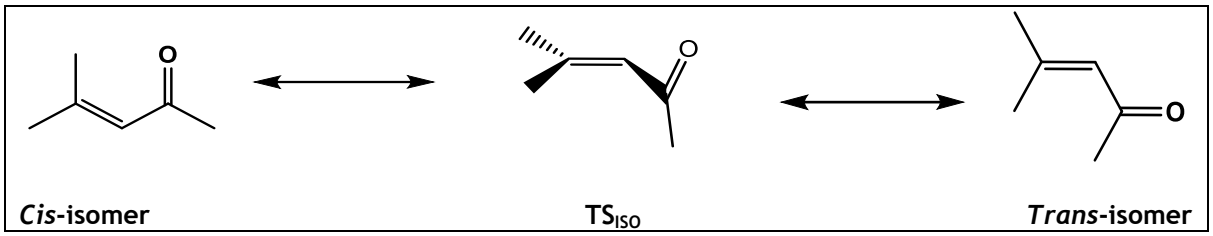

Figure S3: Isomerisation between cis & trans conformers of alkene **10** (Mesityl Oxide) *via a TS_{ISO} barrier.*

During the IRC calculations for some of these cycloaddition (TS_{OZO}) structures, the reactants that are produced are not the lowest energy conformers. In light of this, one very important factor to consider is that the TS_{ISO} barrier may provide an obstacle between the lowest energy conformer and the TS_{OZO} barrier, potentially affecting the k_{ME} values. Many TS_{ISO} barriers are small (< 5 kJ mol^{-1}), such as those seen for Alkenes **2** & **15**, and so are unlikely to act as significant obstacles to reaction. However, as shown in Figure S4, there are alkenes that have larger TS_{ISO} barrier than TS_{OZO} barriers. This could be a significant issue with the O_3 + alkene **5** reaction as the TS_{ISO} barrier is between the lowest energy conformer and the lowest energy TS_{OZO} barrier.

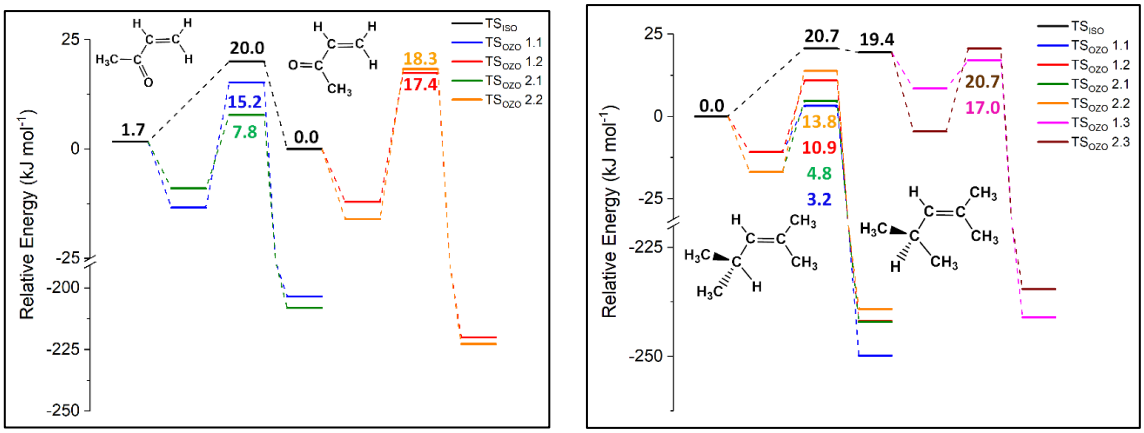

*Figure S4: Potential energy surface of the ozonolyses of Alkene **5** & alkene **8**. This include the different* conformers connected of *via a TS_{ISO} barrier, and which alkene conformer was produced from the IRC calculation of the TS_{OZO} step.*

To determine whether the TS_{ISO} barrier could be a significant obstacle in the cycloaddition step, a test could be run using MESMER's capacity to test the relative importance of different competing pathways in multistep reactions. This test involves constructing new MESMER files that replicate the potential energy surfaces in Figure S4, with the critical inclusion of an isomerization step between the two conformers and having the cycloaddition step that corresponds to each isomer react only with that isomer. If alkene isomerisation essentially freely interconverts, relative to the cycloaddition step then the relative Γ_{THEO} values of the primary ozonide should be the same as for when no isomerisation barrier is included. Furthermore, if the relative Γ_{THEO} values are largely the same with or without the isomerisation barrier then it can be said that this alkene isomerisation has no effect on k_{ME} values too.

But, one difficulty is that including two conformers of the same raw reactant with a TS_{ISO} barrier, in a bimolecular system is beyond the capacity of MESMER. This can be circumnavigated by having within the MESMER input file, a parallel set of pre-reaction complexes augmented with the isomerisation transition states linking the two. These *augmented calculations* replicates the TS_{ISO} barrier seen between the two alkenes but by restricting it to the single bimolecular structure of the pre-reaction complexes, it is within the capacity of MESMER to process. If the obstruction caused by the TS_{ISO} barrier to the TS_{OZO} barrier is significant, the Γ_{THEO} values of the POZ that is formed will drop.

The conformationally—flexible alkenes that are selected to analyse this obstructive capacity are: an alkene that have lots of bulky substituents, alkene **8** ($iPrCH{=}C(CH_3)_2$); and alkenes where the substituent TS_{ISO} rotation would break conjugation between >C=C< and C=O functional groups, alkenes **5** & **10** ($CH_3C(O)CH{=}CH_2$ & $CH_3C(O)CH{=}C(CH_3)_2$). A comparison of the Γ_{THEO} values of the POZ conformers comparing the *augmented*

calculations with the standard MESMER treament for the cycloaddition step of the O_3 reactions with alkenes **5**, **8** & **10**, is found in Table S49.

*Table S49: Comparing different Γ_{THEO} values of the POZs from the ozonolysis of Alkenes **5**, **8** & **10**, using different MESMER treatments.*

	Γ_{THEO}					
Alkene	**Alkene 5**		**Alkene 8**		**Alkene 10**	
Method	**Standard**	**Augmented**	**Standard**	**Augmented**	**Standard**	**Augmented**
Grainsize	20	20	20	20	20	20
POZ 1.1	0.053	0.053	0.723	0.723	0.301	0.301
POZ 1.2	0.018	0.019	0.032	0.032	0.006	0.007
POZ 1.3	N/A	N/A	0.005	0.005	N/A	N/A
POZ 1.1	0.916	0.916	0.234	0.234	0.686	0.685
POZ 1.2	0.012	0.012	0.006	0.006	0.007	0.007
POZ 1.3	N/A	N/A	0.001	0.001	N/A	N/A

The comparison of the standard MESMER treatment with the *augmented calculations*, appears to only diverge from each other to a negligible degree. This may be because TS_{ISO} structures always give lower ΔG barriers than the TS_{OZO} structures (for more details see Section S2). This suggests that the standard MESMER treatment of calculating k_{ME} values, without any reference TS_{ISO} barriers, is very appropriate for determining ozonolysis chemistry, when there are multiple alkene conformers. The standard MESMER treatment is therefore used as the standard method to calculate the k_{ME} values in this study.

S6.2 The Impact of POZ Interconversion on Ozonolysis Chemistry

Throughout this study, all reactions follow a two-step process, where the reactants produce an short-lived intermediate product, usually a cyclic ozonide, which subsequently fragments, due to torsional strain and excess energy. However, the multistep nature of these reactions, such as that seen for the ozonolysis of alkene **18** (*Z*-2-butene) in Figure S5, is that having to involve both a cycloaddition step (TS_{OZO}) and a subsequently a POZ fragmentation step, increases computational cost during MESMER calculations. As only the POZ fragmentation step is irreversible in this MESMER model, this a very costly step to include when determining the Γ_{THEO} values as it involves calculating a lot of computationally intense *reversable reactions*.

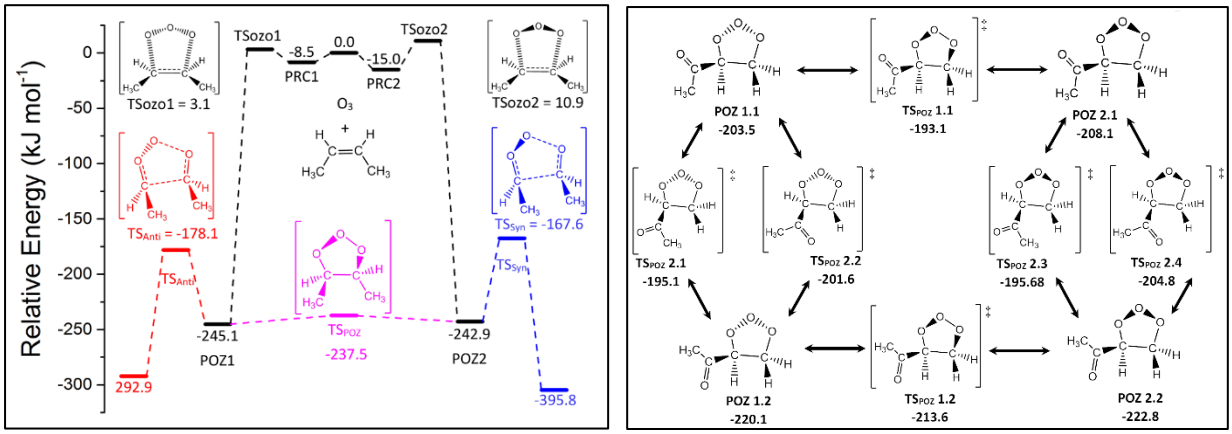

*Figure S5: Comparing the Potential Energy Surface for alkene **18** + O_3 reaction containing only one POZ isomerisation, TS_{POZ}, compared to all the different POZ conformeric isomerisation that the O_3 + alkene **5** potential energy surface would contains [relative energy in kJ mol^{-1}]*

Some alkene ozonolysis reactions have manageable numbers of POZ intermediates an isomerisation transition states such as Alkene **17** + O_3, which has 1 × POZ without any isomerisation transition states (TS_{POZ}), or Alkene **18** + O_3, (featured in Figure S5) which has 2 × POZs and 1 × TS_{POZ}. This means that it is still possible to determine the Γ_{THEO} values using the full potential energy surface, without significant drawbacks in cost either to undertake the computational chemistry calculations or the full MESMER treatment. However this contrast significantly with the ozonolysis of Alkene **5**, which produces 4 × POZs and as many as 6 different TS_{POZ} structures. Alkene **5** + O_3 also is amongst the smaller of these "complex reactions" compared to Alkene **2** + O_3, which produces 6 × POZs and ~12 × TS_{POZ}. This causes significant increases in computational cost in determining the TS_{POZ} structures and goes beyond the capacity of the MESMER software to process.

In the theory, as mapped by the IRC calculations, each cycloaddition pathway produces and each POZ fragmentation pathway emerges from a particular POZ conformer. But with

the ozonolysis of the alkenes, studied here, all each cycloaddition pathway and each POZ fragmentation pathway is interconnected to each POZ conformer due to there isomersation over the TS_{POZ} barriers. As displayed for Alkene **18** + O_3 in Figure S5, the TS_{POZ} barriers calculated for alkene ozonolysis reactions are significantly lower than both cycloaddition and POZ fragmentation barriers.

The structures of the alkenes vary significantly and if the substituent groups are different in character, such as the carbonyl R_1 substituent in the O_3 + Alkene **5** reaction, then the barrier to isomerisation could move upward in energy. This could hypothetically lead to the POZ conformers being chemically distinct. However, as shown in Figure S5, the TS_{POZ} barriers (-213.6 to –193.1 kJ mol^{-1}) are close in energy to POZ (–222.8 to –203.5 kJ mol^{-1}) and significantly lower in energy than both the cycloaddition barriers (7.8 to 18.3 kJ mol^{-1}) and the POZ decomposition barriers (–158.8 to –118.2 kJ mol^{-1}). These results suggest that TS_{POZ} barrier heights are not significantly altered by the presence of the carbonyl R_1 substituent.

This indicates that these POZ conformers interconvert freely, at least to some extent, and therefore the uptake of fragmentation pathways will not discriminate between POZ conformers, to generate multiple sets of final products. This non-discrimination assumption subsequently implies that if the array of POZ conformers and TS_{POZ} barriers in the MESMER file were replaced with a single POZ conformer, with all cycloaddition channels terminating there and all POZ fragmentation pathways originating with that conformer, the same result would emerge. If this “new MESMER treatment” (as it is referred to here) is true then a costs would be reduced significantly, as TS_{POZ} structures would not need to be calculated and such calculations would be significantly within the capacity of the MESMER software to process.

To test this theory, the Γ_{THEO} values of various alkene ozonolysis reactions are determined using three separate treatments which are run on MESMER. These 3 treatments consist of: the full MESMER treatments using all structures on the PES; channelling all cycloaddition and POZ fragmentation channels through the single lowest energy POZ structure, referred to as the “new MESMER treatment”; and where all TS_{POZ} barriers are excluded and all cycloaddition and POZ fragmentation channels run in and out the POZ conformers that the IRC calculations produce, referred to as the “parallel MESMER treatment”. The “parallel MESMER treatment” prevents POZ interconversion and essentially produces two analogous parallel pathways, one for POZ 1 and one for POZ 2, which are analysed as distinct pathways within the MESMER models.

The ozonolysis of Alkenes **1**, **6**, **11**, **13** & **18** ($CH_3CH=CH_2$, $CH_3CH=C(CH_3)_2$, $CF_3CF=CH_2$, *E*-$CF_3CH=CHCl$ and *Z*-$CH_3CH=CHCH_3$) reactions are used because their lack of conformational flexibility produce "simple" PESs, with only 2 × POZs and 1 or 2 × TS_{POZ} structures each. which can be used to compare these two other MESMER treatments to the *full* MESMER treatment. This was undertaken using so many reactions, to make sure the new MESMER treatment was exhaustively tested. This comparison of the different Γ_{THEO} values produced by these MESMER treatments is seen in Table S50.

*Table S50: Comparing different Γ_{THEO} values of the ozonolysis of Alkenes **1**, **6**, **11**, **13** & **18**, using different MESMER treatments. (different CI yields are represented using: Γ_{ANTI} for an anti-conformer; Γ_{SYN} for a syn-conformer; Γ_{FO} for yield of formaldehyde oxide; and Γ_{AO} for yield of dimethyl formaldehyde oxide).*

MESMER Treatment		**Full**	**New**	**Parallel**
Alkene	Channel	All POZs & TS_{POZ}	One POZ & no TS_{POZ}	Multiple POZs & no TS_{POZ}
1	**Grain size**	**25**	**20**	**20**
	Γ_{ANTI}	0.452	0.438	0.562
	Γ_{SYN}	0.276	0.239	0.256
	Γ_{FO} *1*	0.157	0.175	0.080
	Γ_{FO} *2*	0.115	0.148	0.102
6	**Grain size**	**70**	**40**	**40**
	Γ_{ANTI}	0.241	0.216	0.333
	Γ_{SYN}	0.050	0.072	0.053
	Γ_{AO} *1*	0.415	0.509	0.471
	Γ_{AO} *2*	0.294	0.203	0.143
11	**Grain size**	**80**	**40**	**60**
	Γ_{ANTI}	2.48×10^{-7}	2.49×10^{-7}	3.09×10^{-6}
	Γ_{SYN}	2.29×10^{-8}	3.31×10^{-8}	4.43×10^{-7}
	Γ_{FO} *1*	0.531	0.553	0.213
	Γ_{FO} *2*	0.469	0.447	0.787
13 *	**Grain size**	**70**	**40**	**60**
	$\Gamma_{ANTI\text{-}R1}$	0.542	0.604	0.811
	$\Gamma_{SYN\text{-}R3}$	0.119	0.091	0.120
	$\Gamma_{ANTI\text{-}R3}$	0.144	0.108	0.025
	$\Gamma_{SYN\text{-}R1}$	0.194	0.197	0.044
18	**Grain size**	**40**	**30**	**40**
	Γ_{ANTI}	0.872	0.817	0.976
	Γ_{SYN}	0.128	0.183	0.024

** $\Gamma_{ANTI\text{-}R1}$ is for anti-CF_3CHOO; $\Gamma_{SYN\text{-}R1\ is}$ for syn-CF_3CHOO; $\Gamma_{ANTI\text{-}R3}$ is for anti-ClCHOO; $\Gamma_{SYN\text{-}R3}$ is for syn-ClCHOO*

Of these different treatments, the *parallel MESMER treatment*, shows the largest divergence for Γ_{THEO} values in all 5 reactions, except for the anomaly of O_3 + Alkene **6**. Therefore this *parallel MESMER treatment* is not used in the main body of this study.

However, the most important observation between these results is that the new MESMER treatment shows results of similar accuracy to standard MESMER treatment for all alkene ozonolysis reactions studied here. Even the most anomalous result O_3 + Alkene **6** shows agreement enough to be within ~5% of the other results. Much of these degrees of error can be assumed to be due to the changes in grain size. This work was all done with the

lowest possible grainsize that could be possibly processed. This exhaustive analysis of the new MESMER treatment with many different ozonolysis reactions implies that the POZs are mostly freely interconverting and can be treated as essentially one POZ conformer. This is likely because TS_{POZ} barriers are significantly lower in energy than the POZ fragmentation barriers. The high accuracy of this new MESMER treatment of channelling all cycloaddition and POZ fragmentation channels through a single POZ structure has led to it being adopted for determining the Γ_{THEO} values for most of the alkene ozonolysis reactions here. For a full results for the general alkene ozonolysis reactions with what grainsize was used for each Γ_{THEO} result, see Supporting Information Section S2. Standard treatment is often used for simple alkene ozonolysis reactions to calculate the Γ_{THEO} values.

One last noteworthy observation is that during the analysis of the impact of including TS_{POZ} barriers, found here, the O_3 + Alkene **11** reaction had the highest barriers to interconversion (TS_{POZ} 1 & 2 ~ -210.1 & -226.0 kJ mol^{-1}) and this has very little impact on the overall branching ratios.

S6.3 The Impact of CI Interconversion on Ozonolysis Chemistry

The reactions in this study produces many different CIs (and aldehydes & ketones) with various conformeric forms, but for most of these CIs the isomerisation barrier is minor (< 5 kJ mol^{-1}). It is already well established that, due to their contrasting chemistries and their high barrier to interconversion, *syn*- and *anti*-CIs are stereochemically distinct. This leads to them being treated differently in bimolecular sCI analysis and separation of their Γ_{THEO} values into Γ_{ANTI} & Γ_{SYN} values for alkene ozonolysis (see Section S2). However, it is possible that isomerisation (TS_{ISO}) barriers, such as those seen in Figure S6 between *cis*- & *trans*-conformers of *syn*-$CH_3C(O)CHOO$, could prevent free interconversion, like that between *syn*- and *anti*-CIs.

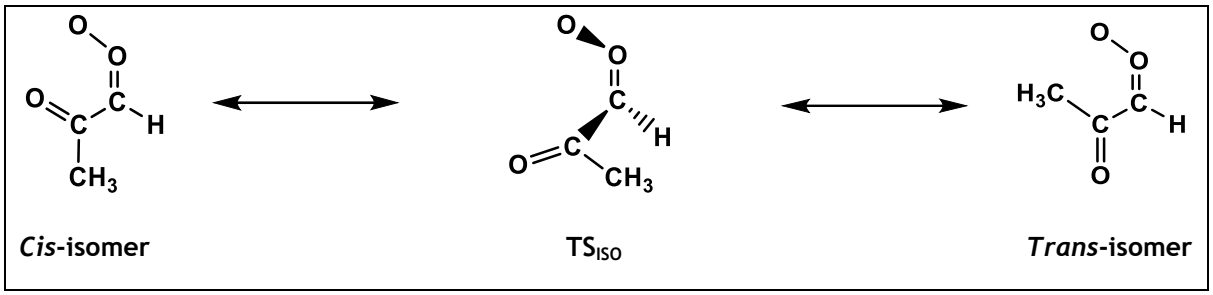

Figure S6: Isomerisation between cis & trans conformers of syn-*$CH_3C(O)CHOO$ via a TS_{ISO} barrier.*

Such CI interconversions are important in sCI unimolecular decomposition, and the different *cis*- & *trans*-conformers can exhibit different bimolecular chemistry.[80] In this section both some key CIs and a single aldehyde ($CH_3C(O)CHO$) from this study are tested to see if the different conformers require different classification or whether the isomers of the aldehyde interconvert post-reaction. The species selected for this comparison are CIs and aldehydes with substituents that make interconversion difficult, such as bulky or conjugated groups. Table S51 displays the computational energies of different conformers and the TS_{ISO} barriers of the species: $CH_3C(O)CHO$, *anti*- & *syn*-$CH_3C(O)CHOO$ and *syn*-iPrCHOO.

Table S51: The zero-point corrected energies various conformers and isomerisation barriers for a variety of Criegee intermediates and aldehydes. All energies are relative to the lower energy conformer of each species.

Chemical	DF-LCCSD(T)-F12a			B3LYP		
	Con 1	TS_{ISO}	Con 2	Con 1	TS_{ISO}	Con 2
***anti*-$CH_3C(O)CHOO$**	0.0	34.2	14.1	0.0	35.3	14.6
***syn*-$CH_3C(O)CHOO$**	0.0	25.7	23.1	0.0	28.1	24.1
$CH_3C(O)CHO$	20.8	23.0	0.0	20.2	28.4	0.0
***syn*-iPrCHOO**	0.0	26.5	9.4			

Aside from the known exception of the barrier between *anti*- & *syn*-CIs, the barriers between the CI and aldehyde conformers studied here are relatively small, especially compared to the excess energy produced from the alkene ozonolysis process. Considering the significant excess energy within a hot CIs, it is assumed here that at least prior to collisional stabilisation, these different hot CI conformers freely interconvert. Despite the fact that $CH_3C(O)CHO$ is likely to see the greater of the TS_{ISO} barriers, the barrier is still relatively small, so the $CH_3C(O)CHO$ conformers are also likely to freely interconvert after ozonolysis too. Therefore, the main manuscript of this study does not refer to specific CI conformer branching ratios (except for *syn* and *anti* conformers), although the pathways that produce specific conformers are identified and their specific yields are noted in Section S2.

S6.4 The Role of the Epoxidation in Alkene Ozonolysis

This section explores whether certain identified transition states identified for O_3 + Alkenes **1** & **5** contribute to the epoxide reaction channels that are found in many alkene ozonolysis reactions . Prior experimental analysis suggests the collective epoxide branching fractions (α_{EPO}) for simple acyclic alkenes are insignificant (<0.006), but that they contribute more significantly to the total reactive outcomes for conjugated dienes such as 1,3-butadiene (0.023) and isoprene (0.039 ± 0.011).[81,82] If the anticipated Γ_{THEO} values for the ozonolysis of Alkenes **1**—**19** are of the same range as isoprene, the analysis in this study should include the relevant epoxide channels. The chemical structures of Alkenes **1** & **5** and examples of the two types of epoxide channel explored in this study are in Figure S7:

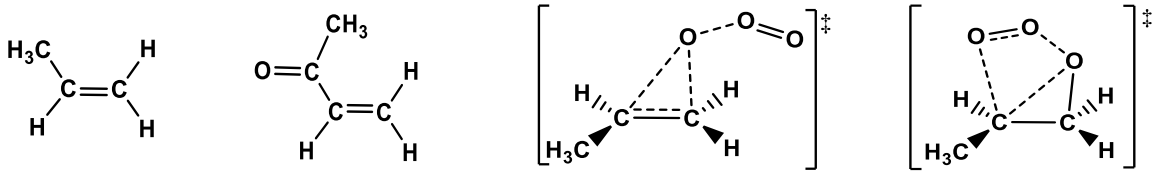

*Figure S7: Chemical Structures of Alkenes **1** & **5** and Example Structures of Epoxidation Channels.*

Given the low experimental α_{EPO} value found for simple acyclic alkenes, this section simply evaluates whether the epoxide reaction channels identified from use of a *B3LYP/aug-cc-pVTZ*-based approach on the simplest alkene, Alkene **1**, to save computational cost. A wider study of the epoxide pathways these alkene ozonolysis reactions can generate is beyond the scope of this investigation. However, there is a prospect that the greater epoxide yields of conjugated dienes could also apply to other conjugated species, including the enones (a type of unsaturated ketones) evaluated in this study. So O_3 + Alkene **5** is also examined to investigate whether enones are also more predisposed to reaction via the epoxide channels. A previous theoretical study by Li *et al.* investigated various epoxidation pathways in the O_3 + 1,3-butadiene reaction, and these calculations produced two types of mechanisms, which are referred to in this study as TS_{EPO} 1 and TS_{EPO} 2.[83] Figure S8 shows some approximate templates for the O_3 + alkene **1** reaction of both the TS_{EPO} 1 channel, which generates the epoxide from the raw reactants via a single TS structure, and the TS_{EPO} 2 channel, which is a POZ fragmentation mechanism. Both epoxide channels are investigated for both O_3 + Alkenes **1** & **5** in this section and, unless otherwise stated, where there are multiple participating TS structures only the lowest energy structure is displayed.

S6.4.1 Challenges with Determining the Energy of Epoxidation TS Structures

During this theoretical analysis of these epoxide pathways for O_3 + Alkenes **1** & **5**, it was noted that the relative energies of the TS_{EPO} structures calculated using *DF-LCCSD(T)-F12/aug-cc-pVTZ* were problematic, as shown in Table S52. This included large differences in energy (sometimes >200 kJ mol^{-1}) between very similar TS_{EPO} structures for both alkenes **1** & **5** without any discernible reason for such an energy disparity. The TS_{EPO} 2.2 & 2.3 structures for O_3 + alkene **5** even yielded relative energies (-153.1 & -152.2 kJ mol^{-1}) lower than the relative energy of the epoxide + O_2 final products (-138.54 kJ mol^{-1}). Many of these TS_{EPO} relative energies were even lower than those recorded for O_3 + 1,3-butadiene (33.5 & -13.4 kJ mol^{-1}), which are already favourable for an epoxide pathway.[83]

*Table S52: Examples of the variations in raw energies between DF-LCCSDT(T)-F12 and B3LYP/aug-cc-pVTZ for the same epoxidation TS structures of Ozonolysis of Alkene **1** & **5**.*

		ΔE (kJ mol^{-1})		
Alkene	**Method**	**DF-LCCSD(T)-F12**	**B3LYP**	**Difference in Relative Energy Between Methods**
1	TS_{OZO} 1	3.9	11.6	-7.7
	TS_{ANTI}	-162.8	-155.0	-7.8
	TS_{FO} 2	-154.1	-144.2	-9.9
	TS_{EPO} 1.1	50.5	50.0	0.5
	TS_{EPO} 2.1	101.9	68.0	33.9
	TS_{EPO} 2.3	94.5	48.9	45.7
5	TS_{OZO} 1.2	17.4	13.5	3.9
	TS_{ANTI} 2	-140.2	-134.5	-5.7
	TS_{FO} 2.1	-139.0	-133.8	-5.2
	TS_{EPO} 1.2	62.6	50.7	11.8
	TS_{EPO} 2.1	-66.7	60.3	-127.0
	TS_{EPO} 2.2	-153.1	67.9	-221.0
	TS_{EPO} 2.3	-152.2	69.7	-221.9
	C_{EPO} 2.1	-138.5	-108.8	-29.8

This lack of consistency on this specific set of transition states for the DF-LCCSD(T)-F12a approach means that only the *B3LYP/aug-cc-pVTZ* energies are used in this section of this limited epoxide pathway examination. The complete relative energies of all TS_{EPO} structures calculated using both the *DF-LCCSD(T)-F12/aug-cc-pVTZ* and the *B3LYP/aug-cc-pVTZ* methods are noted in Section S2.

S6.4.2 Epoxidation During the Ozonolysis of Alkene 1 ($CH_3CH=CH_2$)

While epoxidation geometries identified in the theoretical study of O_3 + 1,3-butadiene by Li *et al.* are used as a template for the TS_{EPO} 1 & 2 structures in this study, the extra conformational flexibility of 1,3-butadiene produces overall larger numbers of TS_{EPO} structures than those seen for O_3 + alkene **1**.[83] However, this additional conformational

flexibility causing an increase in the number of TSs per channel is simply a continuation of the trend observed with both the cycloaddition and POZ fragmentation channels seen earlier in this study. The epoxidation of Alkene **1** by O_3 may compete with other pathways: the *direct reaction* TS_{EPO} 1.1 & 1.2 mechanism competes with the cycloaddition step (as illustrates using the lowest B3LYP/aug-cc-pVTZ energy structures in Figure S8), and the TS_{EPO} 2.1—2.4 pathways compete with other POZ fragmentation channels. This means that reviewing the role of the epoxidation process in k_{ME} is just as important as reviewing the overall epoxide + O_2 branching fraction (α_{EPO}). However, this section is simply a narrow examination of whether epoxide pathways identified may impact, the alkene ozonolysis results presented in this study. A wider computational analysis of all alkene ozonolysis epoxide pathways is beyond the scope of this study.

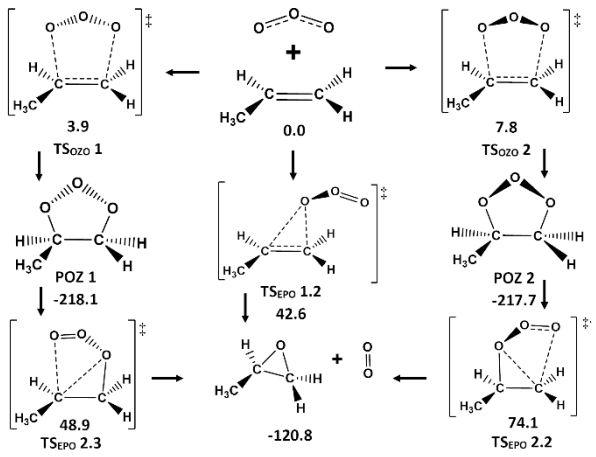

*Figure S8: Schematic of the Lowest Energy (using B3LYP/aug-cc-pVTZ energies) TS_{EPO} 1 & 2 Structures for O_3 + Alkene **1**.*

In spite of the fact that the *direct reaction* TS_{EPO} 1 barriers are lower in energy (42.6 to 50.0 kJ mol^{-1}) relative to the POZ fragmentation TS_{EPO} 2 structures (48.9 to 74.1 kJ mol^{-1}), Figure S8 above shows that the TS_{OZO} 1 & 2 mechanisms are much more favourable to reactant uptake. This is confirmed by the k_{ME} [B3LYP] value for TS_{EPO} 1.1 & 1.2 having a very small contribution (~7.04×10^{-23} cm^3 s^{-1}) to the overall k_{ME} [B3LYP] value (7.37×10^{-16} cm^3 s^{-1}). The TS_{EPO} 2 mechanisms (48.9 to 74.1 kJ mol^{-1}) are much higher compared to other POZ fragmentation processes (-155.0 to -144.2 kJ mol^{-1}), which is reflected in the low overall branching fraction for these epoxide pathways of O_3 + Alkene **1** (α_{EPO} [B3LYP] ~2.22×10^{-8}). However, this section is simply a narrow examination of whether epoxide pathways identified may impact, the alkene ozonolysis results presented in this study. A wider computational analysis of all alkene ozonolysis epoxide pathways is beyond the scope of this study.

S6.4.3 Epoxidation During the Ozonolysis of Alkene 5 ($CH_3C(O)CH=CH_2$)

Alkene **5** (Methyl Vinyl Ketone) is the simplest enone and so has *E*- and *Z*- conformers (similar to 1,3-butadiene), which differ in energy by 0.63 kJ mol^{-1}. This results in four POZs, again similar to 1,3-butadiene, which leads to a large number of epoxidation channels. Some standard epoxide pathway transition states are shown in Figure S9.

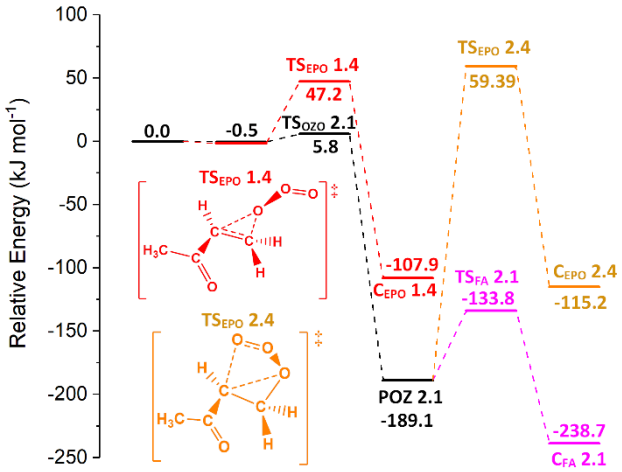

Figure S9: Limited PES comparing low energy ozonolysis and POZ decomposition pathways with lowest energy transition states of the restricted number of epoxidation pathways identified.

Figure S9 displays the significant disparity in energy between the TS_{EPO} 1 (47.2 to 69.7 kJ mol^{-1}) and TS_{OZO} (5.8 to 14.8 kJ mol^{-1}) or TS_{EPO} 2 (59.4 to 105.5 kJ mol^{-1}) and the other POZ breakdown pathways (-148.2 to -110.0 kJ mol^{-1}). These high barriers lead to a low k_{ME} [TS_{EPO} 1] value (1.33×10^{-23} cm^3 s^{-1}) compared to the overall B3LYP k_{ME} value (1.83×10^{-16} cm^3 s^{-1}). These high TS_{EPO} 1 barriers and similarly high TS_{EPO} 2 barriers for POZ decomposition led to a similar low α_{EPO} value for Alkene **5** (~ 7.25×10^{-8}) to that of alkene **1** (2.22×10^{-8}). Even the lowest energy TS_{EPO} 1 and TS_{EPO} 2 structures for O_3 + Alkene **5** calculated for this study (see Figure S10) are much higher than those comparative mechanism for O_3 + 1,3-butadiene calculated in a computational study by Li *et al.* (33.5 & -13.4 kJ mol^{-1}). However, the additional conjugation in the >C=C< bonds within Alkene **5** do not appear to aid these *particular* epoxide formation channels as they do not yield a more than negligible theoretical α_{EPO} value. However, a much wider analysis of alkene ozonolysis epoxide pathways would be required to reflect fully on the role of epoxide formation in these reactions and this is beyond the scope of this study.

One noteworthy observation that requires highlighting from comparing the different TS_{EPO} structures for O_3 + Alkene **5** is that the steric interaction between the ozone group and the substituent group does not wholly dictate energy differences, as shown with the unusually low TS_{EPO} 1.4 & 2.4 barriers. The TS_{EPO} 1.4 & 2.4 structures, shown in Figure S10, have the

similar spatial arrangement of the ketone group and the >C=C< bond being in a *Z*-orientation, in conjunction with the central oxygen in the O_3 inclined towards the —C(O)CH_3 substituent group. These structures, along with TS_{EPO} 2.8, have the orientations of both the electronegative oxygen atom in the ketone group and the O_3 place them into a position where a mutual repulsion would be expected. This is the reason they are described as having "unusually low energies".

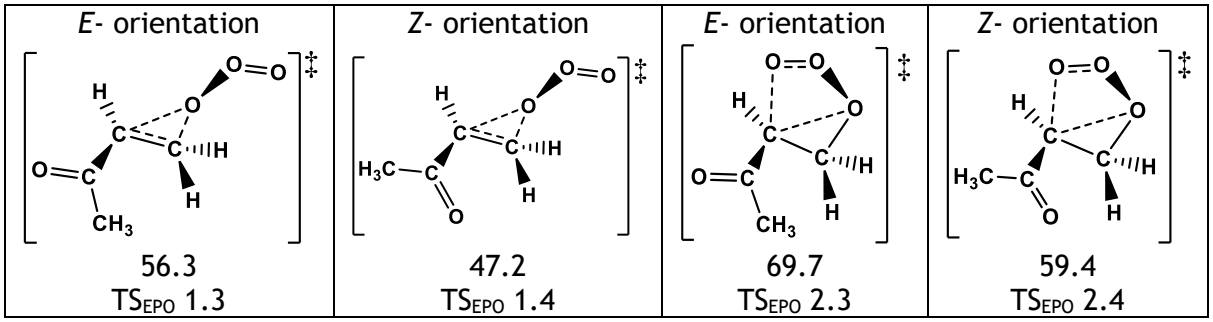

Figure S10: Comparative epoxide subchannel structures, relative B3LYP energies and E- or Z- orientation of alkene 5

If the spatial arrangement is altered slightly such as reverting the ketone group and the >C=C< bond back to an *E*-orientation, such as for TS_{EPO} 1.3 & TS_{EPO} 2.3 in Figure S10, a significant increase in energy is also observed. In sections 3.4.3 & 3.5.4, the TS_{OZO} 2.1 structure in O_3 reactions with both alkenes **5** & **10**, has a similar spatial arrangement for the ketone group, the >C=C< bond and the O_3, with a similarly unusually low energy. This low energy for TS_{OZO} 2.1 is also removed if the orientation of any of these groups change.

S6.4.4 Summary of epoxidation channel

In summary, whilst the conjugated system of the enone does lower the energy of the epoxide pathways in some circumstances, this *B3LYP/aug-cc-pVTZ* only analysis shows that this reduced number of TS_{EPO} pathways have limited impact on the ozonolysis of Alkenes **1** & **5**. Due to this limited impact no further epoxide investigation has not been pursued for Alkenes **2**—**4** & **6**—**19.** If this study included either isoprene or 1,3-butadiene, the epoxide channel would have been included in the investigation of these alkenes due to their high global emission profiles, such that even small branching fractions to these channels may have globally significant impacts.[84,85] The literature often does that these epoxide generating paths are likely to have some kinetic role in alkene ozonolysis process, but any broader expanded analysis of these channels is beyond the scope of this study.

S6.5 A study of the role of stepwise POZ formation and fragmentation processes in the Ozonolysis of Alkenes

In much of the literature about Alkene Ozonolysis there are usually only two significant stages: where ozone reacts with the alkene through a concerted 1,3-cycloaddition to form a primary ozonide (POZ), and a concerted POZ fragmentation process to produce a Criegee intermediate and a carbonyl co-product (either an aldehyde or ketone).[1-3,5,20,23,39-44,86-88] However, in some studies, there is an alternative cycloaddition mechanism in which POZ are formed through the stepwise *DeMore mechanism* through via a very unstable *DeMore species* (Figure S11). While some studies are mixed as to the overall effect of the *DeMore mechanism*, It does appear that these pathways may play some modest role in the cycloaddition kinetics, especially with conjugated alkenes such as isoprene.[89-92]

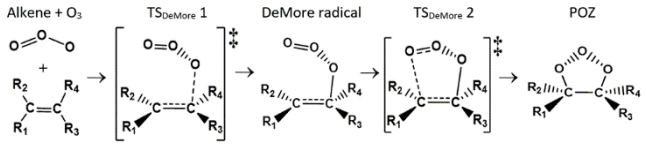

Figure S11: The Stepwise DeMore Mechanism for POZ Formation during Alkene Ozonolysis.

The concerted POZ fragmentation step also has a competing stepwise *O'Neal-Blumstein mechanism* where the POZ breaks down via an ONB radical (see Figure S12). While the concerted mechanism does appear to dominate product branching ratios in the literature, the literature does show a modest role for *O'Neal-Blumstein mechanism* in alkene ozonolysis reactions.[93–95]

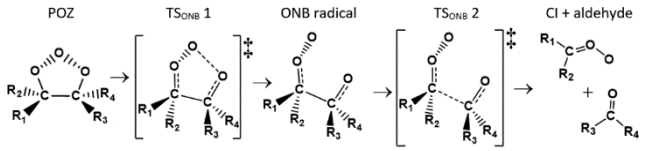

Figure S12: The Stepwise O'Neal-Blumstein Mechanism for POZ Formation during Alkene Ozonolysis.

Given how limited the literature on these two processes are, an investigation into these alkene ozonolysis mechanisms is contained in this section, for the purpose of outlining if such mechanisms should be of interest in the wider study. Much like with the analysis of the epoxidation pathways also included in this supporting information, the exploration of these stepwise pathways are undertaken using *B3LYP/aug-cc-pVTZ* only.

S6.5.1 Stepwise "DeMore" cycloaddition

To determine if stationary points analogous to structures *DeMore* mechanisms identified have important roles on the potential energy surfaces calculated here, many attempts to

obtain transition state geometries but none were located using the conventional *B3LYP/aug-cc-pVTZ* approach. So, a potential energy surface scan was performed (using the *modredundant* function in *Gaussian16*) to produce step-by-step decent from a *DeMore* intermediate species to the primary ozonide. It was inferred from these observations that such *DeMore* transition states would not emerge on these potential energy surfaces by using this *B3LYP/aug-cc-pVTZ* approach. Both of these observations imply that the *DeMore* mechanism does not contribute significantly to the Alkene ozonolysis process.

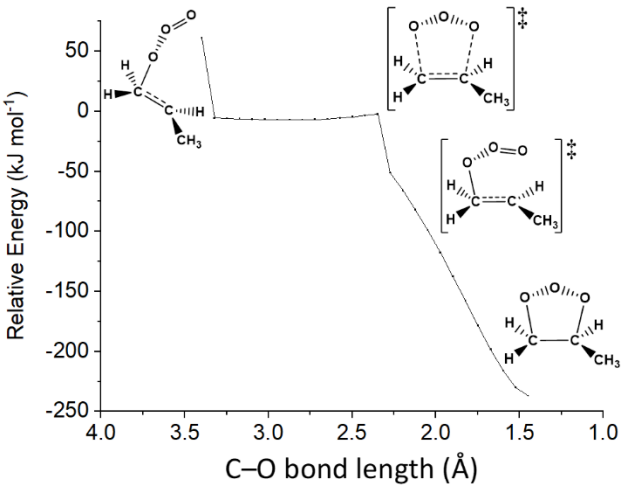

Figure S13: A potential energy surface scan of the POZ formation step of the ozonolysis of propene from a DeMore intermediate.

During an analysis of the epoxidation pathways of the ozonolysis of methyl vinyl ketone in a previous section, the intrinsic reaction coordinates calculations determined that the steepest decent from one of the transition states (TS_{EPO} 2.4) lead to a *DeMore* intermediate structure (see figure below). However, an optimisation of this *DeMore* intermediate was attempted, the *DeMore* intermediate reverted into an epoxide unless the C–O bond length was frozen (using the *Modredundant* function). Given this mixed evidence, it cannot be assumed that TS_{EPO} 2.4 is a *DeMore* mechanism, but given that it is ~50 kJ mol^{-1} greater in energy of the concerted cycloaddition reaction mechanism, it is unlikely that any such identified transition state has an influence on the potential energy surfaces calculated here.

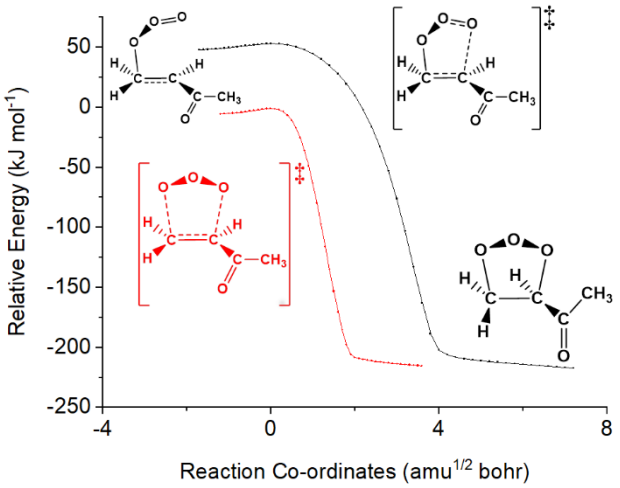

Figure S14: A comparison of a possible DeMore Mechanism, TS_{DEMORE} 2.4, (in Black) and of the concerted 1,3-cycloaddition step (in Red) from the ozonolysis of methyl vinyl ketone.

Considering the evidence given above provided in this section, it is unlikely that any of the *pseudo DeMore* stationary points calculated using this *B3LYP/aug-cc-pVTZ* approach are likely to shape the results presented in this study. But it is quite likely, given the literature precedent that this *DeMore* mechanism does play a role in alkene ozonolysis process, but as stated in the introduction of this study, this a definitive expanded study of these channels was deemed beyond the scope of this study.

S6.5.2 Stepwise "O'Neal-Blumstein" POZ fragmentation:

Both some optimised geometries of the intermediate species and the transition states of the *O'Neal-Blumstein* (ONB) process were calculated the POZ fragmentation of O_3 + propene (see Figure S15 below). In the process of examining O_3 + Propene, the *B3LYP/aug-cc-pVTZ* calculations did yield some optimised geometries similar to literature descriptions of the intermediate species and the transition states of the *O'Neal-Blumstein* (ONB). Although no initial TS_{ONB} 1 mechanisms for forming the ONB intermediate product were isolated, but the energy of structure of the ONB species and the fragmentation step ($TS_{ONB-ANTI}$ 2) were determined and these are shown to be much higher in energy than any concerted fragmentation process. These possible ONB species and fragmentation steps are shown in Figure S15 compared to the much lower energy concerted TS_{ANTI} breakdown mechanism, which produces *anti*-CH_3CHOO + HCHO.

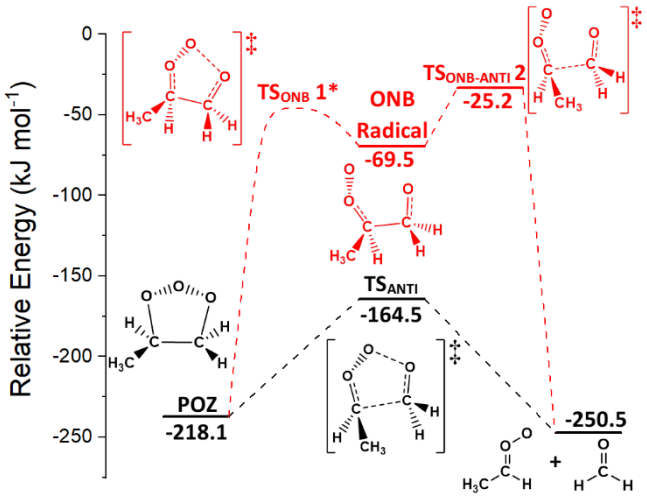

*Figure S15: A Potential Energy Surface of O_3 + Propene showing both the Concerted Mechanism (in black) and the assumed Stepwise O'Neal-Blumstein Mechanism (in Red) for the formation of anti-CH_3CHOO + HCHO. *Note: the TS_{ONB} 1 was not optimised but this is not needed for the purposes of this analysis.*

Several other possible TS_{ONB} structures for O_3 + Alkene **1**, were also found during this study's computational calculations and they are compared to their assumed concerted fragmentation counterparts. Most of them exceed their concerted counterparts by often greater than ~100 kJ mol^{-1}.

Table S53: The B3LYP energies of the transition states barriers for both the concerted and the O'Neal-Blumstein POZ fragmentation processes.

Concerted TS	**TS_{ANTI}**	**TS_{FO} 1**	**TS_{FO} 2**	**TS_{SYN}**
Energy (kJ mol^{-1})	-164.5	-156.8	-154.2	-158.6
ONB TS	**$TS_{ONB-ANTI}$**	**TS_{ONB-FO} 1**	**TS_{ONB-FO} 2**	**$TS_{ONB-SYN}$**
Energy (kJ mol^{-1})	-33.4	-16.02	-24.4	-32.1

From this cursory examination of the possible *O'Neal-Blumstein* stationary points presented here, use of a *B3LYP/aug-cc-pVTZ*-based approach would be suboptimal for a detailed examination of these O'Neal–Blumstein stationary points. According to some studies in the literature, the *O'Neal-Blumstein* mechanism is likely to play some kinetic role in alkene ozonolysis process, any broader expanded study of these channels is beyond the scope of this study.

S7 Effective Rate Constants

S7.1 Effective Rate Constant of Alkene reactions with OH, Cl & NO_3:

Table S54: Table containing the general background abundance of the key atmospheric radicals, OH, Cl & NO_3; the literature rate constant of alkene reactions with OH, Cl & NO_3; and the effective rate constant of alkene reactions with OH, Cl & NO_3 with respect to the atmospheric radical.

	Location	Global Background	Global Background	Location	Global Background	Location	Global Background	ref
	OH conc. (Molec/cm^3)	1.00E+07	*1.00E+06*	Cl conc. (Molec/cm^3)	1.23E+12	NO_3 conc. (Molec/cm^3)	5.70E+08	[3,96]
Alkene No	**k_{EXP} (cm^3 $molec.^{-1}$ s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EXP} (cm^3 $molec.^{-1}$ s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EXP} (cm^3 $molec.^{-1}$ s^{-1})**	**k_{EFF} (s^{-1})**	ref
1	2.63E-11	2.63E-04	2.63E-05	2.30E-10	2.83E+02	9.40E-15	5.36E-06	[3]
2	3.14E-11	3.14E-04	3.14E-05	3.00E-10	3.69E+02	1.30E-14	7.41E-06	[3]
3	3.18E-11	3.18E-04	3.18E-05	-	-	1.40E-14	7.98E-06	[3]
5	2.01E-11	2.01E-04	2.01E-05	-	-	-	-	[3]
6	8.69E-11	8.69E-04	8.69E-05	3.80E-10	4.67E+02	9.40E-12	5.36E-03	[3]
7	8.90E-11	8.90E-04	8.90E-05	-	-	8.50E-12	4.85E-03	[3]
11	1.05E-12	1.05E-05	1.05E-06	7.03E-11	8.65E+01	-	-	[40]
13	4.40E-13	4.40E-06	4.40E-07	5.22E-11	6.42E+01	-	-	[43]
14	9.25E-13	9.25E-06	9.25E-07	4.64E-11	5.71E+01	-	-	[44]
15	6.70E-11	6.70E-04	6.70E-05	-	-	3.90E-13	2.22E-04	[3]
16	6.50E-11	6.50E-04	6.50E-05	-	-	6.80E-13	3.88E-04	[3]
17	6.40E-11	6.40E-04	6.40E-05	3.50E-10	4.31E+02	3.90E-13	2.22E-04	[3]
18	5.64E-11	5.64E-04	5.64E-05	3.40E-10	4.18E+02	3.50E-13	2.00E-04	[3]
19	5.14E-11	5.14E-04	5.14E-05	3.30E-10	4.06E+02	3.40E-13	1.94E-04	[3]

S7.2 Effective Rate Constant of Alkene Ozonolysis respect to Ozone

Table S55: Table containing the abundance of O_3 in different environments; the computational rate constant of alkene reactions with O_3; and the effective rate constant of alkene reactions with O_3 with respect to ozone.

	Location	Rural Europe	Mega-city	Tropical Rainforest	Boreal Forest	Global Background	Summer Houston Peak	Summer Houston Average
	$[O_3]$ (molec. cm^{-3})	1.23E+12	4.93E+12	8.62E+11	1.40E+12	7.30E+11	1.90E+12	1.40E+12
	ref	[56]	[56]	[56]	[56]	[3,57]	[55]	[55]
Alkene No	**k_{THEO} (cm^3 $molec.^{-1}$ s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**
1	3.24E-17	3.99E-05	1.60E-04	2.79E-05	4.54E-05	2.37E-05	6.16E-05	4.54E-05
2	1.03E-16	1.27E-04	5.08E-04	8.88E-05	1.44E-04	7.52E-05	1.96E-04	1.44E-04
3	6.06E-17	7.45E-05	2.99E-04	5.22E-05	8.48E-05	4.42E-05	1.15E-04	8.48E-05
4	2.25E-17	2.77E-05	1.11E-04	1.94E-05	3.15E-05	1.64E-05	4.28E-05	3.15E-05
5	6.90E-17	8.49E-05	3.40E-04	5.95E-05	9.66E-05	5.04E-05	1.31E-04	9.66E-05
6	4.35E-15	5.35E-03	2.14E-02	3.75E-03	6.09E-03	3.18E-03	8.27E-03	6.09E-03
7	5.12E-15	6.30E-03	2.52E-02	4.41E-03	7.17E-03	3.74E-03	9.73E-03	7.17E-03
8	2.44E-16	3.00E-04	1.20E-03	2.10E-04	3.42E-04	1.78E-04	4.64E-04	3.42E-04
9	2.46E-16	3.03E-04	1.21E-03	2.12E-04	3.44E-04	1.80E-04	4.67E-04	3.44E-04
10	1.57E-18	1.93E-06	7.74E-06	1.35E-06	2.20E-06	1.15E-06	2.98E-06	2.20E-06
11	1.14E-20	1.40E-08	5.62E-08	9.83E-09	1.60E-08	8.32E-09	2.17E-08	1.60E-08
12	2.99E-20	3.68E-08	1.47E-07	2.58E-08	4.19E-08	2.18E-08	5.68E-08	4.19E-08
13	1.85E-20	2.28E-08	9.12E-08	1.59E-08	2.59E-08	1.35E-08	3.52E-08	2.59E-08
14	8.11E-21	9.98E-09	4.00E-08	6.99E-09	1.14E-08	5.92E-09	1.54E-08	1.14E-08
15	1.13E-15	1.39E-03	5.57E-03	9.74E-04	1.58E-03	8.25E-04	2.15E-03	1.58E-03
16	2.48E-15	3.05E-03	1.22E-02	2.14E-03	3.47E-03	1.81E-03	4.71E-03	3.47E-03
17	1.81E-16	2.23E-04	8.92E-04	1.56E-04	2.53E-04	1.32E-04	3.44E-04	2.53E-04
18	1.18E-15	1.45E-03	5.82E-03	1.02E-03	1.65E-03	8.61E-04	2.24E-03	1.65E-03
19	1.51E-17	1.86E-05	7.44E-05	1.30E-05	2.11E-05	1.10E-05	2.87E-05	2.11E-05

Table S56: Table containing the abundance of O_3 in different environments; the experimental rate constant of alkene reactions with O_3; and the effective rate constant of alkene reactions with O_3 with respect to ozone.

	Location	Rural Europe	Mega-city	Tropical Rainforest	Boreal Forest	Global Background	Summer Houston Peak	Summer Houston Average	
	$[O_3]$ (molec. cm^{-3})	1.23E+12	4.93E+12	8.62E+11	1.40E+12	7.30E+11	1.90E+12	1.40E+12	
	ref	[56]	[56]	[56]	[56]	[3,57]	[55]	[55]	
Alkene No	**k_{EXP} (cm^3 $molec.^{-1}$ s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**k_{EFF} (s^{-1})**	**ref**
1	9.90E-18	1.22E-05	4.88E-05	8.53E-06	1.39E-05	7.23E-06	1.88E-05	1.39E-05	[5]
5	5.20E-18	6.40E-06	2.56E-05	4.48E-06	7.28E-06	3.80E-06	9.88E-06	7.28E-06	[97]
7	4.65E-16	5.72E-04	2.29E-03	4.01E-04	6.51E-04	3.39E-04	8.84E-04	6.51E-04	[38]
13	1.46E-21	1.80E-09	7.20E-09	1.26E-09	2.04E-09	1.07E-09	2.77E-09	2.04E-09	[43,98]
14	2.81E-21	3.46E-09	1.39E-08	2.42E-09	3.93E-09	2.05E-09	5.34E-09	3.93E-09	[44]

S7.3 Effective Rate Constant with respect to the Alkene:

The effective rate constants calculated here are produced using alkene concentrations obtained from the literature. A survey of these alkene concentrations are found in greater detail in Section S5.

*Table S57: Table containing the abundance of Alkenes in different environments; the computational rate constant of Alkene reactions with O_3; and the effective rate constant of alkene reactions with O_3 with respect to the alkene. Alkenes presented in this table are Alkenes **1-9**, **11** & **13-19**.*

Alkene **1**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	3.24E-17		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	1.10E+11	3.56E-06	57
Rural Europe	1.50E+09	4.86E-08	57
High ponderosapine forest	4.34E+09	1.40E-07	58
Low ponderosapine forest	4.48E+09	1.45E-07	58
Taipei Urban - Summer Daytime	1.38E+10	4.47E-07	59
Taipei Urban - Summer Night-time	2.00E+10	6.46E-07	59
Taipei Urban - Autumn Daytime	1.31E+10	4.23E-07	59
Taipei Urban - Autumn Night-time	1.31E+10	4.23E-07	59
Mexico City - Urban	1.46E+11	4.73E-06	60
Mexico City - Industrial	2.70E+11	8.74E-06	60
Chinese Max	2.02E+11	6.54E-06	60
Karthmandu, Nepal	3.15E+11	1.02E-05	60
Porto Alegre, Brazil	6.97E+11	2.26E-05	60
Meadows and Coniferous forests in Bavaria	4.70E+08	1.52E-08	61
Alkene **2**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	1.03E-16		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	5.70E+10	5.86E-06	57
Rural Europe	5.70E+08	5.86E-08	57
Taipei Urban - Summer Daytime	3.45E+09	3.54E-07	59
Taipei Urban - Summer Night-time	4.43E+09	4.56E-07	59
Taipei Urban - Autumn Daytime	2.96E+09	3.04E-07	59
Taipei Urban - Autumn Night-time	3.20E+09	3.29E-07	59
Taipei, Taiwan	2.22E+10	2.28E-06	60
Chinese Max	5.91E+10	6.07E-06	60
Karachi	2.71E+10	2.78E-06	60
Dallas	7.88E+09	8.10E-07	60
Porto Alegre	1.92E+11	1.97E-05	60
Meadows and Coniferous forests in Bavaria	1.40E+08	1.44E-08	61
Alkene **3**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	6.06E-17		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Taipei Urban - Summer Daytime	7.39E+08	7.59E-08	59
Taipei Urban - Summer Night-time	9.85E+08	1.01E-07	59
Taipei Urban - Autumn Daytime	4.93E+08	5.06E-08	59
Taipei Urban - Autumn Night-time	4.93E+08	5.06E-08	59
General - C5 alkene background	1.28E+09	1.32E-07	60
Alkene **4**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	2.25E-17		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Taipei Urban - Summer Daytime	1.28E+09	1.32E-07	60

Alkene **5**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	6.90E-17		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Borneo	1.11E+10	1.14E-06	57
Rainforest	2.40E+10	2.47E-06	57
Temperate Forest	2.50E+09	2.57E-07	60
Alkene **6**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	4.35E-15		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Taipei Urban - Summer Daytime	1.28E+09	1.32E-07	59
Taipei Urban - Summer Night-time	3.20E+09	1.39E-05	59
Taipei Urban - Autumn Daytime	5.17E+09	2.25E-05	59
Taipei Urban - Autumn Night-time	2.96E+09	1.29E-05	59
Mexico City- Urban	2.96E+09	1.29E-05	60
Mexico City- Industrial	4.16E+10	1.81E-04	60
Porto Alegre Brazil	2.19E+10	9.54E-05	60
Seoul	4.19E+11	1.82E-03	60
Taipei Urban - Summer Daytime	2.46E+10	1.07E-04	59
Alkene **7**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	5.12E-15		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Porto Alegre Brazil	9.85E+10	5.04E-04	60
Porto Alegre Brazil	4.19E+08	2.14E-06	60
Boston	4.19E+11	2.14E-03	60
Boston	1.28E+09	6.56E-06	60
Alkene **8**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	2.44E-16		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Boston	1.72E+08	4.21E-08	60
Boston	7.39E+07	1.81E-08	60
Alkene **9**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	2.46E-16		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Boston	4.68E+08	1.15E-07	60
Boston	9.85E+07	2.42E-08	60
Alkene **11**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	1.14E-20		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Jungfraujoch, Switzerland	7.39E+04	8.39E-16	62
Dubendorf, Switzerland	3.35E+06	3.81E-14	62
Average USA future scenario - summer	1.82E+05	2.07E-15	63,64
Maximum USA future scenario - summer	7.39E+06	8.39E-14	63,64
Alkene **13**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	1.85E-20		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Jungfraujoch, Switzerland	1.97E+05	2.24E-15	62
Dubendorf, Switzerland	2.96E+05	3.36E-15	62
Beijing, China	4.93E+05	5.60E-15	66

Alkene **14**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	8.11E-21		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Jungfraujoch, Switzerland	1.01E+06	2.48E-10	62
Dubendorf, Switzerland	2.29E+07	5.61E-09	62
Alkene **15**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	1.13E-15		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	1.40E+10	1.58E-05	57
Rural Europe	2.00E+07	2.25E-08	57
Taipei Urban - Summer Daytime	2.96E+09	3.33E-06	59
Taipei Urban - Summer Night-time	5.17E+09	5.83E-06	59
Taipei Urban - Autumn Daytime	2.71E+09	3.05E-06	59
Taipei Urban - Autumn Night-time	3.20E+09	3.61E-06	59
Mexico City - Urban	1.82E+10	2.06E-05	60
Mexico City - Industrial	3.35E+10	3.78E-05	60
Chinese Max	1.31E+11	1.47E-04	60
Alkene **16**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	2.48E-15		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	6.90E+09	1.71E-05	57
Rural Europe	1.70E+07	4.22E-08	57
Taipei Urban - Summer Daytime	1.23E+09	3.06E-06	59
Taipei Urban - Summer Night-time	2.22E+09	5.50E-06	59
Taipei Urban - Autumn Daytime	9.85E+08	2.45E-06	59
Taipei Urban - Autumn Night-time	1.23E+09	3.06E-06	59
Mexico City - Urban	9.11E+09	2.26E-05	60
Mexico City - Industrial	1.72E+10	4.28E-05	60
Chinese Max	2.32E+11	5.75E-04	60
Alkene **17**			
k_{THEO} (cm^3 $molec.^{-1}$ s^{-1}):	1.81E-16		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	2.00E+10	3.61E-06	57
Rural Europe	2.00E+08	3.61E-08	57
Taipei Urban - Summer Daytime	2.46E+09	4.45E-07	59
Taipei Urban - Summer Night-time	3.94E+09	7.11E-07	59
Taipei Urban - Autumn Daytime	1.97E+09	3.56E-07	59
Taipei Urban - Autumn Night-time	2.22E+09	4.00E-07	59
Mexico City - Urban	2.59E+10	4.67E-06	60
Mexico City - Industrial	6.11E+10	1.10E-05	60
Chinese Max	8.37E+10	1.51E-05	60
Karachi	7.39E+09	1.33E-06	60
Dallas	1.16E+10	2.09E-06	60
Meadows and Coniferous forests in Bavaria	6.10E+07	1.10E-08	61

Alkene **18**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	1.18E-15		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Mega city	1.50E+10	1.76E-05	[57]
Rural Europe	1.30E+08	1.53E-07	[57]
Taipei Urban - Summer Daytime	2.22E+09	2.61E-06	[59]
Taipei Urban - Summer Night-time	2.96E+09	3.47E-06	[59]
Taipei Urban - Autumn Daytime	1.97E+09	2.32E-06	[59]
Taipei Urban - Autumn Night-time	1.97E+09	2.32E-06	[59]
Mexico City - Urban	2.04E+10	2.40E-05	[60]
Mexico City - Industrial	3.23E+10	3.79E-05	[60]
Chinese Max	6.65E+10	7.82E-05	[60]
Karachi	4.93E+09	5.79E-06	[60]
Dallas	5.91E+09	6.95E-06	[60]
Alkene **19**			
k_{THEO} (cm^3 molec.$^{-1}$ s^{-1}):	1.51E-17		
Location	**[Alkene] (molec. cm^{-3})**	**k_{EFF} (s^{-1})**	**ref**
Taipei Urban - Summer Daytime	9.11E+09	1.38E-07	[59]
Taipei Urban - Summer Night-time	1.26E+10	1.90E-07	[59]
Taipei Urban - Autumn Daytime	1.01E+10	1.53E-07	[59]
Taipei Urban - Autumn Night-time	9.36E+09	1.41E-07	[59]
Mexico City - Urban	7.49E+10	1.13E-06	[60]
Mexico City - Industrial	1.30E+11	1.97E-06	[60]
Chinese Max	9.85E+10	1.49E-06	[60]
Porto Alegre	4.06E+11	6.14E-06	[60]
Meadows and Coniferous forests in Bavaria	4.20E+08	6.35E-09	[61]

S8 Additional Sections Related to Method Specifics:

S8.1 Additional Details on MESMER inputs:

The MESMER calculations of these bimolecular reactions involve the use of an inverse Laplace transform (ILT) approach, and the capture rate pre-exponential provides an upper bound to the rate of pre-reaction complex formation, which is reasonably expected to be close to the gas-kinetic collision frequency. The pre-exponential used throughout this study was 1×10^{-10} cm^3 s^{-1}, and this value has been adopted was selected as the capture limit for MESMER software simulations in many studies of bimolecular reactions.[99–102] A study by Medeiros *et al.* showed that the sensitivity of MESMER rate constant to this capture limit is largely is limited unless the rate constant is shown to be close to the capture limit.[102] Also in previous studies, the rate constants of bimolecular Criegee intermediate reactions were calculated using this same MESMER approach, alongside rate constants of the same reactions calculated using the conventional transition state equations and/or the KiSThelP software package and these results were found to align extremely well, further validating this particularly MESMER approach.[99,103]

As N_2 is the bath gas used in these calculations, with the average, temperature-independent energy lost per collision used here was 300 cm^{-1}. This energy lost per collision value has been in the literature in master equation simulations of both unimolecular and bimolecular gas-phase reactions, including one alkene ozonolysis study, where N_2 is used as the bath gas.[99,100,104–108] It is also well within the range of ~250–500 cm^{-1} for an N_2 recommended in the Glowacki *et al* study outlining how to use the MESMER software.[105]

In this study, when deploying MESMER, the inter-atomic distance and potential energy Lennard-Jones parameter inputs used for the N_2 bath gas were σ = 3.90 Å and ε = 48.0 K respectively, both values which were the MESMER default values but also have much literature precedent with both unimolecular and biomolecular gas-phase reactions.[99,105,107,109,110]

S8.2 Method Verification using Literature Precedent:

As mentioned in Section 2 in the main manuscript, there are many computational chemistry studies of atmospheric reactions, some including analysis of alkene ozonolysis or bimolecular Criegee intermediate reactions. Many of studies based on single-reference methods including here.[111–113] This includes some studies that compare how DFT-based or coupled cluster-based approaches model the ozone + ethene reaction compared with multi-reference treatments and a Gadzhiev *et al.* study states that "single-reference methods are quite adequate" for studying ethene ozonolysis.[111–113]

Furthermore, these studies show that coupled cluster approach gives the good results that close to the results of multireference approximation results" and "that correlated coupled cluster method (CCSD(T)-F12) provides a new standard of accuracy" and the work presented in this manuscript uses such a CCSD(T)-F12 based approach (*DF-LCCSD(T)-F12a/aug-cc-pVTZ*).[111–113] Additionally, in a study by Zhao *et al.*, the hybrid B3LYP functional was found to be high performance functional for these reactions, when using the multi-reference approaches as a standard, and it was found that differences in

structures optimised by C*CSD(T)/cc-pVTZ* and *B3LYP/6-311G(d,p)* have negligible effects on final computed barriers.[111,113]

S8.3 Computational-Experimental Intercomparison:

S8.3.1 Computational-Experimental Sensitivity Study

This *sensitivity analysis* has been assembled here to further underline the validity of the computational approach, *DF-LCCSD(T)-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ* (referred to in this section as the B3LYP-*optimised* approach), when compared with both experimental and theoretical studies. DFT approaches, here B3LYP, are purposely built /or selected largely their capability to model the particular target chemical systems. Two methods are used here to indicate a confidence level for the *B3LYP-optimised* approach: a *scope of agreeability* factor (Δ_{AGREE}) or a *sensitivity variation* factor (Δ_{SENSI}).

The *sensitivity variation* factor (Δ_{SENSI}), the second assessment of reliability, involves determining the relative Gibbs free energy of the TS structures derived from both experimental studies (ΔG_{EXP}) and other theoretical studies (ΔG_{THEO}). By reversing the rate constant equation below, and assuming that P_0 is assumed here to be 1 atmospheres pressure and applying the TS_{OZO} 1 pathway branching ratio produced from this study, the ΔG_{EXP} and ΔG_{THEO} values for TS_{OZO} 1 can be derived:

$$k_{EXP} = \boldsymbol{\kappa}\frac{k_B T}{h} \times \frac{RT}{P_0}\, e^{(-\Delta G_{exp})/RT} \qquad \textit{Equation S12}$$

$$\Delta G_{EXP}\ (TS_{OZO}\ 1) = -\ RT\ ln\left\{[k_{exp}\ \times \Gamma_{THEO}(TS_{AAAH}\ 1)] \times \frac{h}{k_B T\, \boldsymbol{\kappa}} \times \frac{P_0}{RT}\right\} \qquad \textit{Equation S13}$$

The *sensitivity variation* factor which measures differentials between Gibbs free energy barriers of different computational approaches can be derived using Equation 19. Both the *scope of agreeability* and the *sensitivity variation* factor equations feature the two vertical straight lines surrounding a section of the equation ($|\ |$) to convert the number or expression to the absolute value.

$$\Delta_{SENSI} = \frac{\sum(|\Delta G_{TS}\ (\text{B3LYP-}\textit{optimised}\ \text{approach}) - \Delta G_{TS}\ (\text{other approach})|)}{\text{Number of stationary points considered}} \qquad \textit{Equation S14}$$

Due to the nature of this method of determining the ΔG_{EXP} (TS_{OZO} 1) values used here, any differences in the Gibbs free energy for each transition states are likely to be the same across the potential energy surface. For this reason and for the purpose of simplicity only determining and comparing the ΔG_{EXP} for the TS_{OZO} 1 is required here is used here.

To determine the *scope of agreeability* (Δ_{AGREE}) involves finding the relative zero-point corrected energy of the stationary points relative to the raw reactants (ΔE_{SP}) on the potential energy surface using another approach, either using data the literature or calculating the potential energy using another approach. Here the author used the *DF-LCCSD(T)-F12a/aug-cc-pVTZ//M062X/aug-cc-pVTZ* approach, as well as data from other computational studies. This method can only be applied when comparing computational approaches. The difference between the ΔE_{SP} the *B3LYP-optimised* approach and the

alternative approach for each stationary point is determined and then averaged across for each potential energy surface, as shown in the Equation below.

$$\Delta_{AGREE} = \frac{\sum(|\Delta E_{SP}\,(\text{B3LYP-}\textit{optimised}\text{ approach}) - \Delta E_{SP}\,(\text{other approach})|)}{\text{Number of stationary points considered}} \qquad \textit{Equation S15}$$

A *scope of agreeability* factor (Δ_{AGREE}) or a *sensitivity variation* factor (Δ_{SENSI}) for various alkene ozonolysis reactions can be found in this section. Whereas *scope of agreeability* factor can be determined either using any/all stationary points, *sensitivity variation* factor is only be derived using the ozonolysis transition states. The main focus of the Δ_{SENSI} factor here is TS_{OZO} 1/TS_{OZO} 1.1 (see Table S58Table S59), except for Alkene **12**, which uses TS_{OZO} 1.2, as a comparison point as it is the only ozonolysis transition state calculated in the literature computational study, used as a comparison point. However, this is not a traditional error calculation, and instead the Δ_{AGREE} and Δ_{SENSI} values are derived by evaluating numerical discrepancies between *different* overall approaches.

The purely hydrocarbon alkenes included in this study are Propene and *E*- & *Z*-2-butene (Alkenes **1**, **17** & **18**) and, as shown in Table S58Table S59, propene and *E*-2-butene yield small sensitivity factor (Δ_{SENSI} ~ ±1 to ±3 kJ mol^{-1}), when compared to the experimental data, showing a high degree of reliability for the relative Gibbs free energy barriers calculated in this study. Even though the Δ_{SENSI} values for O_3 + *Z*-2-butene is marginally larger (~±5.6 kJ mol^{-1}), it is still the still modest size of Δ_{SENSI} value provide further confidence in this *B3LYP-optimised* approach.

The main alkenone included in this manuscript, methyl vinyl ketone (Alkene **5**), does have a more sizable but still modest *sensitivity variation* (~5 kJ mol^{-1}), similar to that seen for O_3 + *Z*-2-butene. The *sensitivity variations* were also calculated for the ozonolysis of halogenated alkenes, and it was found that Alkenes **11** & **14** had small Δ_{SENSI} values (~ ±1 to ±3.5 kJ mol^{-1}), when compared to the experimental values and the more finely tuned computational analysis of these ozonolysis barriers. In addition, while Alkenes **11** & **14** had larger Δ_{SENSI} values (~ ±3.3 to ±5.5 kJ mol^{-1}), the sensitivity factor are still relatively modest when compared to the variation within the experimental data too.

The literature does contain experimental rate data for many of these alkene ozonolysis reactions but not much in terms of recent computational data, with high level calculations, and so use of this agreeability factor is restricted to a few alkenes, specifically Alkenes **11**-**14**, (this data is found in Table S60Table S63). Both Alkenes **11** & **13**, have only mild differences between the relative zero-point energies, derived from the *CCSD(T)//M062X/6-311++(G(d,p)* approach used in the literature studies, and the relative zero-point energies of the same stationary points calculated for this study. [98,114] This is shown in the quite modest overall Δ_{AGREE} factors found for Alkenes **11** & **13** (~ ±3 - ±5 kJ mol^{-1}). Furthermore, the agreeability factors for the transition states are much smaller than for the minima too, which increases the reliability of the calculations presented here, as transition states are the most important factors when calculating the rate and product yields.

Data from the *Rao and Gejji* study of O_3 + Alkene **12**, does not show broad agreement with our work, when considering the agreeability factor. However, this may be due to the approach used, or due to the fact that this study does not cover as much of the potential

energy surface as explored in this manuscript. In contrast, a McGillen *et al*. study contains energy refined analysis of O_3 + Alkene **14**, including all pathways that we analyse in this study and the zero-point corrected energy barriers calculated show broad agreement with this study (Δ_{AGREE} ~ ±5.9 kJ mol^{-1}).

Overall, the ΔG_{THEO} values calculated using the *B3LYP-optimised* approach are shown to be in considerable alignment with ΔG_{EXP} values from the literature. Also, the overall modest Δ_{AGREE} factors seen when comparing the zero-point corrected energy barriers between this study and the literature, adds to the evidence that the approach adopted here is reliable. However, the main evidence for the reliability of the results calculated in this study is the largely modest *sensitivity variations* found in Table S58Table S59, further validating the use of *DF-HF/DF-LCCSD-F12a//B3LYP/aug-cc-pVTZ* approach used in the main manuscript.

Table S58: Sensitivity study of alkene ozonolysis reactions, comparing computationally generated results to that derived from other rate constants (k_{THEO} & k_{EXP}) by using the rate constant of dominant channel ($\mathbf{kTS_{OZO}\ 1} = k_{EXP} \times \Gamma_{THEO}$), and the computationally-determined tunneling constant ($\boldsymbol{\kappa}$), to determine the relative Gibbs free energy of the dominant channel ($\mathbf{\Delta G\ (TS_{OZO}\ 1)}$) see equations above; and the difference between these computationally/experimentally-derived $\mathbf{\Delta G\ (TS_{OZO}\ 1)}$ values and the ΔG_{THEO} ($\mathbf{TS_{OZO}\ 1}$) from this study produces an "sensitivity" factor (Δ_{SENSI}).

Alkene	**Method of Study**	**T (K)**	$\boldsymbol{k_{THEO}}$ **or** $\boldsymbol{k_{EXP}}$	$\boldsymbol{\Gamma_{THEO}}$	$\boldsymbol{k}\mathbf{TS_{OZO}\ 1}$	$\boldsymbol{\kappa}$	**ΔG TS$_{OZO}$ 1**	$\boldsymbol{\Delta_{SENSI}}$	**Ref**
			(cm^3 s^{-1})	**TS$_{OZO}$ 1**	**(cm^3 s^{-1})**		**kJ mol^{-1}**		
$CH_3CH=CH_2$ (Alkene **1**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	3.24×10^{-18}	0.842	2.73×10^{-17}	1.033	57.0	—	This study
	Experimental (298 K) * — IUPAC	**298.15**	1.05×10^{-18}		8.84×10^{-18}		59.8	-2.8	[115]
	Experimental (295 K) — *Avzianova & Ariya*	**298.15**	9.90×10^{-18}		8.34×10^{-18}		59.9	-3.0	[5]
	Experimental (295 K) — Neeb and Moortgat	**298.15**	1.15×10^{-18}		9.68×10^{-18}		59.6	-2.6	[13]
	B3LYP/aug-cc-pVTZ	298.15	7.42×10^{-16}	0.812	6.02×10^{-16}		49.3	7.7	This study
$CH_3C(O)CH=CH_2$ (Alkene **5**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	6.90×10^{-17}	0.916	6.32×10^{-17}	1.039	54.9	—	This study
	Experimental (298 K) * — IUPAC	298.15	5.20×10^{-18}		4.77×10^{-18}		61.3	-6.4	[97]
	Experimental (287 K) * — Ren *et al.* (2017)	287	5.10×10^{-18}		4.67×10^{-18}		59.0	-4.1	[23]
	Experimental (292 K) * — Grosjean *et al.* (1993)	292.18	4.72×10^{-18}		4.33×10^{-18}		60.3	-5.4	[24]
	Experimental (296 K) * — Grosjean and Grosjean (1999)	291	5.84×10^{-18}		5.35×10^{-18}		59.5	-4.6	[22]
	B3LYP/aug-cc-pVTZ	298.15	1.73×10^{-16}	0.823	1.42×10^{-16}		52.9	2.0	This study
E-$CH_3CH=CHCH_3$ (Alkene **17**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	3.61×10^{-16}	0.500	1.81×10^{-16}	1.042	52.3	—	This study
	Experimental (298 K) * — IUPAC	**298.15**	2.00×10^{-16}		1.00×10^{-16}		53.8	-1.5	[116]
	Experimental (298 K) — *Avzianova & Ariya (298)*	298.15	1.86×10^{-16}		9.30×10^{-17}		53.9	-1.6	[5]
	Experimental (298 K) * — Wegener et al 2007	298.15	2.38×10^{-16}		1.19×10^{-16}		53.3	-1.0	[9]
	B3LYP/aug-cc-pVTZ	298.15	5.05×10^{-15}	0.500	2.52×10^{-15}		45.7	6.6	This study
Z-$CH_3CH=CHCH_3$ (Alkene **18**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	1.18×10^{-15}	0.972	1.14×10^{-15}	1.017	47.7	—	This study
	Experimental (298 K) * — IUPAC	**298.15**	1.30×10^{-16}		1.26×10^{-16}		53.1	-5.5	[117]
	Experimental (298 K) * — Alam 2011	**298.15**	1.19×10^{-16}		1.16×10^{-16}		53.3	-5.7	[14]
	B3LYP/aug-cc-pVTZ	298.15	8.36×10^{-15}	0.964	8.06×10^{-15}		42.8	4.8	This study

Table S59: Sensitivity study of alkene ozonolysis reactions, comparing computationally generated results to that derived from other rate constants (k_{THEO} & k_{EXP}) by using the rate constant of dominant channel ($\mathbf{kTS_{OZO}\ 1} = k_{EXP} \times \Gamma_{THEO}$), and the computationally-determined tunneling constant ($\boldsymbol{\kappa}$), to determine the relative Gibbs free energy of the dominant channel ($\mathbf{\Delta G\ (TS_{OZO}\ 1)}$) see equations above; and the difference between these computationally/experimentally-derived $\mathbf{\Delta G\ (TS_{OZO}\ 1)}$ values and the ΔG_{THEO} ($\mathbf{TS_{OZO}\ 1}$) from this study produces an "sensitivity" factor (Δ_{SENSI}).

Alkene	Method of Study	T (K)	k_{THEO} or k_{EXP}	Γ_{THEO}	$k\mathbf{TS_{OZO}\ 1}$	κ	$\mathbf{\Delta G\ TS_{OZO}\ 1}$	Δ_{SENSI}	Ref
			(cm^3 s^{-1})	$\mathbf{TS_{OZO}\ 1}$	(cm^3 s^{-1})		kJ mol^{-1}		
$CF_3CF=CH_2$ (Alkene **11**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	1.14×10^{-20}	0.188	2.13×10^{-21}	1.082	80.5	—	This study
	Experimental (298 K) * — McGillen *et al.*	**296**	2.56×10^{-21}		4.80×10^{-22}		83.6	-3.1	[106]
	Experimental (298 K) * — Nielsen *et al.* (2007)	**298.15**	2.77×10^{-21}		5.20×10^{-22}		84.0	-3.5	[40]
	CCSD(T)//M06-2X/6-311++G(d,p) - Paul *et al.*	**298.15**	9.50×10^{-21}	1.000	9.50×10^{-21}		76.8	3.7	[114]
	M06-2X/6-311++G(d,p) - Paul *et al.*	**298.15**	3.11×10^{-18}		3.11×10^{-18}		62.5	18.1	[114]
	B3LYP/aug-cc-pVTZ	298.15	3.66×10^{-20}	0.285	1.04×10^{-20}		76.6	3.9	This study
$CF_3CF_2CH=CH_2$ (Alkene **12**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	2.99×10^{-20}	0.499	1.49×10^{-20}	1.033	75.6	—	This study
	Experimental (298 K) * — Sulbaek Andersen *et al.*	**298.15**	2.00×10^{-19}		9.98×10^{-20}		70.9	4.7	[42]
	Experimental (298 K) * — Soto *et al.*	**298.15**	2.34×10^{-19}		1.17×10^{-19}		70.5	5.1	[41]
	CCSD(T)/6-311G(d,p)//M06-2x/6-311++G(d,p) - Rao *et al*	298.15	1.01×10^{-19}	1.000	1.01×10^{-19}		70.8	4.7	[98]
	B3LYP/aug-cc-pVTZ	298.15	1.04×10^{-19}	0.474	4.92×10^{-20}		72.7	2.9	This study
E-$CF_3CH=CHCl$ (Alkene **13**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	1.85×10^{-20}	0.727	1.34×10^{-20}	1.085	76.0	—	This study
	Experimental (298 K) * — Sulbaek Andersen *et al.*	**295**	1.46×10^{-21}		1.06×10^{-21}		81.4	-5.4	[43]
	CCSD(T)/6-311G(d,p)//M06-2x/6-311++G(d,p) - Rao *et al*	298.15	5.00×10^{-20}	1.000	5.00×10^{-20}		72.7	3.3	[98]
	B3LYP/aug-cc-pVTZ	298.15	3.29×10^{-21}	0.531	1.75×10^{-21}		81.0	-5.1	This study
E-$CF_3CH=CHF$ (Alkene **14**)	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	298.15	8.11×10^{-21}	0.536	4.35×10^{-21}	1.063	78.7	—	This study
	Experimental (298 K) * — McGillen *et al.*	**298.15**	2.19×10^{-21}		1.17×10^{-21}		82.0	-3.2	[106]
	Experimental (298 K) * — Søndergaard *et al.*, 2007	298.15	2.81×10^{-21}		1.51×10^{-21}		81.3	-2.6	[44]
	B3LYP/aug-cc-pVTZ	298.15	2.76×10^{-20}	0.546	1.5×10^{-20}		75.7	3.1	This study

*Table S60: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of O_3 + 2,3,3,3-tetra-fluoropropene (Alkene **11**) relative to different computational chemistry approaches both from this study and the literature (Δ_{AGREE}).*

O_3 + 2,3,3,3-tetra-fluoropropene (Alkene **11**)			Zero-point corrected energy (kJ mol^{-1})							Ref
Study	**Approach**		PRC	TS_{OZO} 1	POZ 1	TS_{anti}	Anti-CF_3CFOO + HCHO	$TS_{fo}1$	HCHOO + CF_3FO	
This Study	*DF-LCCSD-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ*	ΔE	-18.5	31.3	-248.0	-120.9	-181.2	-188.1	-267.4	-
Paul *et al.*	*CCSD(T)//M062X/6-311++(G(d,p)*	ΔE	-	27.2	-237.7	-120.4	-182.1	-187.8	-263.8	114
Overall Δ_{AGREE} 3.28		Δ_{AGREE}	-	-4.1	10.3	0.5	-1.0	0.2	3.6	
Paul *et al.*	*DFT – only M06-2X/6-311++(G(d,p))*	ΔE	-	12.9	-306.9	-152.0	-229.2	-221.7	-308.6	114
Overall Δ_{AGREE} 38.53		Δ_{AGREE}	-	-18.4	-58.8	-31.1	-48.0	-33.6	-41.2	
This Study	*DFT – only B3LYP/aug-cc-pVTZ*	ΔE	-1.1	27.3	-225.5	-108.4	-199.0	-174.1	-275.7	-
Overall Δ_{AGREE} 13.79		Δ_{AGREE}	17.4	-3.9	22.5	12.6	-17.8	14.0	-8.4	

*Table S61: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of O_3 + 3,3,4,4,4-penta-fluoro-1-butene (Alkene **12**) relative to different computational chemistry approaches both from this study and the literature (Δ_{AGREE}).*

O_3 + 3,3,4,4,4-penta-fluoro-1-butene (Alkene **12**)			Zero-point corrected energy (kJ mol^{-1})							Ref
Study	**Approach**		PRC	TS_{OZO} 1.1	POZ 1.1	TS_{anti}	Anti-CF_3CF_2CHOO + HCHO	$TS_{fo}1$	HCHOO + CF_3CF_2CHO	
This study	*DF-LCCSD-F12a/aug-cc-pVTZ// B3LYP/aug-cc-pVTZ*	ΔE	-9.0	26.5	-209.3	-113.4	-176.5	-141.0	-196.8	-
Rao and Gejji	*CCSD(T)/6-311G(d,p)// M06-2x/6-311++G(d,p)*	ΔE	-14.9	20.9	-272.9	-149.7	-272.9	-180.6	-241.3	118
Overall Δ_{AGREE} ±41.72		Δ_{AGREE}	-5.9	-5.6	-63.7	-36.4	-96.4	-39.6	-44.5	
This study	*DFT – only B3LYP/aug-cc-pVTZ*	ΔE	-1.2	23.6	-192.0	-105.9	-191.1	-132.3	-209.4	-
Overall Δ_{AGREE} ±10.18		Δ_{AGREE}	7.8	-2.9	17.2	7.5	-14.6	8.7	-12.6	

*Table S62: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of O_3 + E-1-,chloro-3,3,3-tri-fluoro-1-butene (Alkene **13**) relative to different computational chemistry approaches both from this study and the literature (Δ_{AGREE}).*

O_3 + E-1-,chloro-3,3,3-tri-fluoro-1-butene (Alkene **13**)			Zero-point corrected energy (kJ mol^{-1})							Ref
Study	**Approach**		PRC	TS_{OZO} 1	POZ 1	TS_{ANTI}1	Anti-CF_3CHOO + ClCHO	TS_{SYN}1	syn-ClCHOO + CF_3CHO	
This study	*DF-LCCSD-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ*	ΔE	-12.0	26.2	-223.9	-148.1	-229.5	-136.4	-209.6	-
Rao and Gejji	*CCSD(T)/6-311G(d,p)//M06-2x/6-311++G(d,p)*	ΔE	-15.9	23.0	-216.7	-146.9	-216.7	-134.3	-205.9	98
Overall Δ_{AGREE} ±4.9		Δ_{AGREE}	-3.9	-3.2	7.2	1.3	12.7	2.1	3.8	
This study	*DFT – only B3LYP/aug-cc-pVTZ*	ΔE	1.3	31.2	-201.1	-136.5	-250.7	-115.2	-224.0	-
Overall Δ_{AGREE} ±15.7		Δ_{AGREE}	13.3	5.1	22.8	11.6	-21.2	21.2	-14.4	

*Table S63: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of O_3 + E-1-3,3,3-tetra-fluoro-1-butene (Alkene **14**) relative to different computational chemistry approaches both from this study and the literature (Δ_{AGREE}).*[106]

O_3 + E-1-3,3,3-tetra-fluoro-1-butene (Alkene **14**)			Zero-point corrected energy (kJ mol^{-1})												
Study	**Approach**		PRC1	TS_{OZO}1	POZ 1	PRC2	TS_{OZO}2	POZ 2	TS_{ANTI} 1	Anti-CF_3CHOO + FCHO	TS_{syn} 1	syn-FCHOO + CF_3CHO	TS_{ANTI} 2	anti-FCHOO + CF_3CHO	TS_{syn} 2	syn-CF_3CHOO + FCHO
This Study	*DF-LCCSD-F12a/aug-cc-pVTZ// B3LYP/aug-cc-pVTZ*	ΔE	-9.0	30.7	-245.4	-10.7	29.6	-235.0	-173.5	-266.4	-144.1	-211.4	-143.9	-207.6	-166.3	-263.0
McGillen *et al.*	*ωB97X-D/cc-pVTZ*	ΔE	-7.0	25.6	-259.4	-8.9	24.2	-248.1	-174.1	-275.0	-142.0	-220.9	-144.9	-219.5	-164.7	-269.6
Overall Δ_{AGREE} ±5.9		Δ_{AGREE}	2.0	-5.0	-14.0	1.8	-5.4	-13.1	-0.5	-8.6	2.1	-9.5	-1.0	-11.9	1.6	-6.6
This Study	*B3LYP/aug-cc-pVTZ* only	ΔE	1.0	28.1	-222.1	-0.1	26.6	-211.7	-160.9	-276.0	-129.3	-219.3	-131.8	-225.3	-150.1	-268.6
Overall Δ_{AGREE} ±5.5		Δ_{AGREE}	10.1	-2.6	23.3	10.5	-3.1	23.3	12.7	-9.6	14.8	-7.9	12.0	-17.7	16.3	-5.5

S8.3.2 Further Comparison of Computational & Experimental Rate Constants

To further support the evidence provided in this sensitive study, a log–log plot of the literature experimental rate coefficients as a function of the results of the calculated rate constants is provided in Figure S16, with errors of the experimental data representing the experimental uncertainties.[1,2,5,12,20,40,41,43,44,87,97,106,115–117,119,120] The numerical values of these experimental rate coefficients and calculated rate constants are found in Table 2 in the main manuscript.

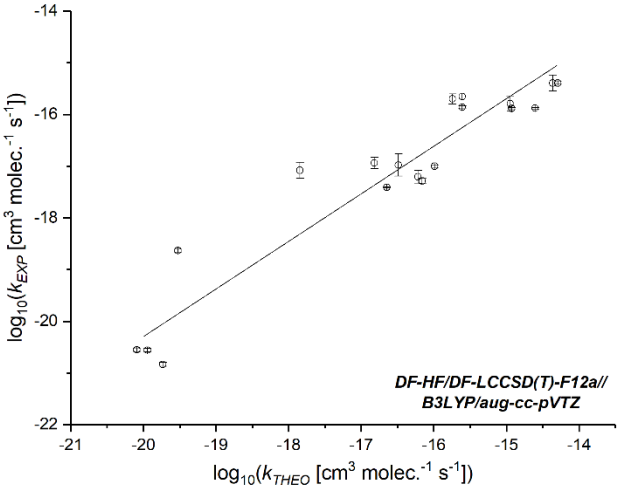

Figure S16: The present theoretical rate coefficients for alkene ozonolysis reactions plotted as a function of the rate constants determined with the present CTST calculations using the results of barrier heights obtained at the

The relationships between the experimental & theoretical rate constants shows a clear and strong linearity in the log–log plot and using a linear least-squares analysis the fit results parameters of this plot is a slope of 0.870 ± 0.073 and an intercept of -2.709 ± 1.215. As with any model, there is some variation in the exact accuracy of this approach's capability to model different alkenes as is shown by the fact that the intercept is a notable non-negligible offset k_{EXP}-k_{THEO} relationship shown on the log-log graph. However, the slope of the fitted line of the log-log plot, while smaller than unity, is still considered close enough to a 1-to-1 relationship that the B3LYP-based approach is considered to produce rate constants with a higher accuracy, when using other log-log plots of k_{EXP}-k_{THEO} relationships in the literature as a benchmark.[39]

Furthermore, this log–log plot showing a strong linearity with a correlation coefficient of ~0.945, which is near enough to unity. This adds to the evidence that the master equation rate constants based on the DF-HF/DF-LCCSD(T)-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ approach used in this study is quite effective at ascertaining the relative reactivities of ozone with a wide variety of alkenes. Additionally, the sensitivity study also shows that this *B3LYP*-based approach provides relative barrier heights in close proximity (within 6-8 kJ mol^{-1}) to the recent literature for both experimental and theoretical results, a degree of variation acceptable for a computational chemistry study.

S8.3.3 Literature Precedent for Alkene Ozonolysis at Standard Temperature and Pressure

The *International Union of Pure and Applied Chemistry* (IUPAC) group produces a series preferred values for rate constants at standard temperature and pressure for a significant array of the alkene ozonolysis reactions, including many of the reactions studied here.[97,115–117,119,121–124] The research found in the IUPAC task evaluations shows that alkene ozonolysis produces rate constants (10^{-18} – 10^{-16}) large enough that these reactions is likely an important process at ground level (standard pressure), occur at a range of atmospheric temperatures around standard temperature.[97,115–117,119,121–123]

The literature shows that ozone and alkenes have a significant tropospheric abundance at ground level because many of the prominent rural and urban sources of Alkenes are ground-based (e.g. vehicle exhausts, chemical plants and foliage) and ground-based anthropogenic activity (e.g. wood-burning) also produces significant O_3 emissions.[125–129] As mentioned previously, in situ detection of sCIs is difficult in the troposphere, due to their short-lifetimes, but studies have identified definitive signatures of sCI-specific reaction products in the troposphere, including the products of sCI reactions with organic acid.[130–133]

As alkene ozonolysis is the main source of atmospheric sCIs, these product signatures provide more evidence showing that alkene ozonolysis occurs at and conditions quite proximate to standard atmosphere temperature-pressure. Given this and that the IUPAC standard preferred values are derived for standard atmosphere temperature-pressure, during this study, unless stated otherwise, all rate constants and product branching ratios in this manuscript were calculated using standard pressure and temperature

S8.4 Additional Literature Details on CI fragmentation and OH yields

S8.4.1 Importance of *syn*-CIs as sources of OH

As discussed in the main manuscript of this article, in the aftermath of alkene ozonolysis, the CIs react/fragment so swiftly that the CI yields have to be determined indirectly using the branching fraction of the carbonyl co-product.[3,134-136] However, many CIs, such as CH_3CHOO, form into *anti*- & *syn*-conformer that do not interconvert, and the carbonyl co-product yields only provide the collective branching fractions of the of these two conformers. The *anti* & *syn* conformers CIs often fragment via different mechanisms to produce different secondary products, and so within this study and much of the literature, relative conformer yields are instead inferred from the products of the unimolecular decay.[3,137]

The key secondary product used to infer *syn*-CI yields in this study are OH radicals, which are understood to be the result of a *syn*-CI, like *syn*-CH_3CHOO & *syn*-EtCHOO (but not *syn*-iPrCHOO & *syn*-tBuCHOO), breaking down through an α-H atom on a *syn*-alkyl group transferring to the terminal oxygen on the carbonyl oxide.[3] This 1,4 H-transfer mechanism forms a vinyl hydroperoxide (VHP), which then fragments to release an OH radical.[57,80,103,138,139] For the OH radical yield to be generated from the CI there firstly has to an α-H atom on a *syn*-alkyl group and then the 1,4 H-transfer mechanism has to be energetically favourable compared to other mechanism.

For example, both *anti*-CH_3CHOO & *anti*-EtCHOO do not have *syn*-alkyl groups and so they cannot react via the 1,4 H-transfer mechanism and their most energetically favourable mechanism for these CIs is the 1,3-cyclisation that produces a short-lived dioxirane species.[140] In contrast, according to a study by Vereecken *et al.*, while *syn*-CIs can both break down via the 1,3-cyclisation, for CIs with smaller *syn*-alkyl groups, this process significantly slower than 1,4-H-migration and so the VHP channel dominates the breakdown of *syn*-CH_3CHOO & *syn*-EtCHOO.[57] The high reactivity of the 1,4-H-migration is reflected in the rapid decay of a CIs with α-H atom on a *syn*-alkyl group (*syn*-CH_3CHOO, *syn*-EtCHOO & $(CH_3)_2COO$) over those without (*anti*-CH_3CHOO, *anti*-EtCHOO & CH_2OO) displayed in Table S64.

Table S64: Unimolecular rate constants (k_{UNI}) of Criegee Intermediates in this study derived by Vereecken et al.[57]

k_{uni} (s^{-1})	CH_3CHOO	EtCHOO	^{i}PrCHOO	^{t}BuCHOO	CH_2OO	$(CH_3)_2COO$
Syn-	136	205	6.7	0.01	0.3	478
Anti-	53	74	102	111		

The speed of the 1,4-H-migration, reflected in their high unimolecular decay rates, implies that a high OH yield from an alkene ozonolysis reaction can indicate a higher yield of *syn*-CH_3CHOO or *syn*-EtCHOO over their *anti*-CI equivalents. Furthermore, so even if, as some studies suggest, the *anti*-CH_3CHOO or *anti*-EtCHOO can breakdown to produce slight yields of OH radicals, these yields would be negligible compared to any OH yield from a significant *syn*-CH_3CHOO or *syn*-EtCHOO branching fraction.[140]

However, also seen in Table S64 is that the greater unimolecular decay rates seen for *syn*-CIs over *anti*-CIs does not continue for iPrCHOO & tBuCHOO. This is partially due to the fact that, as observed by Vereecken *et al.*, as the alkyl group *anti*-CIs becomes more substituted the 1,3-ring closure barrier lowers, increasing the decay rate of *anti*-iPrCHOO & *anti*-tBuCHOO over *anti*-CH_3CHOO & *anti*-EtCHOO.[57]

The small rate constant for *syn*-tBuCHOO is largely due to the fact that as *syn*-alkyl group no longer has any α-H atom, it cannot proceed via the swift 1,4 H-transfer mechanism or produce significant OH yields. Furthermore, whereas the position of the tBu group on the *anti*-CI counterpart is far away from the active sight of the 1,3-ring closure, the bulk of the *syn* orientated tBu group will significantly inhibit the movement within any 1,3 ring-closure mechanism.

While *syn*-iPrCHOO can breakdown via a 1,4-H-migration, the *syn*-iPr group has one α-H atom this reducing the propitious of this VHP channel. Vereecken *et al.* reports that as a sizeable the CI population adopts substituent orientations that diminish the favourability of 1,4-H-migration (such as if the H atom adopts an anti-orientation to the carbonyl oxide group).[57] The VHP channel still dominates the breakdown of *syn*-iPrCHOO but the slower rate of reaction may lead to some CI stabilisation marginally may impact OH yields.[57] So, it is likely that if there is some OH yield from the ozonolysis of an alkene, like Alkene **3**, where no other OH source is likely, this could be indicative of a significant *syn*-iPrCHOO branching fraction. However, determining the impact of this slower rate on OH yields is beyond the scope of this study.

S8.4.2 Potential other CI sources of OH yield

Broadly, any Criegee intermediate with α-H atoms in a *syn*-alkyl group such as a *syn*-CH_3, will have a potential decay pathway where the α-H transfers to the terminal oxygen on the COO pathway to produce a vinyl hydroperoxide (VHP). Much of the literature agrees that this is the dominant pathway for the breakdown of *syn*-CH_3CHOO and *syn*-EtCHOO (DOI: 10.1039/C7CP05541B).[57,141] Often, this leads to the COOH group seeing a O-O bond fission, generating an OH radical. This "VHP pathway" decay process is agreed to be the dominant source of OH radicals from CI decay and it as a pathway is inaccessible to most "anti-CIs" as they do not have α-H atoms in a *syn*-alkyl group.[57]

However, the issue is that a slower minor mechanism does generate OH radicals from other CIs without α-H atoms in a *syn*-alkyl group as shown in the IUPAC datasheet of the unimolecular decay of CH_2OO.[121,140,142] In some of the literature that the unimolecular fragmentation of CH_2OO with excess energy and some *anti*-CI species like anti-CH_3CHOO, proceeds largely through a 1,3-cyclisation, producing an $RHCO_2$ ring known as a dioxirane.[106,140] This highly energised dioxirane subsequently reopens to form a bisoxy O–C–O biradical and then rearranges to produce a "hot" RC(O)OH acid, and this is why it is referred to as a "hot acid" channel.[143] One minor decay pathway considered for this "hot" RC(O)OH acid is that it sees an O-O bond fission to produce RCO radicals and a marginal OH.[140,142]

However, the OH yield from the "hot acid" pathway is much more marginal, with a maximum yield of 15-18% under the most favourable of circumstances (according to IUPAC datasheet of O_3 + ethene: *Ox_VOC5*), as CH_2OO and *anti*-CIs are much more likely to

breakdown via other routes or stabilise and react further.[121,121,140] Whereas it is worth emphasizing here that the “VHP pathway” decay from *syn*-CIs are both much more rapid and are thought to produce very high yield of OH radicals (sometimes >99%).[57,144] Therefore it is still the case that high OH yields are significantly indicative of yields of *syn*-CH3CHOO, *syn*-EtCHOO over their anti-counterparts.

S8.5 Additional Computational Details on the Kinetics of *syn*-CI fragmentation

When considering the product branching fractions found in Tables 3 & 4 in the main body of the manuscript, it is clear that the relevance of this TS_{SYN} pathway decreases sequentially as we transition from Alkene **1** to **4**. To determine the factors involved in this declining importance it is advisable to assess the different kinetic or thermodynamics effects involved in the competing POZ fragmentation processes. To review the different factors involved the thermochemical properties relating to heat of formation of these O_3 + Alkene **1**-**4** reactions, which are found in Table S65.

*Table S65: Thermochemical properties of the Ozonolysis of Alkenes **1**-**4**. Thermodynamic energy parameters for the 1,3-cycloadditon step are set relative to raw reactants. All thermodynamic energy parameters listed for the POZ fragmentation process are obtained set as relative to the POZ intermediate. Calculated using computational approach DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ.*

Alkene 1 + O_3	**Heat of Formation of Product (kJ mol^{-1})**		**Alkene 2 + O_3**	**Heat of Formation of Product (kJ mol^{-1})**	
Reaction Channels	**ΔH_{298}**	**ΔG_{298}**	**Reaction Channels**	**ΔH_{298}**	**ΔG_{298}**
Alkene **1** + O_3 → POZ 1	-240.9	-186.4	Alkene **2** + O_3 → POZ 1.3	-242.2	-187.1
Alkene **1** + O_3 → POZ 2	-241.5	-186.3	Alkene **2** + O_3 → POZ 2.3	-243.8	-188.0
POZ 1 → *anti*-CH_3CHOO+CH_2O	7.6	-47.3	POZ 2.3 → *anti*-EtCHOO +CH_2O	9.9	-45.8
POZ 1 → *syn*-CH_3CHOO +CH_2O	-7.1	-61.0	POZ 2.3 → *syn*-EtCHOO +CH_2O	-2.6	-58.0
POZ 1 → CH_3CHO + CH_2OO	1.9	-55.3	POZ 2.3 → EtCHO + CH_2OO	2.5	-55.5
Alkene 3 + O_3	**Heat of Formation of Product (kJ mol^{-1})**		**Alkene 4 + O_3**	**Heat of Formation of Product (kJ mol^{-1})**	
Reaction Channels	**ΔH_{298}**	**ΔG_{298}**	**Reaction Channels**	**ΔH_{298}**	**ΔG_{298}**
Alkene **3** + O_3 → POZ 1.1	-239.3	-183.6	Alkene **4** + O_3 → POZ 1	-240.7	-185.3
Alkene **3** + O_3 → POZ 2.2	-243.6	-187.0	Alkene **4** + O_3 → POZ 2	-241.5	-185.0
POZ 2.3 → *anti*-iPrCHOO+CH_2O	12.0	-44.8	POZ 1 → *anti*-tBuCHOO +CH_2O	8.4	-48.5
POZ 2.3 → *syn*-iPrCHOO+CH_2O	1.6	-53.8	POZ 1 → *syn*-tBuCHOO +CH_2O	6.6	-48.0
POZ 2.3 → iPrCHO + CH_2OO	4.8	-54.4	POZ 1 → tBuCHO + CH_2OO	0.0	-59.4

It is clear that for each of reaction, that the POZ formation is highly exothermic (ΔH_{298} < -200 kJ mol^{-1}) and the drop in Gibbs free energy (ΔG_{298} < -180 kJ mol^{-1}) suggests that the reaction is spontaneous. The excess of the energy from exothermicity of the first step leads to the barrier of the POZ fragmentation steps being surmounted, as described in the main body of the text.

However, when considering POZ fragmentation steps alone, the enthalpy of formation of the products (also found in Table S65), it can be inferred that both the formation pathways that produce the *anti*-R_1CHOO + CH_2O (ΔH_{298} ~ 7 – 11 kJ mol^{-1}) and the CH_2OO + RCHO (ΔH_{298} ~ 0 – 5 kJ mol^{-1}) products are all mildly endothermic, relative to the lowest energy POZ. However, the *syn*- R_1CHOO + CH_2O enthalpy of formation of Alkene **1** + O_3 is negative and therefore is mildly exothermic. But the relative heat of formation of the *syn*-R_1CHOO + CH_2O products increases incrementally from Alkene **1** to **4**, to the point that *syn*-tBuCHOO + CH_2O is mildly endothermic. However, the ΔG_{298} values for all CI + aldehyde products are below that of the lowest energy POZ and therefore this process is inferred to be thermodynamically spontaneous.

The heat of reaction for the *syn*-CI does become more unfavourable progressively from Alkene **1** to **4**, principally because the greater bulk of the *syn*-R group increase steric interaction with the COO group, which increases the energy of the CI molecule. This is in contrast to the *anti*- R_1CHOO + CH_2O and the CH_2OO + RCHO product pairs, which see little difference in their relative heat of formations across the O_3 + Alkene **1** to **4** reactions. This broadly indicates that the branching fraction of *syn*-CH_3CHOO from O_3 + Alkene **1**, is much greater than that of *syn*-tBuCHOO from O_3 + Alkene **4**, an assumption that is broadly in agreement with the results in the manuscript. However, despite the fact that *syn*-CH_3CHOO + CH_2O has the lowest heat of formation of the three product pairs, the *syn*-CH_3CHOO yield from O_3 + Alkene **1** is still smaller than that of both *anti*- R_1CHOO + CH_2O and the CH_2OO + R_1CHO. This increases the evidence for the α-H atoms providing some stabilisation to the *syn*-CH_3CHOO species. This shows that while the relative heat of formations does have some impact on the favourability on CI branching fractions, it does not dictate product yield.

When determining the factors in the decline in *syn*-CI yields both the number of pathways and the favourability of those pathways needs to be considered and therefore the energy, enthalpy and free energy barriers and the product branching fractions of POZ fragmentation pathway barriers for O_3 + Alkenes **1**-**4** are displayed in Table S66. The number of pathways is particularly important when considering the yield of CH_2OO + R_1CHO from O_3 + Alkene **1** to **4**. For example, it is clear that the TS_{SYN} barrier, for O_3 + Alkenes **1**, is lower than both TS_{FO} barriers, but, as there are multiple TS_{FO} barriers, the yield of CH_2OO + CH_3CHO is higher than that of *syn*-CH_3CHOO + CH_2O. Whereas, the yield for *anti*-CH_3CHOO is greater than *syn*-CH_3CHOO simply because of the lower TS_{ANTI} barrier (see Table S66).

*Table S66: Relative Energies (ΔE), zero-point corrected energies (ΔZPE), relative enthalpy at 298 K ($\Delta H_{298.15}$), relative Gibbs free energy ($\Delta G_{298.15}$), and product branching fractions of POZ fragmentation pathway barriers for O_3 + Alkenes **1**-**4**, with a particular focus on TS_{SYN} pathways. Calculated using computational approach DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ.*

Alkene No.	TS	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**	**Γ_{THEO}**
Alkene **1**	TS_{ANTI}	-172.3	-162.8	-167.5	-114.4	0.438
	TS_{FO} (range)	*-167 to -164*	*-157 to -154*	*-162 to -159*	*-108 to -106*	0.323
	TS_{SYN}	-171.2	-161.1	-166.2	-112.1	0.239
Alkene **2**	*TS_{ANTI} (range)*	*-174 to -172*	*-164 to -162*	*-169 to -165*	*-115 to -113*	0.427
	TS_{FO} (range)	*-168 to -164*	*-158 to -155*	*-163 to -160*	*-109 to -106*	0.373
	TS_{SYN} 1	-172.1	-162.5	-167.2	-112.4	0.089
	TS_{SYN} 2	**-160.3**	**-150.7**	**-155.4**	**-100.9**	**0.051**
	TS_{SYN} 3	-173.3	-163.3	-168.0	-113.3	0.092
Alkene **3**	*TS_{ANTI} (range)*	*-173 to -170*	*-164 to -161*	*-168 to -165*	*-114 to -111*	0.431
	TS_{FO} (range)	*-168 to -163*	*-160 to -155*	*-164 to -159*	*-110 to -104*	0.454
	TS_{SYN} 1	**-160.1**	**-150.5**	**-155.2**	**-100.1**	**0.026**
	TS_{SYN} 2	-170.9	-161.1	-165.7	-110.0	0.072
	TS_{SYN} 3	**-159.6**	**-149.5**	**-154.1**	**-98.7**	**0.020**
Alkene **4**	TS_{ANTI}	-173.1	-164.1	-168.0	-113.9	0.470
	TS_{FO} (range)	*-169 to -164*	*-160 to -155*	*-164 to -159*	*-108 to -106*	0.471
	TS_{SYN}	**-160.8**	**-151.5**	**-155.9**	**-100.3**	**0.059**

It is important to note here that the -R_1 groups on Alkenes **2** & **3** are augmented to a point where each POZ fragmentation pathway exists in triplicate, due to the increased

conformational flexibility. However, Alkene **4** has much restricted conformational flexibility and so does not display POZ fragmentation pathways in triplicate. When reviewing the overall chemistry of O_3 + Alkene **2** or **3**, each TS_{ANTI} pathway only varies a little between these different "subchannels", with the zero-point corrected TS_{ANTI} 1-3 barriers remaining largely within ~3-5 kJ mol^{-1} of each other and not varying too much between Alkenes **1**-**4** either (see Table S66). The same could be said for the multiple TS_{FO} barriers, which also only vary by a small ~3-6 kJ mol^{-1} both within the same ozonolysis reaction and largely between the different O_3 + Alkene **1**-**4** reactions.

However, as the -R_1 group is incrementally augmented from Alkenes **1** to **4**, the TS_{SYN} barriers can alter in energy, with the TS_{SYN} barriers falling into two categories a lower energy group (ΔZPE ~ -163 to -160 kJ mol^{-1}) and a higher energy mechanism (ΔZPE ~ -152 to -149 kJ mol^{-1}), which are in bold in Table S66. Furthermore, the prevalence of the higher energy mechanism increases as the -R_1 group sequentially increases in bulk, to the point where the only TS_{SYN} barrier on the O_3 + Alkene **4** potential energy surface is a higher energy mechanism. No analogous increase is reflected in either TS_{ANTI} or TS_{FO} channels. So it is clear that the increased prevalence of this higher TS_{SYN} energy mechanism is responsible for the stepwise decline in *syn*-R_1CHOO yields from O_3 reactions with Alkenes **1** to **4**.

When considering how much of the change in product distribution of *syn*-R_1CHOO is due to the kinetic effects or thermodynamic impacts, it is important to review the any enthalpy or exergonic changes, which are found in the $\Delta H_{298.15}$ & $\Delta G_{298.15}$ values of the TS barrier. It is clear that the differences between lower energy TS_{SYN} barriers and high energy TS_{SYN} barriers are ~10 kJ mol^{-1} within the same reaction but this ~10 kJ mol^{-1} difference in energy between high and low energy TS_{SYN} barriers is seen in the zero-point corrected energy and is maintained in both the $\Delta H_{298.15}$ & $\Delta G_{298.15}$ values. Viewing these results it would appear that there is little increase in thermodynamically spontaneity of the TS_{SYN} mechanism and that most of the increase in reaction barrier is likely due to increased kinetic effects, particularly steric interactions.

When reviewing the over transition state structures for Alkene **1**, there is likely some steric interaction and this continues throughout both the low & high energy TS_{SYN} mechanism for the ozonolysis reactions of Alkenes **1**-**4**. The first high energy TS_{SYN} mechanism is TS_{SYN} 2 on Alkene **2** and, as seen in Figure S17, there is one structural difference are very clear structural difference compared to the low energy TS_{SYN} mechanisms. That is the orientation of the -Et group inwards towards the POZ structure, particularly the the terminal oxygen on the COO group. While the intramolecular distances do not alter drastically, that orientation distorts the overall POZ structure and increasing the reaction barrier. (For any further details on geometric distances seen within stationary point structures, all cartesian co-ordinates of all stationary points are found in SI Section 10)

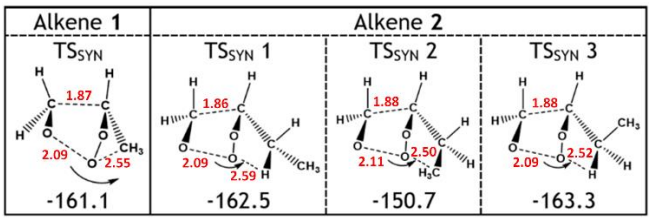

*Figure S17: Geometries and energies of the different TS_{SYN} structures of the O_3 reactions with Alkenes **1** & **2**. The arrows in the figure show the movement that takes place as the molecule proceeds through the transition states and indicates what steric interactions might result. Also included are selected intramolecular distances in the POZ structure in the C-C bond fission, the O-O bond fission and the distance between the terminal oxygen of the CI and the R_1 group (Å). Energies (in kJ mol^{-1}) are relative to raw reactants.*

This is further reflected in TS_{SYN} 1 & 3 on Alkene **3** which both see this greater steric interaction between the alkyl -iPr group at certain orientations and the active site of the TS_{SYN} structure. Therefore, both TS_{SYN} 1 & 3 see an increase in barrier heights and a concurrent drop in overall *syn*-iPrCHOO yields for O_3 + Alkene **3** (Γ_{SYN} ~0.115). This culminates in the bulky -tBu group on Alkene **4** causing the ozonolysis reaction to have the only TS_{SYN} barrier be high in energy (-160.8 kJ mol^{-1}) and therefore the yield for syn-tBuCHOO is very low (Γ_{SYN} ~0.059).

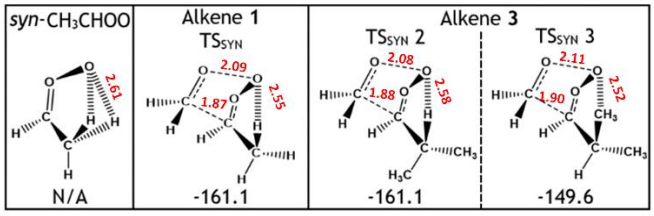

*Figure S18: Schematic featuring the stabilising role of a-H atoms in a syn-CHR_2 group in relation to the terminal oxygens in the carbonyl oxide group, using the ozonolysis of Alkenes **1** & **3**. Also included are selected intramolecular distances in the POZ structure in the C-C bond fission, the O-O bond fission and the distance between the terminal oxygen of the CI and the R_1 group (Å).*
Energies (in kJ mol^{-1}) are relative to raw reactants.

Overall, it is clear that the greater steric interaction between the alkyl -R_1 group at certain orientations and the active site of the TS_{SYN} structure causes distortions in the TS structure and increase in energy for the TS_{SYN} barrier of ~10 kJ mol^{-1}. Also, Alkenes **1** to **4** sees a stepwise increase the proportion of transition states with these steric interactions and concurrent increase the number of higher energy TS_{SYN} barrier, with Alkene **4** only having a higher energy TS_{SYN} barrier. Therefore, it is clear that the increased dominance of this higher TS_{SYN} energy mechanism is responsible for the stepwise decline in *syn*-R_1CHOO yields from O_3 reactions with Alkenes **1** to **4**.

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S10.0 Cartesian Coordinates And IRCs of the Alkene Ozonolysis Reactions

S10.1 Reactants

S10.1.1 Ozone

Compound: O_3	**Energy (Hartree)** -225.232118853147
Reaction Coordinates: 8 -0.000000 0.000000 0.429077 8 0.000000 1.077304 -0.214539 8 -0.000000 -1.077304 -0.214539	**Frequencies (cm^{-1}):** 745.8860, 1189.8635, 1249.1307

S10.1.2 Alkenes

Compound: 1-Propene (Alkene 1)	**Energy (Hartree)** -117.734202583006
Reaction Coordinates: 6 -1.230938 0.162150 0.000000 6 0.133754 -0.452181 0.000000 6 1.278183 0.219838 0.000000 1 2.233452 -0.287527 0.000000 1 1.300084 1.303347 0.000000 1 0.166634 -1.537973 0.000000 1 -1.180079 1.250999 -0.000004 1 -1.803043 -0.153849 -0.876177 1 -1.803039 -0.153842 0.876181	**Frequencies (cm^{-1}):** 204.9479, 425.8636, 592.517, 924.196, 947.717, 950.3007, 1027.4886, 1075.0243, 1192.5587, 1330.7287, 1409.8921, 1452.5855, 1479.5898, 1494.4211, 1708.0283, 3014.1612, 3054.976, 3090.0181, 3122.2949, 3128.6327, 3208.6582

Compound: 1-Butene con 1 (Alkene 2)	**Energy (Hartree)** -156.990868091369
Reaction Coordinates: 6 -0.536459 -0.517092 0.305759 6 0.720848 0.298931 0.330086 6 1.858817 -0.019671 -0.274312 1 1.960541 -0.935339 -0.845149 1 2.729712 0.619667 -0.219444 1 0.667703 1.230181 0.888931 6 -1.728322 0.242406 -0.290499 1 -2.633603 -0.365138 -0.259588 1 -1.925489 1.162189 0.263200 1 -1.537492 0.514803 -1.329163 1 -0.363084 -1.438686 -0.254199 1 -0.787596 -0.815119 1.329209	**Frequencies (cm^{-1}):** 109.5259, 228.1782, 317.2718, 433.7871, 654.5041, 797.6579, 857.8692, 950.0516, 991.6019, 1019.2921, 1035.3656, 1095.9436, 1201.3788, 1291.9326, 1324.9038, 1347.1325, 1409.6417, 1459.0333, 1483.6329, 1498.3084, 1506.7266, 1703.7339, 3001.7445, 3024.8565, 3045.1892, 3085.1411, 3091.1432, 3111.3755, 3126.3992, 3207.0069

Compound: 1-Butene con 2 (Alkene 2)	**Energy (Hartree)** -156.990759930222
Reaction Coordinates: 6 0.638811 0.717833 0.000002 6 -0.854431 0.555674 -0.000001 6 -1.533105 -0.585545 0.000001 1 -1.044066 -1.550718 0.000003 1 -2.614680 -0.591931 -0.000001 1 -1.413272 1.487408 -0.000005 6 1.454633 -0.570783 -0.000001 1 2.521758 -0.347745 0.000001 1 1.242067 -1.177482 0.881388 1 1.242069 -1.177476 -0.881395 1 0.915341 1.327440 -0.867565 1 0.915339 1.327437 0.867571	**Frequencies (cm^{-1}):** 160.259, 257.6184, 275.4325, 547.3184, 564.6587, 805.1812, 837.0941, 947.1934, 998.2798, 1032.782, 1038.5949, 1110.213, 1146.5461, 1293.5114, 1334.6517, 1381.0385, 1411.6583, 1456.0652, 1475.7496, 1499.0556, 1508.9344, 1703.3793, 2995.8815, 3008.4799, 3029.2014, 3087.4202, 3091.1398, 3117.9322, 3140.3888, 3214.7309

Compound: 3-methyl-1-Butene con 1 (Alkene 3)	**Energy (Hartree)** -196.250016454020
Reaction Coordinates: 6 -0.369797 -0.000000 -0.307860 6 0.949413 -0.000003 0.412744 6 2.145751 -0.000001 -0.161515 1 3.056614 -0.000003 0.422167 1 2.257390 0.000004 -1.239614 1 0.886880 -0.000008 1.499171 1 -0.165906 0.000000 -1.382726 6 -1.174768 -1.264206 0.028387 1 -0.628045 -2.165889 -0.248287 1 -1.387431 -1.316605 1.098771 1 -2.129533 -1.267701 -0.500422 6 -1.174763 1.264209 0.028389 1 -0.628035 2.165890 -0.248285 1 -2.129527 1.267709 -0.500419 1 -1.387425 1.316608 1.098773	**Frequencies (cm^{-1}):** 98.8235, 222.6742, 239.6225, 313.4523, 321.4543, 347.0894, 504.5264, 697.5098, 801.1446, 930.7808, 932.2227, 951.0227, 963.7819, 1007.3587, 1036.2437, 1115.241, 1185.2275, 1218.5117, 1322.1315, 1337.3236, 1342.1606, 1396.8721, 1416.4007, 1461.1698, 1488.9058, 1489.881, 1501.9278, 1510.7555, 1701.7048, 3009.9448, 3016.5794, 3020.9294, 3073.2624, 3079.7035, 3090.4561, 3091.8414, 3102.8104, 3125.4857, 3205.8722

Compound: 3-methyl-1-Butene con 2 (Alkene 3)	**Energy (Hartree)** -196.249609684300
Reaction Coordinates: 6 0.471638 -0.018352 -0.417232 6 -0.896450 -0.628921 -0.257404 6 -1.985773 -0.052916 0.237060 1 -2.918762 -0.595435 0.310334 1 -1.994966 0.971569 0.584568 1 -0.966572 -1.663115 -0.585257 1 0.708452 -0.064473 -1.487926 6 0.562071 1.443577 0.017004 1 -0.142226 2.070983 -0.530164 1 0.352517 1.552418 1.083076 1 1.565193 1.831589 -0.163949 6 1.521043 -0.879191 0.306284 1 1.478788 -1.918362 -0.023504 1 2.528122 -0.506270 0.113506 1 1.354279 -0.864087 1.385038	**Frequencies (cm^{-1}):** 114.6497, 235.0579, 260.5161, 286.8624, 350.9344, 382.2605, 539.2118, 674.5589, 781.4482, 923.1806, 932.5024, 950.0535, 969.3309, 1033.2886, 1043.7479, 1117.0369, 1154.9103, 1207.1747, 1319.3983, 1339.8844, 1369.4212, 1399.9641, 1416.4501, 1457.613, 1490.4591, 1493.7712, 1503.9212, 1513.9373, 1699.5984, 2972.0167, 3019.9562, 3025.481, 3080.4557, 3084.0765, 3086.0992, 3090.2351, 3110.3928, 3140.0824, 3214.3701

Compound: 3,3-dimethyl-1-Butene (Alkene 4)	**Energy (Hartree)** -235.509880163998
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.351150 -0.001909 -0.000000 6 1.009060 0.660323 0.000000 6 2.201853 0.078085 0.000000 1 2.326643 -0.996421 -0.000000 1 3.108508 0.668311 -0.000000 1 0.969826 1.747386 0.000000 6 -1.115401 0.467384 -1.254902 1 -2.127636 0.058245 -1.262419 1 -1.193783 1.555680 -1.284174 1 -0.609550 0.142645 -2.165026 6 -0.262357 -1.531765 0.000002 1 -1.263343 -1.965983 0.000003 1 0.260348 -1.901743 -0.883122 1 0.260348 -1.901740 0.883127 6 -1.115403 0.467388 1.254900 1 -2.127638 0.058248 1.262417 1 -0.609553 0.142651 2.165025 1 -1.193785 1.555684 1.284168	104.7515, 226.713, 264.1669, 285.0811, 291.744, 314.8559, 350.0099, 385.3784, 402.5624, 526.5443, 699.9181, 714.1615, 883.0131, 927.0951, 938.5748, 951.0736, 963.7101, 1016.7692, 1039.6134, 1050.5989, 1091.827, 1222.6682, 1231.8623, 1291.626, 1341.9136, 1395.8354, 1399.3707, 1423.351, 1457.8098, 1481.6925, 1488.1651, 1491.7312, 1504.8251, 1504.9522, 1522.0759, 1697.4588, 3016.3606, 3019.0744, 3027.0225, 3076.5819, 3080.1217, 3085.1923, 3085.4136, 3089.3936, 3089.6833, 3104.2194, 3139.7976, 3213.9846

Compound: Methyl Vinyl Ketone (Alkene 5) Con 1	**Energy (Hartree)** -230.947246392397
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.745082 -0.601228 0.000001 6 -0.443184 0.165775 -0.000002 6 0.804450 -0.656380 -0.000002 6 2.012398 -0.101726 0.000001 1 2.913228 -0.699634 0.000002 1 2.117137 0.975614 0.000003 1 0.689509 -1.734043 -0.000003 8 -0.413644 1.379339 -0.000000 1 -2.586099 0.086258 -0.000007 1 -1.798052 -1.250785 -0.877062 1 -1.798056 -1.250767 0.877077	91.2067, 125.0188, 267.7951, 416.1738, 459.9243, 601.345, 686.5542, 778.0401, 959.5856, 1019.3789, 1027.227, 1047.4258, 1085.647, 1196.2019, 1329.7897, 1385.1429, 1439.4219, 1464.5645, 1474.0063, 1667.5026, 1764.2385, 3025.0855, 3075.4149, 3139.8447, 3141.3414, 3155.0215, 3231.2254

Compound: Methyl Vinyl Ketone (Alkene 5) Con 2	**Energy (Hartree)** -230.948123255856
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.862592 1.290436 0.000000 6 0.541735 -0.188772 -0.000000 6 -0.876762 -0.629762 0.000000 6 -1.935118 0.176610 -0.000000 1 -2.941959 -0.218702 0.000000 1 -1.840063 1.254225 -0.000001 1 -0.997314 -1.706492 0.000002 8 1.425408 -1.024458 -0.000000 1 1.941376 1.417331 -0.000003 1 0.440003 1.779118 -0.879457 1 0.440009 1.779115 0.879462	115.3929, 125.8373, 279.3674, 434.0748, 492.6237, 538.0067, 701.2258, 760.6503, 946.7066, 997.4841, 1043.5912, 1051.9594, 1075.0319, 1271.0386, 1311.8244, 1390.2797, 1448.5287, 1473.5799, 1479.6845, 1681.4643, 1740.3039, 3036.7015, 3090.9528, 3141.4545, 3142.9025, 3164.6944, 3223.3275

Compound: 2-methyl-2-Butene (Alkene 6)	**Energy (Hartree)** -196.253938354277
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.624503 1.452410 0.000000 6 -0.447140 -0.041432 -0.000000 6 0.730526 -0.670603 0.000000 1 0.707689 -1.757034 0.000000 6 2.106934 -0.077806 0.000000 1 2.671834 -0.409494 0.875668 1 2.671834 -0.409494 -0.875668 1 2.106436 1.010167 -0.000000 6 -1.736975 -0.818574 0.000000 1 -1.562432 -1.893791 0.000000 1 -2.343659 -0.571524 0.876361 1 -2.343659 -0.571524 -0.876361 1 0.315041 1.998972 -0.000000 1 -1.198069 1.769879 -0.875725 1 -1.198068 1.769879 0.875725	119.287, 142.8596, 184.9092, 265.3825, 296.142, 384.9177, 457.0872, 527.2405, 770.054, 832.394, 957.7479, 968.7794, 1018.083, 1066.3741, 1068.8734, 1105.8277, 1129.4731, 1234.5111, 1376.8706, 1411.2291, 1415.4366, 1423.97, 1472.9828, 1481.779, 1483.9397, 1492.3166, 1496.9433, 1498.3233, 1733.8621, 3003.315, 3010.4859, 3012.6748, 3040.3203, 3044.1971, 3044.5477, 3095.0622, 3099.7183, 3115.5834, 3123.0159

Compound: 2-methyl-2-pentene (Alkene 7) con 1	**Energy (Hartree)** -235.510710308254
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.520310 0.221336 -0.523304 6 -0.234286 -0.525718 -0.322966 6 0.979796 -0.045824 -0.041200 6 2.155079 -0.971745 0.130221 1 2.945285 -0.739424 -0.590032 1 2.599420 -0.861198 1.123880 1 1.871746 -2.015220 -0.001392 6 1.312561 1.411770 0.128122 1 1.755509 1.590707 1.112078 1 2.060720 1.721688 -0.607412 1 0.451197 2.066543 0.024353 1 -0.327786 -1.605616 -0.414792 1 -1.363805 1.298498 -0.469677 1 -1.892183 0.018473 -1.533586 6 -2.603355 -0.188153 0.484308 1 -3.543315 0.327818 0.282390 1 -2.795928 -1.261654 0.438934 1 -2.297778 0.049388 1.504166	51.8385, 134.0678, 155.563, 211.3092, 213.2614, 306.3294, 360.6327, 413.2072, 486.1891, 512.7563, 751.3242, 825.2312, 864.3378, 915.4111, 962.8715, 1013.2655, 1020.6581, 1082.2278, 1094.991, 1105.6605, 1141.043, 1231.6042, 1293.7294, 1338.8625, 1390.3168, 1407.4913, 1412.798, 1421.2303, 1473.0816, 1479.5445, 1490.5559, 1492.0726, 1497.0068, 1498.9707, 1507.1527, 1728.9667, 2997.3477, 3003.3894, 3011.1735, 3022.168, 3040.5651, 3044.3677, 3062.2916, 3084.0155, 3087.4197, 3094.8892, 3103.9654, 3119.1194

Compound: 2-methyl-2-pentene (Alkene 7) con 2	**Energy (Hartree)** -235.503965311762
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.587139 -0.824293 -0.000001 6 -0.081647 -0.918267 -0.000000 6 0.912688 -0.025175 0.000000 6 2.343751 -0.505934 0.000002 1 2.410754 -1.592876 0.000003 1 2.881410 -0.131116 -0.876192 1 2.881410 -0.131114 0.876194 6 0.803464 1.476984 0.000000 1 1.315239 1.889798 0.874584 1 1.315248 1.889799 -0.874579	49.3885, 126.9372, 178.6736, 240.3712, 261.9161, 312.6675, 336.2853, 394.4681, 465.0377, 618.9179, 748.0852, 774.9348, 878.4081, 891.3665, 960.6299, 1023.4086, 1032.3807, 1075.0986, 1104.4448, 1111.0341, 1145.5448, 1214.3884, 1313.6081, 1377.6798, 1398.9989, 1410.8834, 1420.1532, 1427.8634, 1474.1226, 1477.3024,

1 -0.212815 1.848888 -0.000005 1 0.238029 -1.958104 0.000000 1 -1.939778 -1.398553 -0.864851 1 -1.939779 -1.398552 0.864850 6 -2.299938 0.526588 -0.000002 1 -3.379324 0.366789 -0.000002 1 -2.058735 1.117812 0.883316 1 -2.058734 1.117811 -0.883319	1485.5748, 1492.4022, 1499.7359, 1510.3612, 1515.345, 1731.9196, 2985.1506, 2994.8608, 3002.3228, 3010.713, 3030.2095, 3038.2199, 3040.7653, 3082.8631, 3091.5868, 3096.9833, 3101.0623, 3177.4209

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 1	**Energy (Hartree)** -274.769873729866
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.247137 0.237315 -0.000023 6 0.055240 -0.516336 0.000036 6 1.304219 -0.044270 0.000000 6 2.483373 -0.981511 0.000076 1 3.116709 -0.814425 -0.876310 1 3.116702 -0.814291 0.876442 1 2.171798 -2.025197 0.000155 6 1.676813 1.413854 -0.000112 1 2.287634 1.652389 0.875439 1 2.287647 1.652251 -0.875692 1 0.817731 2.079795 -0.000171 1 -0.064196 -1.598538 0.000122 1 -1.048296 1.310326 -0.000120 6 -2.059584 -0.087816 -1.263421 1 -1.512045 0.185139 -2.165993 1 -2.280533 -1.156454 -1.318240 1 -3.010384 0.448795 -1.265264 6 -2.059568 -0.087590 1.263445 1 -1.512019 0.185529 2.165960 1 -3.010369 0.449020 1.265201 1 -2.280514 -1.156218 1.318458	40.2249, 121.1126, 149.4513, 199.6047, 207.6406, 226.1775, 255.9976, 301.8987, 397.8943, 400.2782, 449.0185, 504.6168, 514.9766, 806.8098, 857.8554, 875.9431, 929.9461, 952.8705, 960.5746, 964.6545, 1019.0613, 1088.314, 1105.6218, 1114.5094, 1138.028, 1192.67, 1236.2331, 1330.4358, 1338.1236, 1392.9908, 1395.7476, 1409.608, 1418.7341, 1421.6929, 1473.2079, 1485.7607, 1488.1608, 1489.7061, 1492.0437, 1495.6178, 1502.5374, 1509.3166, 1727.2033, 3003.3271, 3010.867, 3014.1397, 3018.2239, 3035.8106, 3040.5823, 3044.3118, 3070.1314, 3078.284, 3086.8013, 3087.8307, 3091.1843, 3098.6926, 3117.9913

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 2	**Energy (Hartree)** -274.764773946885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.338433 -0.567560 0.000010 6 0.151295 -0.871346 0.000013 6 1.201254 -0.045119 0.000000 6 2.605061 -0.593296 0.000008 1 3.160641 -0.246154 -0.876346 1 3.160641 -0.246130 0.876353 1 2.616229 -1.682291 0.000023 6 1.139328 1.459171 -0.000022 1 1.658226 1.860516 0.875499 1 1.658232 1.860490 -0.875551 1 0.128892 1.853883 -0.000031 1 0.385053 -1.932121 0.000028 1 -1.833136 -1.542711 0.000028 6 -1.817961 0.150147 1.272820 1 -1.517384 -0.398512 2.166038 1 -1.410784 1.157939 1.352519 1 -2.906959 0.231618 1.277280 6 -1.817964 0.150102 -1.272825	66.9975, 125.3714, 167.3352, 197.0113, 208.3577, 234.3454, 237.9794, 308.8628, 376.8418, 393.88, 406.0858, 495.3459, 620.8043, 769.1911, 838.2769, 853.7765, 930.0836, 959.0098, 961.2789, 977.2296, 1015.9067, 1076.2022, 1105.3816, 1123.0582, 1129.0872, 1205.0421, 1226.7452, 1357.6722, 1380.4474, 1384.5308, 1398.2498, 1410.817, 1419.5341, 1423.837, 1473.4915, 1483.5955, 1487.1637, 1490.7858, 1493.4414, 1500.0646, 1505.225, 1511.4668, 1719.997, 3003.0185, 3005.6275, 3011.4461, 3022.5044, 3026.9414, 3040.039, 3044.0641, 3079.6144,

1 -1.517391 -0.398590 -2.166024 1 -2.906961 0.231577 -1.277284 1 -1.410783 1.157890 -1.352561	3082.613, 3094.0631, 3096.8454, 3097.0983, 3113.8644, 3143.5006

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 3	**Energy (Hartree)** -274.763016073451
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.354661 -0.223774 -0.415572 6 -0.094184 -0.657937 -0.362243 6 -1.244757 -0.062819 -0.031566 6 -1.455245 1.355444 0.429559 1 -2.147931 1.871342 -0.242215 1 -0.548740 1.942733 0.494055 1 -1.929641 1.358110 1.415440 6 -2.532425 -0.848604 -0.098538 1 -2.370389 -1.873330 -0.429355 1 -3.241417 -0.376719 -0.785509 1 -3.022654 -0.878803 0.879146 1 -0.189436 -1.703443 -0.648756 1 1.711274 -0.559693 -1.397350 6 1.684710 1.267854 -0.327831 1 1.503045 1.669764 0.669539 1 1.114195 1.856119 -1.046219 1 2.744118 1.416640 -0.544683 6 2.165233 -1.012286 0.630230 1 1.876956 -0.717367 1.641064 1 3.234763 -0.826539 0.513981 1 1.997901 -2.086085 0.536625	35.6181, 112.23, 149.6262, 212.6158, 225.555, 262.282, 307.951, 329.8406, 358.5092, 409.1844, 425.0623, 505.6342, 613.6757, 770.3826, 844.3845, 874.9328, 931.9043, 954.6786, 960.6706, 976.4238, 1023.5399, 1084.2207, 1100.8448, 1105.1482, 1144.7, 1207.7566, 1227.8653, 1326.0417, 1376.3833, 1395.1516, 1402.1973, 1410.7867, 1422.7879, 1428.191, 1474.0691, 1484.0705, 1488.9555, 1495.1297, 1496.138, 1500.0458, 1511.7552, 1517.2955, 1725.4607, 2968.4206, 3002.7538, 3011.2398, 3017.7296, 3026.6285, 3038.9404, 3041.6594, 3076.0373, 3081.171, 3083.6741, 3088.9647, 3096.5764, 3100.5859, 3178.7312

Compound: 2,4,4-trimethyl-2-pentene (Alkene 9) con 1	**Energy (Hartree)** -314.024563428501
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.137021 -0.070215 0.000000 6 -0.259379 -0.689851 0.000001 6 -1.471838 -0.127696 0.000001 6 -2.706834 -0.992971 -0.000001 1 -3.328600 -0.786757 0.876368 1 -3.328602 -0.786750 -0.876367 1 -2.460715 -2.053740 -0.000005 6 -1.777139 1.346640 0.000001 1 -2.379148 1.607658 -0.875378 1 -2.379196 1.607648 0.875349 1 -0.896633 1.979490 0.000028 1 -0.251207 -1.776368 0.000001 6 2.159436 -1.222334 -0.000016 1 2.038628 -1.853302 -0.882604 1 2.038636 -1.853320 0.882560 1 3.179848 -0.835652 -0.000017 6 1.381325 0.778784 -1.263983 1 1.232401 0.181059 -2.164341 1 0.712537 1.635696 -1.321966 1 2.406761 1.155494 -1.275302 6 1.381335 0.778758 1.263999 1 1.232421 0.181014 2.164346 1 2.406769 1.155471 1.275316	64.6822, 125.8305, 167.2823, 186.8965, 206.5533, 231.1321, 251.6629, 291.7571, 307.6043, 324.4647, 353.3254, 377.9719, 425.5823, 444.5562, 507.1322, 563.6174, 763.512, 822.3046, 852.0831, 926.4871, 929.8539, 947.305, 960.7913, 962.3601, 1016.111, 1050.8404, 1050.9084, 1102.2743, 1105.3059, 1178.0627, 1223.8857, 1250.4395, 1272.6268, 1390.6545, 1398.7861, 1400.4123, 1411.3526, 1423.0565, 1433.9231, 1473.2339, 1481.7288, 1482.5287, 1489.4142, 1489.436, 1493.4063, 1497.3553, 1507.9296, 1508.2509, 1520.1388, 1714.1334, 3003.1763, 3011.9746, 3016.3659, 3019.786, 3026.3564, 3040.1157, 3044.466, 3075.8264, 3077.4012, 3080.487, 3085.2659, 3097.2579, 3103.8216, 3105.2391, 3109.5045, 3148.4459

1 0.712543 1.635666 1.322006	

Compound: 2,4,4-trimethyl-2-pentene (Alkene 9) con 2	**Energy (Hartree)** -314.022840256808
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.153931 -0.048669 -0.000000 6 -0.259750 -0.606740 0.000000 6 -1.493679 -0.091407 0.000000 6 -1.908958 1.356708 -0.000000 1 -2.533187 1.564475 -0.874234 1 -1.088057 2.060881 -0.000004 1 -2.533181 1.564477 0.874237 6 -2.680455 -1.026650 0.000000 1 -2.378564 -2.072788 0.000001 1 -3.312543 -0.853912 -0.876221 1 -3.312544 -0.853911 0.876221 1 -0.228806 -1.694896 0.000000 6 1.866263 -0.602670 -1.253503 1 2.918543 -0.310396 -1.258443 1 1.820595 -1.692529 -1.283641 1 1.402786 -0.222853 -2.165068 6 1.297257 1.478281 0.000006 1 0.850274 1.929994 0.885386 1 0.850277 1.930000 -0.885373 1 2.357218 1.740226 0.000008 6 1.866266 -0.602679 1.253498 1 1.402792 -0.222868 2.165066 1 2.918546 -0.310405 1.258436 1 1.820598 -1.692538 1.283628	37.8322, 101.7978, 141.0677, 207.7913, 226.2622, 241.0601, 279.2297, 282.177, 331.5456, 352.9526, 362.9578, 394.6266, 425.29, 447.2463, 523.6109, 571.5711, 759.7664, 816.9911, 886.0609, 919.5083, 921.9658, 952.2851, 959.7541, 963.041, 1024.7654, 1047.0804, 1049.2022, 1102.2659, 1105.0826, 1175.1177, 1218.0621, 1242.0655, 1293.024, 1395.1699, 1395.2076, 1402.1578, 1411.0855, 1425.6459, 1434.4024, 1474.1451, 1482.1272, 1483.267, 1487.6212, 1493.7567, 1495.2499, 1501.5745, 1505.6236, 1513.9309, 1524.0001, 1720.2484, 3002.9985, 3011.4962, 3014.5969, 3017.7374, 3027.3661, 3038.9553, 3041.8064, 3074.9884, 3075.9104, 3081.1704, 3084.0698, 3084.7163, 3088.8554, 3099.5563, 3100.8475, 3183.575

Compound: Mesityl oxide (Alkene 10) Con 1	**Energy (Hartree)** -309.465790128374
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.817766 1.181570 0.000004 6 1.405239 -0.276388 0.000000 6 -0.006648 -0.723675 0.000002 6 -1.179688 -0.066779 0.000000 6 -2.458820 -0.860839 0.000002 1 -3.064594 -0.611789 0.875663 1 -3.064593 -0.611795 -0.875662 1 -2.276783 -1.933168 0.000006 6 -1.408062 1.417055 -0.000004 1 -2.002887 1.696951 -0.873831 1 -2.002883 1.696956 0.873824 1 -0.505647 2.013372 -0.000008 1 -0.048320 -1.807120 0.000003 8 2.271136 -1.136768 -0.000004 1 2.903580 1.226157 0.000009 1 1.437161 1.699458 -0.881230 1 1.437152 1.699457 0.881235	31.6247, 80.284, 143.1236, 213.5149, 230.804, 244.7836, 321.059, 373.1935, 471.6983, 524.2838, 583.3977, 584.7874, 781.0513, 876.1255, 885.7522, 956.6211, 1006.7854, 1015.2786, 1050.1668, 1092.0784, 1104.8031, 1202.7335, 1285.404, 1375.525, 1390.6008, 1409.8701, 1419.9382, 1467.8219, 1470.9895, 1483.6426, 1484.0559, 1495.1889, 1501.6001, 1683.5878, 1710.2959, 3012.6049, 3021.673, 3036.5958, 3051.1468, 3056.0309, 3095.4893, 3115.1414, 3134.563, 3146.8775, 3184.7417

Compound: Mesityl oxide (Alkene 10) Con 2	**Energy (Hartree)** -309.469316688066

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.560147 -0.799843 -0.000136 6 1.332280 0.091641 0.000049 6 0.040736 -0.632293 0.000085 6 -1.203331 -0.120263 -0.000002 6 -2.391119 -1.040052 0.000042 1 -3.018807 -0.851288 0.875172 1 -3.018660 -0.851563 -0.875252 1 -2.103278 -2.089720 0.000231 6 -1.539236 1.340342 -0.000146 1 -2.153759 1.574849 -0.874336 1 -2.153184 1.575136 0.874378 1 -0.657914 1.969542 -0.000496 1 0.133320 -1.712859 0.000161 8 1.450441 1.304942 0.000166 1 3.459067 -0.189878 -0.000173 1 2.556494 -1.450538 0.877320 1 2.556331 -1.450413 -0.877685	5.8179, 86.0289, 114.2669, 145.7257, 205.0671, 210.6334, 339.0034, 375.819, 442.647, 469.8649, 601.5013, 628.5367, 825.3514, 856.2612, 913.0507, 957.5863, 970.9409, 1005.165, 1042.746, 1096.5757, 1108.4228, 1188.3377, 1241.1667, 1381.198, 1390.1797, 1413.3283, 1415.1672, 1463.24, 1467.3951, 1473.9688, 1476.0118, 1487.7439, 1503.8996, 1660.1472, 1744.6457, 3010.4657, 3017.3443, 3025.9074, 3047.5875, 3056.8968, 3077.1295, 3107.6752, 3136.3004, 3139.6793, 3169.7428

Compound: HFO-1234yf (Alkene 11)	**Energy (Hartree)** -514.464460739210
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.585281 -0.043725 -0.000000 6 0.922986 -0.027137 -0.000000 6 1.716238 -1.077688 -0.000001 1 2.788511 -0.953648 -0.000000 1 1.298487 -2.070706 -0.000001 9 1.389017 1.232144 -0.000000 9 -1.057966 -1.299622 0.000000 9 -1.077228 0.584609 1.083539 9 -1.077230 0.584609 -1.083538	66.5226, 234.0701, 236.7274, 365.1414, 415.2527, 493.7216, 570.3112, 611.2868, 679.7835, 755.144, 787.2174, 932.9654, 956.2932, 1141.1345, 1151.7237, 1178.4052, 1353.311, 1423.1767, 1747.7183, 3179.6402, 3276.2088

Compound: HFO-1345fz (Alkene 12) con 1	**Energy (Hartree)** -652.907119469829
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.406520 0.464064 0.041056 6 -1.522801 -0.339034 0.631669 6 -2.575775 -0.740538 -0.061205 1 -2.684659 -0.515610 -1.112637 1 -3.364589 -1.307849 0.411851 1 -1.404735 -0.563074 1.683356 6 0.950218 -0.293991 -0.013799 9 1.922772 0.493908 -0.477940 9 1.293377 -0.712595 1.214935 9 0.854506 -1.364889 -0.812109 9 -0.680637 0.869707 -1.226395 9 -0.191880 1.585372 0.793853	65.4496, 74.8184, 198.6928, 219.6502, 276.1685, 313.3121, 354.3534, 378.6851, 459.1658, 522.8383, 564.6134, 580.3317, 645.5624, 729.0861, 768.6396, 1006.1183, 1021.6304, 1023.5818, 1037.8805, 1126.2012, 1182.7922, 1193.0461, 1246.4826, 1313.0904, 1326.6004, 1455.9826, 1714.5074, 3154.9201, 3185.8, 3241.5178

Compound: HFO-1345fz (Alkene 12) con 2	**Energy (Hartree)** -652.904303093187
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.373774 0.636304 -0.000001 6 -1.766832 0.091752 0.000022 6 -2.127041 -1.181547 -0.000001 1 -1.418307 -1.996261 -0.000041	75.3476, 82.8866, 175.3097, 217.682, 288.051, 308.1011, 346.8878, 415.779, 426.4018, 498.141, 573.3491, 587.1223,

1 -3.174403 -1.448473 0.000018 1 -2.505479 0.884601 0.000061 6 0.805569 -0.372781 0.000002 9 1.971435 0.276945 -0.000013 9 0.761617 -1.156981 1.087333 9 0.761605 -1.157009 -1.087307 9 -0.198970 1.436160 -1.095537 9 -0.198947 1.436192 1.095505	651.4742, 710.5058, 760.9488, 980.9817, 1000.8456, 1023.0824, 1090.7632, 1132.2297, 1182.4404, 1183.2641, 1198.8206, 1316.4318, 1376.3369, 1472.9663, 1719.0547, 3157.1139, 3167.5889, 3242.3767

Compound: HFO-1233zd (Alkene 13)	**Energy (Hartree)** -874.459906302694
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.304166 0.037365 0.000000 6 -0.124015 0.475233 0.000000 6 -1.124569 -0.388198 0.000000 17 -2.785458 0.098196 -0.000000 1 -0.988720 -1.458223 0.000001 1 -0.277597 1.544740 -0.000001 9 1.958514 0.511736 -1.083528 9 1.958515 0.511740 1.083526 9 1.448039 -1.301504 0.000002	81.6682, 155.5861, 167.9512, 299.2645, 393.6749, 400.4923, 547.4506, 563.4267, 660.1194, 833.3308, 851.3053, 872.8286, 968.2956, 1117.8281, 1125.0475, 1261.1857, 1285.3608, 1322.7518, 1697.9469, 3203.4882, 3220.3034

Compound: HFO-1234ze(E) (Alkene 14)	**Energy (Hartree)** -514.467255920440
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.843476 0.031705 0.000000 6 -0.560694 0.526254 -0.000001 6 -1.592866 -0.296119 -0.000000 9 -2.847722 0.166306 -0.000000 1 -1.543881 -1.375091 0.000000 1 -0.689768 1.598797 -0.000001 9 1.521177 0.474285 -1.082808 9 1.521177 0.474288 1.082807 9 0.926942 -1.314295 0.000002	85.0572, 191.9601, 193.4258, 386.5226, 409.7951, 418.4184, 554.7289, 577.4385, 690.8616, 869.6416, 879.7608, 963.0113, 1084.8443, 1116.9275, 1187.7224, 1257.587, 1321.8206, 1346.0002, 1742.5088, 3208.2322, 3218.0848

Compound: *E*-2-pentene (Alkene 15) con 1	**Energy (Hartree)** -196.251071480094
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.295855 0.556837 -0.220006 6 0.066116 -0.044855 -0.400279 6 1.169904 0.338239 0.233138 1 1.102628 1.160771 0.941527 6 2.527626 -0.268169 0.055375 1 3.250426 0.475332 -0.291259 1 2.912725 -0.659893 1.000639 1 2.509533 -1.084536 -0.667014 1 0.130587 -0.869626 -1.107825 6 -2.338349 -0.455703 0.270882 1 -3.323589 0.005142 0.355288 1 -2.423089 -1.298008 -0.418354 1 -2.064921 -0.854290 1.248704 1 -1.235300 1.394648 0.478403 1 -1.635656 0.972367 -1.174770	95.1208, 174.4694, 207.0285, 212.393, 302.7287, 410.1315, 488.8208, 766.8394, 817.5183, 884.3052, 949.8826, 1000.5831, 1029.2249, 1072.7703, 1080.2898, 1102.139, 1179.992, 1278.1465, 1322.7711, 1338.3681, 1369.4151, 1409.1436, 1414.9778, 1479.9028, 1483.1445, 1493.0503, 1497.8229, 1505.8295, 1731.9048, 2998.0422, 3010.7105, 3022.8968, 3041.7622, 3049.2851, 3082.4761, 3085.5294, 3088.4103, 3097.267, 3111.8101

Compound: *E*-2-pentene (Alkene 15) con 2	**Energy (Hartree)** -196.250612583247
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.396132 0.663057 0.000001 6 -0.105953 0.719991 -0.000000 6 -0.948189 -0.308269 0.000000 1 -0.553348 -1.319353 0.000002 6 -2.442134 -0.192208 -0.000000 1 -2.877019 -0.680561 -0.876242 1 -2.877019 -0.680548 0.876250 1 -2.762895 0.849873 -0.000007 1 -0.524143 1.724290 -0.000002 6 2.019655 -0.729366 -0.000000 1 3.107809 -0.660621 0.000001 1 1.723368 -1.300060 0.881425 1 1.723371 -1.300058 -0.881429 1 1.761409 1.223907 -0.867778 1 1.761408 1.223905 0.867781	130.3313, 201.3828, 203.2816, 221.8668, 292.7763, 366.5152, 583.9821, 717.6484, 835.4658, 855.006, 951.5287, 1007.0597, 1039.5076, 1072.8252, 1082.5013, 1109.8349, 1145.4322, 1294.0792, 1323.984, 1342.7188, 1382.2184, 1413.543, 1417.3128, 1478.2158, 1480.4696, 1494.103, 1499.2672, 1507.7024, 1732.3268, 2992.3715, 3003.9092, 3010.0394, 3027.5453, 3048.3419, 3085.3026, 3085.8294, 3088.8917, 3102.4869, 3133.8875

Compound: *Z*-2-pentene (Alkene 16) con 1	**Energy (Hartree)** -196.249290990363
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.010746 -0.198222 0.561353 6 0.013678 0.811731 0.134129 6 1.302108 0.614454 -0.141415 1 1.882671 1.481361 -0.442343 6 2.071878 -0.670389 -0.086180 1 2.529282 -0.887960 -1.054905 1 2.891397 -0.599267 0.634145 1 1.457110 -1.523846 0.192647 1 -0.365072 1.825551 0.033681 1 -0.563596 -1.186428 0.670085 1 -1.385389 0.078640 1.552669 6 -2.199758 -0.275580 -0.405698 1 -2.952628 -0.978457 -0.046177 1 -2.679137 0.698708 -0.517042 1 -1.877596 -0.600271 -1.395899	56.5887, 136.8691, 214.5953, 260.9216, 300.6178, 474.1665, 572.161, 720.4797, 795.9926, 863.0838, 935.7132, 1013.6785, 1025.7052, 1051.4266, 1067.852, 1093.8952, 1172.2047, 1282.5784, 1302.9043, 1340.4758, 1406.7983, 1411.0139, 1442.7749, 1482.5483, 1484.6711, 1494.972, 1498.104, 1507.0336, 1721.314, 3000.5883, 3015.1258, 3023.4597, 3050.2094, 3061.1266, 3085.2081, 3088.8849, 3102.8509, 3109.9953, 3132.9181

Compound: *Z*-2-pentene (Alkene 16) con 2	**Energy (Hartree)** -196.243578385811
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.346035 0.530063 -0.000000 6 -0.042625 1.114177 -0.000001 6 -1.264818 0.580769 0.000000 1 -2.082808 1.296181 0.000001 6 -1.727065 -0.846757 -0.000000 1 -2.354640 -1.039431 0.874611 1 -2.354674 -1.039418 -0.874590 1 -0.921974 -1.572409 -0.000021 1 -0.017015 2.201089 -0.000001 1 1.870389 0.952186 -0.865216 1 1.870386 0.952185 0.865219 6 1.547001 -0.983835 0.000000 1 2.613861 -1.212224 0.000005	70.7599, 118.6826, 241.8645, 305.955, 324.6422, 411.6616, 677.3082, 681.0786, 792.0716, 810.5278, 924.8355, 1023.3636, 1048.4103, 1056.5721, 1069.0422, 1110.8488, 1144.3627, 1310.0689, 1316.5031, 1394.6609, 1406.1158, 1417.3797, 1448.2938, 1475.2148, 1486.6778, 1493.1653, 1507.6348, 1514.9225, 1727.0842, 2988.5174, 2999.203, 3015.111, 3030.9911, 3045.5051, 3084.559, 3094.3334, 3097.6924, 3119.4895, 3159.5188

1 1.112653 -1.452330 0.883057 1 1.112661 -1.452329 -0.883061	

Compound: *E*-2-butene (Alkene 17)	**Energy (Hartree)** -156.994340303979
Reaction Coordinates: 6 1.956867 -0.079076 0.000000 6 0.535689 0.393027 -0.000000 6 -0.535689 -0.393028 -0.000000 1 -0.389176 -1.470660 -0.000000 6 -1.956867 0.079076 0.000000 1 -2.496480 -0.289912 -0.876354 1 -2.496480 -0.289912 0.876354 1 -2.016423 1.167743 0.000000 1 0.389176 1.470659 -0.000000 1 2.016423 -1.167742 -0.000001 1 2.496480 0.289913 -0.876353 1 2.496480 0.289912 0.876354	**Frequencies (cm^{-1}):** 176.4585, 229.7314, 245.7757, 281.793, 501.7962, 763.4185, 874.6193, 990.2857, 998.622, 1071.1443, 1072.9916, 1074.3046, 1167.8269, 1334.2191, 1336.5376, 1414.0301, 1415.6287, 1479.5634, 1480.1443, 1488.9859, 1497.3116, 1736.0464, 3010.5495, 3010.8238, 3048.8673, 3049.5438, 3084.2729, 3085.8189, 3106.0668, 3115.5896

Compound: *Z*-2-butene (Alkene 18)	**Energy (Hartree)** -156.992617941268
Reaction Coordinates: 6 1.587222 -0.520466 -0.000000 6 0.665981 0.661426 -0.000000 6 -0.665981 0.661426 -0.000000 1 -1.160946 1.627759 0.000000 6 -1.587222 -0.520466 -0.000000 1 -2.241381 -0.500797 0.875770 1 -2.241383 -0.500795 -0.875768 1 -1.059134 -1.471929 -0.000002 1 1.160946 1.627759 0.000000 1 1.059134 -1.471929 -0.000004 1 2.241384 -0.500794 -0.875768 1 2.241379 -0.500798 0.875771	**Frequencies (cm^{-1}):** 126.2, 142.7478, 287.1418, 400.5225, 572.897, 698.0489, 867.8641, 978.3282, 1010.4684, 1025.3172, 1067.0026, 1067.6084, 1160.0865, 1295.2903, 1395.5841, 1418.5863, 1440.7993, 1482.7723, 1485.7588, 1489.9577, 1495.1634, 1726.0624, 3014.0643, 3016.1249, 3049.918, 3050.1832, 3096.2508, 3110.3152, 3117.6898, 3139.0122

Compound: *Z*-2-pentene (Alkene 19) con 1	**Energy (Hartree)** -235.506682457045
Reaction Coordinates: 6 -0.484550 -0.779889 -0.638230 6 0.525983 -0.847958 0.469686 6 1.696144 -0.218366 0.564952 1 2.289756 -0.408075 1.454327 6 2.316438 0.730764 -0.415159 1 2.526540 1.692914 0.059377 1 3.275525 0.345477 -0.771905 1 1.688328 0.916275 -1.284034 1 0.248846 -1.503141 1.291820 6 -1.881700 -0.342377 -0.162983 6 -1.943829 1.106751 0.315921 1 -1.261216 1.279437 1.148810 1 -1.667935 1.796144 -0.485117 1 -2.949401 1.369846 0.647015 1 -2.589075 -0.485136 -0.983701	**Frequencies (cm^{-1}):** 41.2889, 109.1277, 138.6313, 200.7807, 254.3338, 306.0596, 362.8515, 478.4332, 574.6806, 710.7203, 774.1094, 859.1837, 893.2596, 913.9097, 971.1405, 1016.7575, 1058.8693, 1066.8111, 1068.3942, 1096.9851, 1172.2002, 1248.8115, 1285.6173, 1303.9926, 1352.9883, 1376.1035, 1409.2313, 1414.0569, 1441.3499, 1481.0826, 1484.2795, 1491.0118, 1493.7543, 1500.092, 1507.7222, 1721.092, 2997.5177, 3011.7554, 3015.048, 3021.8142, 3037.2674, 3049.8747,

1 -2.208956 -1.008607 0.640698 1 -0.149721 -0.113664 -1.435121 1 -0.573613 -1.775028 -1.087295	3058.0268, 3078.8452, 3089.2331, 3100.7837, 3109.1404, 3131.3534

Compound: Z-2-pentene (Alkene 19) con 2	**Energy (Hartree)** -235.506435572184
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.434966 -0.117017 0.541223 6 -0.768923 -0.917198 0.140474 6 -1.998500 -0.479536 -0.127223 1 -2.738429 -1.222625 -0.409177 6 -2.506265 0.930013 -0.085721 1 -2.920030 1.219735 -1.055210 1 -3.319095 1.026870 0.639157 1 -1.736662 1.652390 0.178752 1 -0.594362 -1.986289 0.053094 6 1.602087 -0.256493 -0.448454 6 2.853014 0.499733 -0.006021 1 2.652727 1.568128 0.098353 1 3.213119 0.136792 0.958923 1 3.663324 0.384110 -0.727068 1 1.839604 -1.316616 -0.574572 1 1.280249 0.101120 -1.429809 1 0.185006 0.938803 0.656687 1 0.776276 -0.459438 1.525215	49.398, 89.8889, 131.3736, 200.6305, 237.2598, 284.6984, 367.1046, 472.5868, 573.9975, 716.265, 749.0739, 874.3506, 897.4234, 914.7403, 996.5133, 1016.423, 1046.2213, 1064.9359, 1067.7578, 1112.9827, 1173.4844, 1258.5156, 1296.0617, 1307.5407, 1327.4771, 1377.8452, 1409.382, 1413.0443, 1441.3848, 1481.8697, 1484.5099, 1492.062, 1495.9796, 1499.292, 1509.8532, 1721.1738, 2989.8003, 3013.0685, 3014.9788, 3019.3197, 3036.2808, 3050.028, 3059.6606, 3078.2852, 3082.9867, 3101.9921, 3110.5017, 3132.9048

Compound: Z-2-pentene (Alkene 19) con 3	**Energy (Hartree)** -235.505472702575
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.387333 -0.463961 0.701236 6 0.465392 0.714968 0.330713 6 1.730961 0.707319 -0.087526 1 2.184208 1.668259 -0.312315 6 2.630709 -0.473982 -0.290862 1 2.983197 -0.515716 -1.324889 1 3.522305 -0.393583 0.336840 1 2.147545 -1.422526 -0.065533 1 -0.016601 1.683692 0.414440 6 -1.568144 -0.714092 -0.257091 6 -2.602649 0.410309 -0.293766 1 -3.008865 0.603567 0.701753 1 -2.175461 1.342466 -0.664852 1 -3.437593 0.151168 -0.946170 1 -1.177074 -0.884773 -1.263410 1 -2.060679 -1.642297 0.044550 1 0.216477 -1.369984 0.755883 1 -0.791076 -0.303631 1.707472	34.3897, 103.3731, 134.5315, 214.2817, 240.4438, 292.9596, 379.8072, 506.8255, 563.1399, 726.9086, 753.4922, 864.2882, 874.0456, 921.5376, 976.0881, 1019.525, 1054.0488, 1067.4956, 1069.3503, 1115.1616, 1159.276, 1254.0333, 1286.6668, 1309.7021, 1351.7153, 1373.443, 1408.4598, 1415.8675, 1443.9916, 1483.8179, 1484.6204, 1490.4358, 1496.0546, 1502.4863, 1508.8898, 1718.1454, 2993.7939, 3013.0809, 3015.0794, 3021.7087, 3042.6046, 3049.9742, 3066.3489, 3079.0806, 3088.2713, 3103.7062, 3117.7216, 3139.4572

Compound: Z-2-pentene (Alkene 19) con 4	**Energy (Hartree)** -235.500658574891
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.577039 0.946865 0.000000 6 -0.916425 1.144905 -0.000000	66.6089, 98.5924, 158.6739, 174.6908, 243.1529, 288.2919,

6 -1.956113 0.309862 -0.000000 1 -2.932908 0.786052 0.000000 6 -2.028114 -1.188752 0.000000 1 -2.583132 -1.539328 0.874654 1 -2.583145 -1.539328 -0.874646 1 -1.060683 -1.677803 -0.000007 1 -1.177357 2.200314 0.000000 1 0.973702 1.492334 -0.865662 1 0.973702 1.492333 0.865663 6 1.181178 -0.457355 -0.000001 6 2.709439 -0.418085 0.000000 1 3.132589 -1.423346 -0.000000 1 3.091038 0.102388 -0.880903 1 3.091036 0.102385 0.880906 1 0.836567 -1.010323 0.876289 1 0.836569 -1.010321 -0.876293	375.6707, 405.2788, 677.6753, 691.5656, 774.183, 816.3684, 889.4815, 912.7182, 991.5727, 1024.0328, 1052.5046, 1068.8351, 1075.9989, 1128.5062, 1151.1806, 1278.6814, 1306.2328, 1333.9822, 1339.9285, 1407.242, 1410.6888, 1415.8065, 1447.3686, 1471.9223, 1489.4133, 1490.9556, 1498.713, 1500.125, 1513.8684, 1726.4224, 2977.137, 2988.1787, 3014.9054, 3019.1809, 3024.2171, 3045.3647, 3052.6144, 3080.9261, 3084.2604, 3094.2598, 3119.4523, 3158.768

Compound: Isobutene (Alkene 20)	**Energy (Hartree)**
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.272479 -0.676792 0.000000 6 0.000000 0.123854 0.000000 6 0.000001 1.454624 0.000000 1 0.922183 2.021321 0.000000 1 -0.922183 2.021320 0.000000 6 1.272479 -0.676794 0.000000 1 2.153824 -0.037282 0.000000 1 1.321461 -1.329357 0.876282 1 1.321461 -1.329357 -0.876282 1 -2.153825 -0.037281 0.000000 1 -1.321462 -1.329356 -0.876282 1 -1.321462 -1.329356 0.876282	172.7829, 211.2397, 381.0088, 439.3224, 442.8878, 706.3756, 814.459, 924.6733, 961.7242, 988.287, 1022.3943, 1086.1878, 1108.4808, 1296.388, 1409.6995, 1415.2186, 1444.6997, 1471.8573, 1483.628, 1489.6004, 1502.8985, 1712.7565, 3007.5773, 3013.0906, 3047.6689, 3050.2723, 3100.6528, 3102.2216, 3129.5895, 3206.5032

S10.2 Products

S10.2.1 Criegee Intermediates

Compound: sCI1 (HCHOO)	**Energy (Hartree)** -189.400847568329
Reaction Coordinates: 6 -1.068412 0.202194 -0.000000 8 -0.003231 -0.459294 -0.000000 8 1.179333 0.194958 0.000000 1 -1.021445 1.284352 -0.000000 1 -1.976903 -0.382830 0.000002	**Frequencies (cm^{-1}):** 527.7609,673.7578, 912.8476, 951.0664, 1242.0554, 1402.0013, 1543.5428, 3118.1651, 3267.9600

Compound: *Anti*-CH_3CHOO	**Energy (Hartree)** -228.668481416675
Reaction Coordinates: 6 1.768337 -0.098013 0.000000 6 0.380636 0.408005 -0.000001 8 -0.571402 -0.409277 -0.000001 8 -1.854416 0.073325 0.000001 1 0.119269 1.462625 -0.000001 1 2.303633 0.275054 0.877345 1 1.786152 -1.185114 -0.000027 1 2.303652 0.275101 -0.877313	**Frequencies (cm^{-1}):** 159.9851, 257.6665, 324.381, 553.5978, 867.7539, 893.0654, 968.3519, 1067.3161, 1157.1901, 1344.2119, 1414.9461, 1458.644, 1462.7974, 1577.2586, 3019.4822, 3060.7084, 3131.6411, 3145.1519

Compound: *Syn*-CH_3CHOO	**Energy (Hartree)** -228.674137895205
Reaction Coordinates: 6 1.364404 -0.472563 -0.000000 6 0.481825 0.697474 0.000000 8 -0.774763 0.588713 -0.000000 8 -1.295881 -0.676150 0.000000 1 0.816554 1.727871 0.000000 1 2.410795 -0.181137 -0.000003 1 1.130215 -1.098354 0.866933 1 1.130211 -1.098357 -0.866930	**Frequencies (cm^{-1}):** 185.3271, 295.7077, 460.8721, 674.8786, 756.9638, 900.7617, 982.6906, 1046.5977, 1110.553, 1349.2256, 1398.9588, 1437.3442, 1460.4744, 1559.818, 3015.3924, 3049.5183, 3140.3388, 3177.8251

Compound: *Anti*-EtCHOO con 1	**Energy (Hartree)** -267.925413397257
Reaction Coordinates: 6 -1.238387 0.671859 0.000001 6 0.243293 0.716298 -0.000001 8 0.906784 -0.346617 0.000001 8 2.280006 -0.267327 -0.000000 1 0.808677 1.644807 -0.000003 1 -1.577933 1.251548 0.867130 1 -1.577935 1.251550 -0.867126 6 -1.855251 -0.723194 -0.000000 1 -1.551814 -1.289222 -0.879384 1 -1.551811 -1.289225 0.879380 1 -2.941441 -0.647683 0.000001	**Frequencies (cm^{-1}):** 130.9388, 193.1388, 202.5138, 272.6768, 419.6176, 620.8898, 744.3949, 897.1681, 918.3676, 925.3618, 1025.6913, 1105.3439, 1123.1071, 1275.1458, 1339.7654, 1387.5666, 1425.6198, 1450.0468, 1498.9388, 1504.5907, 1574.7551, 2994.2524, 3005.7603, 3048.8185, 3114.4836, 3114.5196, 3135.7266

Compound: *Anti*-EtCHOO con 2	**Energy (Hartree)** -267.924722060814
Reaction Coordinates: 6 1.131391 0.597027 0.114323 6 -0.186195 -0.013288 0.406647 8 -1.174188 0.269041 -0.313495 8 -2.384882 -0.310259 -0.030725 1 -0.357920 -0.717017 1.217757 1 1.021985 1.290943 -0.718380 1 1.434653 1.179175 0.991339 6 2.208737 -0.460271 -0.182091 1 2.315531 -1.161616 0.645772 1 1.963229 -1.027476 -1.078988 1 3.171487 0.024934 -0.337014	**Frequencies (cm^{-1}):** 79.1142, 195.2713, 205.3122, 327.0348, 409.9348, 538.219, 777.8747, 908.9061, 921.1754, 935.6995, 1017.6514, 1089.1869, 1177.5842, 1277.7692, 1321.9142, 1366.6797, 1416.2125, 1471.0462, 1499.8413, 1504.8533, 1566.5471, 3007.5733, 3039.1061, 3086.2792, 3107.0306, 3111.9258, 3132.8426

Compound: *Syn*-EtCHOO con 1	**Energy (Hartree)** -267.929199725584
Reaction Coordinates: 6 0.923269 0.426502 0.547182 6 -0.273025 0.951814 -0.133366 8 -1.335917 0.288133 -0.280028 8 -1.378535 -0.987515 0.215939 1 -0.343576 1.943872 -0.565754 1 0.578050 -0.104376 1.437841 1 1.555704 1.264174 0.840694 6 1.714340 -0.561104 -0.339827 1 2.094886 -0.069777 -1.234859 1 2.563010 -0.947994 0.222458 1 1.080044 -1.394116 -0.631598	**Frequencies (cm^{-1}):** 112.796, 197.0713, 243.4832, 323.9713, 537.4759, 652.1667, 811.3089, 833.6176, 890.6056, 905.7836, 1009.4333, 1081.9342, 1145.8927, 1289.6824, 1331.79, 1370.0543, 1401.7209, 1460.3766, 1495.3906, 1511.5641, 1558.8684, 3032.0107, 3044.775, 3087.3063, 3106.9797, 3135.4246, 3164.4414

Compound: *Syn*-EtCHOO con 2	**Energy (Hartree)** -267.930089984566
Reaction Coordinates: 6 -0.773628 -0.439742 0.000000 6 0.143905 0.707537 0.000000 8 1.397747 0.574971 -0.000000 8 1.895135 -0.701219 -0.000000 1 -0.172097 1.745490 0.000000 1 -0.499810 -1.066484 0.857959 1 -0.499809 -1.066484 -0.857958 6 -2.249706 -0.054174 -0.000000 1 -2.510613 0.531063 -0.882579 1 -2.873539 -0.946390 -0.000000 1 -2.510613 0.531063 0.882579	**Frequencies (cm^{-1}):** 94.1884, 200.9246, 218.1471, 362.392, 465.8496, 689.645, 707.4179, 830.1912, 890.317, 935.7901, 1047.473, 1098.5582, 1140.771, 1248.8554, 1320.9428, 1370.6582, 1424.9606, 1430.752, 1503.458, 1505.6674, 1561.5455, 3000.6382, 3006.4657, 3036.0444, 3092.694, 3108.5153, 3159.5381

Compound: *Anti*-iPrCHOO con 1	**Energy (Hartree)** -307.183903025558
Reaction Coordinates: 6 -0.965724 -0.022320 -0.415928 6 0.451044 -0.471047 -0.343096 8 1.340114 0.284155 0.114105	**Frequencies (cm^{-1}):** 86.4377, 189.3429, 195.2162, 220.6261, 257.4231, 334.5273, 436.9484, 442.9461, 601.9411,

8 2.635957 -0.175402 0.163739 1 0.771661 -1.457371 -0.671117 1 -1.230765 -0.073551 -1.480983 6 -1.862506 -1.041551 0.316090 1 -1.662940 -1.031784 1.387934 1 -2.910430 -0.786411 0.161324 1 -1.704546 -2.055839 -0.051424 6 -1.180802 1.407058 0.078694 1 -0.932701 1.496751 1.136303 1 -0.565070 2.118627 -0.469045 1 -2.225846 1.686708 -0.050311	826.139, 920.3659, 928.242, 940.115, 971.1987, 975.1866, 1108.5286, 1140.3406, 1205.1665, 1300.8512, 1342.4565, 1373.2338, 1407.8302, 1429.2624, 1488.4416, 1492.5379, 1504.3735, 1510.6035, 1563.7815, 2968.5051, 3033.1315, 3042.4617, 3098.7008, 3102.9851, 3106.8174, 3112.9375, 3128.3525

Compound: *Anti*-iPrCHOO con 2	**Energy (Hartree)** -307.183504223503
Reaction Coordinates: 6 0.887613 0.000000 -0.323680 6 -0.461359 0.000004 0.300578 8 -1.485439 -0.000003 -0.422869 8 -2.720692 0.000002 0.178783 1 -0.621403 0.000012 1.377128 1 0.743561 -0.000001 -1.405313 6 1.653916 1.271480 0.084187 1 1.786741 1.320883 1.166272 1 2.642925 1.267849 -0.374361 1 1.131562 2.171757 -0.237300 6 1.653908 -1.271483 0.084190 1 1.786732 -1.320886 1.166275 1 1.131549 -2.171758 -0.237296 1 2.642918 -1.267859 -0.374358	**Frequencies (cm^{-1}):** 67.3615, 184.8015, 204.221, 214.3213, 266.4091, 317.491, 416.6544, 477.3281, 523.4987, 851.3703, 925.6943, 939.2119, 947.0572, 947.6788, 968.204, 1099.3011, 1182.723, 1198.2556, 1322.2851, 1333.6178, 1365.1658, 1401.9082, 1423.0427, 1488.3999, 1490.9307, 1502.5096, 1510.1752, 1566.1929, 3029.6121, 3031.5752, 3054.3653, 3091.6977, 3098.037, 3105.4845, 3106.3581, 3123.2305

Compound: *Syn*-iPrCHOO con 1	**Energy (Hartree)** -307.187971815102
Reaction Coordinates: 6 0.685393 0.034039 -0.266093 6 -0.344387 -0.746961 0.451159 8 -1.585539 -0.578006 0.306437 8 -2.016369 0.391930 -0.560956 1 -0.114839 -1.533111 1.164189 6 0.802253 1.443751 0.358578 1 1.186654 1.387829 1.377879 1 1.496498 2.039857 -0.233659 1 -0.164773 1.940955 0.364631 1 0.294160 0.167642 -1.279557 6 2.024152 -0.706031 -0.288280 1 1.937024 -1.684752 -0.761394 1 2.759440 -0.129507 -0.848813 1 2.416638 -0.849099 0.720696	**Frequencies (cm^{-1}):** 97.301, 196.6638, 208.2676, 232.3478, 275.8028, 335.1623, 411.9805, 546.8364, 672.2183, 838.1781, 850.88, 889.9471, 939.4327, 950.3204, 975.7047, 1109.0713, 1173.5297, 1192.4754, 1308.2468, 1321.5635, 1371.7229, 1393.551, 1423.2907, 1486.691, 1494.8823, 1502.364, 1514.2539, 1559.3308, 3019.6062, 3027.3683, 3035.1978, 3086.2642, 3096.0502, 3100.9662, 3127.9019, 3149.0892

Compound: *Syn*-iPrCHOO con 2	**Energy (Hartree)** -307.184639319810
Reaction Coordinates: 6 -0.878257 -0.000001 0.485811 6 0.510830 -0.000004 1.017271	**Frequencies (cm^{-1}):** 106.1975, 196.259, 198.7294, 229.4144, 235.9845, 341.1971,

8 1.575267 -0.000002 0.342536 8 1.514281 0.000004 -1.025788 1 0.720729 -0.000010 2.082327 6 -1.177955 1.278802 -0.323492 1 -0.549243 1.326970 -1.208037 1 -2.225039 1.263930 -0.627045 1 -1.013352 2.175651 0.274198 1 -1.521789 -0.000004 1.368946 6 -1.177958 -1.278799 -0.323500 1 -1.013357 -2.175652 0.274185 1 -2.225042 -1.263922 -0.627054 1 -0.549245 -1.326963 -1.208045	417.1591, 539.501, 742.4056, 798.3226, 843.7334, 886.6389, 941.3455, 964.4005, 971.288, 1097.8197, 1123.9389, 1195.8952, 1336.5111, 1368.1737, 1388.3097, 1393.6817, 1417.9274, 1482.0393, 1493.91, 1502.4489, 1522.3991, 1558.6615, 3028.4394, 3037.2438, 3039.1962, 3094.1619, 3095.4681, 3138.4912, 3140.7073, 3150.7961

Compound: *Anti*-tBuCHOO	**Energy (Hartree)** -346.443987742296
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.789980 -0.001899 0.000000 6 -0.622216 -0.490941 0.000001 8 -1.586526 0.307444 0.000001 8 -2.866746 -0.202482 0.000000 1 -0.868477 -1.551112 0.000002 6 1.474988 -0.578024 1.260488 1 1.413826 -1.666766 1.287820 1 2.529747 -0.300726 1.258757 1 1.020181 -0.186446 2.170246 6 1.474983 -0.578019 -1.260493 1 1.020172 -0.186437 -2.170247 1 2.529741 -0.300720 -1.258765 1 1.413821 -1.666760 -1.287829 6 0.864650 1.528339 0.000003 1 0.381929 1.950817 -0.880399 1 0.381933 1.950814 0.880409 1 1.908986 1.840905 0.000002	72.1401, 188.151, 188.2131, 214.2437, 266.0175, 267.9342, 327.4276, 336.7752, 351.7125, 453.0763, 462.9141, 555.678, 774.9509, 910.7703, 922.1565, 926.7502, 954.2772, 959.5186, 972.3446, 1042.6824, 1064.7891, 1212.059, 1227.8809, 1295.2272, 1357.7122, 1399.7857, 1408.0789, 1435.3288, 1480.5727, 1487.9721, 1488.4896, 1503.0707, 1504.3892, 1518.7856, 1561.5817, 3027.2938, 3029.8872, 3040.5647, 3091.6685, 3095.4354, 3100.5416, 3100.793, 3105.6391, 3110.5258, 3121.737

Compound: *Syn*-tBuCHOO	**Energy (Hartree)** -346.444793572179
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.674006 0.018836 0.000000 6 -0.425399 -0.994158 0.000003 8 -1.667963 -0.782312 0.000003 8 -2.155760 0.497368 -0.000001 1 -0.213619 -2.059710 0.000006 6 0.570336 0.896137 1.269013 1 0.678505 0.293952 2.172053 1 1.379325 1.627869 1.253432 1 -0.382295 1.416647 1.304163 6 0.570338 0.896124 -1.269022 1 1.379325 1.627858 -1.253445 1 0.678513 0.293930 -2.172055 1 -0.382294 1.416630 -1.304181 6 2.009587 -0.742745 0.000005 1 2.110730 -1.374102 -0.884612 1 2.837661 -0.034600 0.000001 1 2.110729 -1.374091 0.884630	114.1607, 194.1886, 205.8697, 232.2877, 242.8082, 264.5474, 311.7319, 373.5137, 391.4703, 393.826, 547.4009, 663.0079, 788.1158, 844.621, 883.7145, 925.5938, 937.5768, 946.5911, 973.0925, 1045.3904, 1059.5755, 1212.9554, 1234.9867, 1273.5478, 1387.4046, 1388.6852, 1398.869, 1427.9961, 1474.7784, 1491.2046, 1492.4225, 1498.8999, 1508.6258, 1525.3289, 1552.4378, 3023.8797, 3030.5664, 3033.6024, 3083.1399, 3088.7935, 3089.4156, 3101.4749, 3138.0935, 3139.3703, 3141.242

Compound: *Anti*-OCH-CHOO con 1	**Energy (Hartree)** -341.874794351903
Reaction Coordinates: 6 -1.380256 1.277703 -0.000000 1 -0.955960 1.770134 0.876375 1 -0.955957 1.770135 -0.876373 1 -2.460742 1.386745 -0.000002 6 -1.036272 -0.186163 0.000000 6 0.387585 -0.587014 0.000002 8 1.273575 0.315950 0.000000 8 2.568387 -0.027599 -0.000001 1 0.693149 -1.627188 0.000001 8 -1.860316 -1.079225 -0.000001	**Frequencies (cm^{-1}):** 89.6551, 146.6518, 186.4248, 224.6185, 399.2977, 500.0396, 564.1078, 570.7829, 831.647, 915.5553, 1012.7049, 1032.2613, 1049.9935, 1243.359, 1341.157, 1401.107, 1462.5227, 1471.3513, 1484.672, 1737.9924, 3041.5794, 3095.8339, 3149.8163, 3178.9853

Compound: *Anti*-OCH-CHOO con 2	**Energy (Hartree)** -341.869209743485
Reaction Coordinates: 6 2.127294 -0.803805 -0.000000 1 2.079125 -1.451555 0.878536 1 2.079127 -1.451553 -0.878537 1 3.064887 -0.256073 0.000001 6 0.975759 0.169274 -0.000000 6 -0.372747 -0.463275 -0.000000 8 -1.386227 0.292533 -0.000000 8 -2.603355 -0.254499 0.000000 1 -0.548493 -1.533793 0.000002 8 1.107522 1.371942 0.000000	**Frequencies (cm^{-1}):** 102.3254, 112.5058, 191.0887, 212.4039, 376.1871, 466.8569, 565.8761, 617.4788, 888.5896, 915.1229, 943.8324, 1043.1568, 1059.09, 1199.1456, 1355.7011, 1393.137, 1461.9568, 1471.3795, 1484.65, 1758.0848, 3027.5069, 3078.7494, 3148.8069, 3160.3167

Compound: *Syn*-OCH-CHOO con 1	**Energy (Hartree)** -341.871502609295
Reaction Coordinates: 6 0.824684 1.415296 0.000001 1 0.252348 1.748952 0.866525 1 1.823703 1.843568 0.000003 1 0.252351 1.748953 -0.866524 6 0.938768 -0.075163 -0.000000 6 -0.264153 -0.958412 0.000001 8 -1.493315 -0.652057 0.000001 8 -1.908490 0.625605 -0.000002 1 -0.094945 -2.028110 0.000003 8 1.998149 -0.674010 -0.000002	**Frequencies (cm^{-1}):** 53.3101, 199.8905, 242.9936, 325.1407, 348.3545, 498.05, 591.87, 671.4057, 819.5133, 854.8213, 929.5827, 1042.2661, 1048.7575, 1258.0221, 1357.3156, 1402.6209, 1440.6406, 1453.1665, 1487.5244, 1727.3454, 3041.8082, 3094.7872, 3143.9874, 3190.0379

Compound: *Syn*-OCH-CHOO con 2	**Energy (Hartree)** -341.862276812340
Reaction Coordinates: 6 2.212569 -0.366213 -0.000000 1 2.378486 -0.992625 -0.879375 1 2.922410 0.455584 -0.000001 1 2.378487 -0.992624 0.879375 6 0.805815 0.192945 0.000000 6 -0.249500 -0.850623 0.000000 8 -1.514104 -0.688513 0.000000 8 -2.085057 0.507733 -0.000000	**Frequencies (cm^{-1}):** 56.8625, 95.6231, 211.2354, 295.931, 342.9427, 470.109, 603.6244, 693.3941, 806.2389, 873.8416, 987.0687, 1009.6464, 1039.5672, 1182.516, 1373.8337, 1390.1633, 1461.4244, 1473.5334, 1484.3973, 1748.4762, 3027.9802, 3080.2331, 3147.2836, 3182.6552

1 0.007673 -1.902228 -0.000001 8 0.561616 1.377686 0.000000	

Compound: $(CH_3)_2COO$	**Energy (Hartree)** -267.942546539936
Reaction Coordinates: 6 -0.072626 1.465423 -0.000000 6 -0.377947 0.024683 -0.000000 8 0.567304 -0.816015 -0.000001 8 1.858053 -0.326037 0.000001 6 -1.751450 -0.541461 0.000000 1 -2.301504 -0.192862 -0.877682 1 -1.721850 -1.628087 -0.000001 1 -2.301501 -0.192865 0.877685 1 -0.976897 2.068002 -0.000002 1 0.555520 1.695182 0.865234 1 0.555523 1.695181 -0.865232	**Frequencies (cm^{-1}):** 154.7878, 180.6109, 277.8128, 307.6135, 363.4465, 483.1866, 597.9012, 812.4888, 924.0134, 934.3173, 985.9827, 1070.4539, 1093.8612, 1305.1876, 1393.4045, 1409.3403, 1438.2555, 1458.0039, 1469.8151, 1476.4709, 1560.106, 3020.3234, 3025.0231, 3060.3596, 3065.9584, 3134.9818, 3137.2227

Compound: *Anti*-CF_3CF_2CHOO con 1	**Energy (Hartree)** -763.819838560287
Reaction Coordinates: 6 0.069149 0.627138 0.022159 6 -1.236224 0.079680 0.533411 8 -2.153739 -0.114622 -0.301088 8 -3.332105 -0.597276 0.118248 1 -1.394430 -0.148462 1.580273 9 -0.061230 1.131744 -1.217459 9 0.470150 1.617642 0.864146 6 1.205189 -0.440766 -0.006928 9 1.356875 -0.964924 1.217947 9 0.885110 -1.420835 -0.855647 9 2.354927 0.108299 -0.387810	**Frequencies (cm^{-1}):** 44.3986, 57.0473, 153.6216, 185.5355, 220.3238, 244.4913, 329.0152, 354.6629, 373.6292, 403.3591, 478.9045, 533.1629, 588.2807, 625.4113, 728.0104, 825.9083, 883.5367, 987.1218, 1053.852, 1139.4701, 1192.9705, 1206.8077, 1241.3348, 1298.0137, 1341.3819, 1534.4801, 3187.8179

Compound: *Anti*-CF_3CF_2CHOO con 2	**Energy (Hartree)** -763.818682766641
Reaction Coordinates: 6 -0.209949 0.769713 -0.000001 6 1.290692 0.714352 0.000016 8 1.865913 -0.400862 -0.000009 8 3.206432 -0.449944 0.000003 1 1.873935 1.628647 0.000047 9 -0.609897 1.470190 1.094503 9 -0.609877 1.470174 -1.094524 6 -0.963428 -0.591937 0.000002 9 -0.648973 -1.297686 -1.088456 9 -0.648980 -1.297676 1.088469 9 -2.277449 -0.364442 -0.000003	**Frequencies (cm^{-1}):** 54.871, 70.3267, 116.3479, 177.129, 217.1967, 256.1066, 336.8535, 365.3074, 376.2775, 393.3915, 477.5585, 530.2372, 590.7708, 641.6927, 692.4777, 787.0862, 887.8686, 984.3691, 1107.5422, 1114.7433, 1175.4569, 1209.0797, 1211.1947, 1337.2608, 1347.8549, 1544.616, 3173.6706

Compound: *Syn*-CF_3CF_2CHOO con 1	**Energy (Hartree)** -763.816355614179
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.003801 0.701424 -0.128518 6 1.241007 0.658922 0.730098 8 2.241648 -0.082513 0.545868 8 2.274088 -0.974731 -0.450052 1 1.322895 1.331879 1.571843 9 0.288532 0.805216 -1.437493 9 -0.663474 1.832436 0.250099 6 -1.007627 -0.478856 0.080434 9 -1.264414 -0.596419 1.394913 9 -2.148787 -0.207742 -0.554718 9 -0.525885 -1.629365 -0.367297	27.0324, 94.7261, 149.4391, 189.9634, 212.3468, 276.2901, 314.8169, 354.514, 426.5154, 464.8876, 494.3785, 559.4939, 582.4453, 648.1925, 750.1928, 774.9641, 830.5958, 945.864, 1066.2727, 1126.2644, 1181.1031, 1213.9794, 1227.7939, 1289.1019, 1369.3086, 1532.2685, 3212.718

Compound: *Syn*-CF_3CF_2CHOO con 2	**Energy (Hartree)** -763.816743925882
Reaction Coordinates: 6 0.151655 -0.282103 0.000000 6 1.047244 0.934668 0.000000 8 2.306717 0.869749 0.000000 8 2.931888 -0.310367 -0.000000 1 0.652384 1.939972 0.000000 9 0.361554 -1.039417 1.099463 9 0.361554 -1.039418 -1.099462 6 -1.345243 0.140891 0.000000 9 -1.609795 0.881573 -1.086690 9 -2.134980 -0.926063 -0.000000 9 -1.609795 0.881573 1.086690	**Frequencies (cm^{-1}):** 63.5645, 71.6863, 136.7132, 216.3012, 216.6225, 246.917, 298.1751, 360.9537, 404.6534, 470.2807, 542.1749, 556.7641, 594.1608, 602.749, 751.3958, 767.793, 875.8626, 958.276, 1030.5662, 1141.6776, 1183.7528, 1188.334, 1237.0489, 1326.2237, 1377.1304, 1533.5921, 3218.195

Compound: *Anti*-CF_3CHOO	**Energy (Hartree)** -526.205978402574
Reaction Coordinates: 6 -0.814124 -0.010987 0.000000 6 0.599627 -0.529934 0.000001 8 1.532385 0.307937 -0.000000 8 2.803565 -0.122750 -0.000000 1 0.814702 -1.591587 0.000002 9 -0.871266 1.317793 -0.000001 9 -1.465219 -0.472475 -1.084562 9 -1.465219 -0.472472 1.084563	**Frequencies (cm^{-1}):** 53.4225, 186.5103, 191.8874, 388.9843, 394.1412, 416.4183, 552.7580, 560.7356, 699.8777, 883.4653, 889.1822, 988.9465, 1131.2630, 1171.7198, 1270.0033, 1355.9541, 1546.1599, 3188.0668

Compound: *Syn*-CF_3CHOO	**Energy (Hartree)** -526.205009675300
Reaction Coordinates: 6 0.544326 0.408563 0.000000 6 -0.965669 0.489858 0.000000 8 -1.720767 -0.517005 -0.000000 8 -1.205470 -1.752491 -0.000000 1 -1.466000 1.447260 0.000000 9 1.014961 -0.207422 1.087387 9 1.014961 -0.207422 -1.087387 9 1.014961 1.672420 0.000000	**Frequencies (cm^{-1}):** 83.4264, 179.3385, 247.1426, .2827, 478.5065, 507.3023, ,536.2006, 591.5612, 758.0400, 772.8798, 885.1813, 947.2031, 1151.7894, 1176.1918, 1243.1084, 1364.7774, 1539.7613, ,3220.6741

Compound: *Anti*-ClCHOO	**Energy (Hartree)** -648.567491157440
Reaction Coordinates: 6 0.000000 0.446097 0.000000 17 -1.534775 -0.276709 0.000000 1 0.093739 1.524821 0.000000 8 1.012621 -0.284105 -0.000000 8 2.237057 0.346936 -0.000000	**Frequencies (cm^{-1}):** 229.5392, 303.4732, 458.6682, 865.92, 891.9082, 915.5859, 1291.2838, 1476.5172, 3188.0722

Compound: *Syn*-ClCHOO	**Energy (Hartree)** -648.572181521575
Reaction Coordinates: 6 0.000000 0.842892 -0.000000 17 -1.279322 -0.251963 -0.000000 1 -0.196377 1.904658 -0.000000 8 1.205128 0.491035 0.000000 8 1.537978 -0.825865 0.000000	**Frequencies (cm^{-1}):** 241.5659, 471.9135, 657.3934, 752.0452, 869.6006, 902.2343, 1330.4159, 1460.2303, 3220.2157

Compound: *Anti*-FCHOO	**Energy (Hartree)** -288.578114161732
Reaction Coordinates: 6 0.000000 0.583824 -0.000000 9 -1.138700 1.222551 0.000000 1 0.914897 1.162472 -0.000000 8 -0.034852 -0.649166 0.000000 8 1.201527 -1.309381 -0.000000	**Frequencies (cm^{-1}):** 268.0562, 334.6853, 573.9602, 880.5495, 899.7337, 1214.4299, 1317.8767, 1591.5708, 3211.2991

Compound: *Syn*-FCHOO	**Energy (Hartree)** -288.580107921778
Reaction Coordinates: 6 0.000000 0.819490 0.000000 9 1.262219 0.529738 -0.000000 1 -0.281417 1.862464 0.000000 8 -0.878953 -0.056851 0.000000 8 -0.505866 -1.386529 -0.000000	**Frequencies (cm^{-1}):** 290.6308, 484.5048, 767.7453, 782.9853, 845.1627, 1204.4974, 1343.3329, 1593.0432, 3233.2806

Compound: *Anti*-CF_3CFOO	**Energy (Hartree)** -625.3783361
Reaction Coordinates: 6 -0.277404 -0.919423 0.000000 6 0.018963 0.571292 0.000000 8 1.190937 0.987253 0.000000 8 1.417147 2.337638 0.000000 9 -0.997920 1.369496 0.000000 9 0.847756 -1.621862 0.000000 9 -0.997920 -1.235503 1.084149 9 -0.997920 -1.235503 -1.084149	**Frequencies (cm^{-1}):** 41.8080, 154.2443, 183.9192, 293.0541, 346.5294, 372.3393, 406.8758, 515.4784, 576.4030, 659.0393, 728.8220, .5490, 906.9387, 1155.2541, 1155.7283, 1229.1869, 1400.7892, 1601.0242

Compound: *Syn*-CF_3CFOO	**Energy (Hartree)** -625.3731138

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.267347 0.734443 0.000000 6 -0.668190 -0.480912 0.000000 8 -0.317071 -1.670141 0.000000 8 1.031885 -1.966693 0.000000 9 -1.951916 -0.250006 0.000000 9 1.031885 0.735046 1.087938 9 1.031885 0.735046 -1.087938 9 -0.480015 1.843635 0.000000	58.8820, 180.2110, 218.4479, 269.2791, 292.9260, ,363.8515, 484.2548, 493.0742, 582.0033, 631.0249, 653.9584, 780.2000, 927.2456, 1158.8972, 1195.1079, 1198.3764, 1398.0465, 1580.9318

Compound: *Anti*-nPrCHOO con 1	**Energy (Hartree)** -307.181067012075
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.512711 0.900051 0.352587 6 -0.628351 -0.044175 0.360780 8 -1.716841 0.306294 -0.158476 8 -2.763993 -0.578758 -0.157008 1 -0.595133 -1.044241 0.783547 1 0.162162 1.860325 -0.024729 1 0.838722 1.047214 1.388447 6 1.718464 0.404885 -0.478611 6 2.382827 -0.859440 0.063106 1 3.259263 -1.116297 -0.531656 1 1.712335 -1.719384 0.037988 1 2.712380 -0.722061 1.094869 1 1.396438 0.248513 -1.509889 1 2.446591 1.217711 -0.501882	57.3891, 98.1852, 175.8113, 241.148, 301.1324, 334.5312, 458.2627, 544.0796, 763.1513, 849.6596, 856.3487, 940.4958, 944.6979, 1007.685, 1050.9046, 1112.5895, 1152.3069, 1253.9629, 1290.3338, 1328.9757, 1361.0412, 1386.524, 1422.7998, 1470.609, 1493.4645, 1503.5391, 1508.228, 1561.8709, 3002.7804, 3027.4275, 3034.0535, 3062.0201, 3088.5795, 3090.9573, 3095.4269, 3144.4718

Compound: *Anti*-nPrCHOO con 2	**Energy (Hartree)** -307.181954702062
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.510416 -0.533809 0.254420 6 0.840671 0.037982 0.448086 8 1.770608 -0.289874 -0.328431 8 3.012643 0.262072 -0.141466 1 1.086723 0.754922 1.227730 1 -0.472029 -1.276942 -0.542405 1 -0.796891 -1.051416 1.177147 6 -1.567881 0.545744 -0.055130 6 -2.969708 -0.045433 -0.182435 1 -3.699685 0.732311 -0.406218 1 -3.277932 -0.536078 0.742463 1 -3.015348 -0.785044 -0.983366 1 -1.554761 1.301450 0.733842 1 -1.292079 1.056298 -0.979674	65.6742, 89.2984, 168.4161, 243.394, 300.3373, 336.3777, 384.6076, 578.5347, 746.1612, 846.8403, 880.0363, 938.8091, 948.3238, 1020.8924, 1041.6515, 1105.6554, 1178.063, 1258.6457, 1293.9097, 1328.312, 1357.0746, 1379.8877, 1418.2676, 1469.9779, 1494.2577, 1500.3118, 1508.8923, 1564.8337, 3000.1766, 3026.0869, 3029.1671, 3055.7101, 3083.0873, 3092.4341, 3096.6082, 3133.3991

Compound: *Anti*-nPrCHOO con 3	**Energy (Hartree)** -307.182121254065
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.583661 -1.015023 -0.296147 6 0.655972 -0.483752 0.314407 8 1.529564 0.052851 -0.409267 8 2.668870 0.538519 0.182102	62.869, 105.9322, 178.42, 247.2197, 279.0519, 351.7739, 450.114, 537.3536, 779.941, 818.5202, 880.1877, 936.78, 946.9433,

1 0.863698 -0.521736 1.381395 1 -0.529327 -0.889808 -1.377961 1 -0.623362 -2.089912 -0.087585 6 -1.857765 -0.353276 0.271306 6 -1.987456 1.124798 -0.088758 1 -2.911020 1.540876 0.313614 1 -2.001321 1.266544 -1.170706 1 -1.158714 1.712369 0.309177 1 -2.715896 -0.907662 -0.112369 1 -1.874067 -0.478120 1.356905	992.711, 1057.1994, 1095.1244, 1175.9777, 1240.3839, 1283.5495, 1334.2517, 1363.6115, 1384.7879, 1424.3973, 1467.8791, 1491.9958, 1501.1848, 1504.7684, 1565.4296, 3004.7632, 3026.2427, 3029.5516, 3057.3638, 3083.074, 3091.2354, 3096.2382, 3129.9569

Compound: *Anti*-nPrCHOO con 4	**Energy (Hartree)** -307.182218473013
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.559948 0.837680 -0.000000 6 -0.918625 0.737439 0.000000 8 -1.477565 -0.384116 -0.000000 8 -2.852427 -0.435356 0.000000 1 -1.571559 1.606789 0.000000 1 0.843478 1.448114 -0.867398 1 0.843478 1.448115 0.867397 6 1.322417 -0.486724 0.000000 1 1.026689 -1.072181 0.871978 1 1.026688 -1.072181 -0.871977 6 2.834935 -0.276625 -0.000000 1 3.159938 0.279201 -0.881610 1 3.159939 0.279202 0.881610 1 3.359235 -1.231903 0.000000	80.3561, 138.497, 143.0562, 240.1337, 251.5122, 326.4856, 403.5991, 665.0471, 720.2753, 833.6513, 861.1925, 937.5239, 940.597, 998.8708, 1045.9112, 1121.6527, 1140.4928, 1253.3391, 1318.7091, 1328.0623, 1356.1445, 1408.6418, 1420.5347, 1447.5595, 1493.6704, 1502.631, 1509.4189, 1572.6658, 2984.0156, 2995.7929, 3024.5283, 3042.6179, 3064.2164, 3088.9886, 3096.4366, 3133.4776

Compound: *Anti*-nPrCHOO con 5	**Energy (Hartree)** -307.181910880642
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.646564 1.168582 -0.106263 6 0.768963 0.764035 -0.290550 8 1.199600 -0.297590 0.216017 8 2.527302 -0.619712 0.046251 1 1.487956 1.366564 -0.840453 1 -0.630307 2.096041 0.481611 1 -1.028713 1.471754 -1.088351 6 -1.574819 0.138873 0.543976 1 -1.135445 -0.201561 1.482741 1 -2.501802 0.652459 0.804851 6 -1.892095 -1.060996 -0.349071 1 -2.356891 -0.742406 -1.284364 1 -0.996497 -1.630938 -0.593310 1 -2.586423 -1.736456 0.150573	91.5103, 128.6726, 165.1414, 234.3122, 257.2545, 335.2353, 437.5822, 621.3027, 783.9881, 804.6133, 853.8654, 931.7261, 944.3601, 979.8758, 1064.9686, 1098.3415, 1142.0294, 1243.1641, 1299.4352, 1342.5786, 1382.6938, 1397.2192, 1421.2839, 1446.0822, 1492.1839, 1502.4825, 1509.8679, 1575.5467, 2983.9653, 3006.4971, 3029.6857, 3040.2365, 3068.1115, 3091.056, 3106.8837, 3131.9858

Compound: *Syn*-nPrCHOO con 1	**Energy (Hartree)** -307.186319485581
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.285432 0.668228 0.497870 6 -1.049098 0.941684 -0.057703 8 -1.935563 0.055268 -0.203460	75.9689, 108.778, 192.5411, 242.726, 304.6045, 370.2883, 530.2874, 660.9098, 761.4841, 813.2105, 890.0174, 891.9084,

8 -1.639564 -1.228243 0.172804 1 -1.383861 1.917230 -0.392884 1 0.151341 -0.015671 1.340227 1 0.723466 1.603842 0.847870 6 1.227476 -0.005676 -0.532167 6 2.575066 -0.359093 0.090501 1 2.452742 -1.064906 0.913237 1 3.231716 -0.819367 -0.648175 1 3.081132 0.526489 0.480114 1 0.737878 -0.902983 -0.907260 1 1.373348 0.668309 -1.378889	911.7306, 1005.6927, 1028.0212, 1100.0583, 1155.1074, 1267.776, 1303.4333, 1333.2206, 1362.6453, 1371.794, 1415.3463, 1458.7502, 1495.6888, 1499.5993, 1506.1713, 1555.9629, 3023.2799, 3024.8293, 3035.9697, 3072.9839, 3081.5503, 3093.742, 3104.0287, 3163.9706

Compound: *Syn*-nPrCHOO con 2	**Energy (Hartree)** -307.185660079521
Reaction Coordinates: 6 0.255765 0.313774 0.974048 6 -0.680101 0.949916 0.031150 8 -1.668082 0.350781 -0.476881 8 -1.873039 -0.962135 -0.146435 1 -0.613517 1.980706 -0.298130 1 -0.350753 -0.266871 1.674525 1 0.794575 1.095047 1.511994 6 1.261262 -0.649544 0.291947 6 2.244554 0.048632 -0.644547 1 2.816105 0.820118 -0.123847 1 2.956281 -0.666984 -1.056694 1 1.735636 0.520847 -1.486956 1 1.806084 -1.156271 1.090092 1 0.695661 -1.412427 -0.240044	**Frequencies (cm^{-1}):** 63.9642, 119.7899, 188.0012, 242.8649, 326.7743, 372.7058, 539.8268, 665.4507, 760.6731, 816.3104, 886.1695, 891.8698, 897.229, 987.3466, 1043.8406, 1103.3874, 1134.3635, 1258.1987, 1280.6656, 1344.6388, 1361.5194, 1380.9147, 1419.4438, 1457.1881, 1496.5986, 1502.6063, 1506.2974, 1555.4388, 3020.8301, 3023.7021, 3044.9949, 3069.0258, 3079.3221, 3090.5231, 3105.7184, 3166.487

Compound: *Syn*-nPrCHOO con 3	**Energy (Hartree)** -307.184497672213
Reaction Coordinates: 6 0.329268 0.946748 0.574690 6 -0.751053 0.871057 -0.426047 8 -1.657962 -0.005345 -0.447450 8 -1.670995 -0.987455 0.506390 1 -0.849684 1.579057 -1.242648 1 0.018056 0.383627 1.452914 1 0.457681 1.999678 0.838805 6 1.679790 0.406595 0.037861 6 1.673698 -1.090419 -0.260631 1 0.934583 -1.348461 -1.019795 1 2.651756 -1.409754 -0.622303 1 1.432513 -1.668026 0.630983 1 1.961357 0.967869 -0.856843 1 2.435180 0.634528 0.792128	**Frequencies (cm^{-1}):** 53.7657, 98.8056, 189.4119, 258.0978, 308.7251, 375.9105, 540.1885, 641.0404, 781.6319, 802.1913, 877.5309, 884.4448, 910.571, 974.2216, 1048.7562, 1097.0622, 1167.4631, 1247.3852, 1279.0684, 1345.898, 1366.9992, 1386.6266, 1428.171, 1462.0446, 1488.4836, 1499.0387, 1501.4274, 1559.5203, 3020.3561, 3029.6266, 3034.852, 3055.1886, 3093.766, 3104.5469, 3108.2332, 3155.7172

Compound: *Syn*-nPrCHOO con 4	**Energy (Hartree)** -307.187234925581
Reaction Coordinates: 6 0.262782 -0.150022 0.000003 6 -0.870210 0.784104 0.000002	**Frequencies (cm^{-1}):** 84.7541, 97.7522, 149.1674, 245.1554, 319.834, 395.4879, 464.8931, 686.4635,

8 -2.070834 0.399027 -0.000001 8 -2.298821 -0.951664 -0.000001 1 -0.773220 1.864746 0.000003 1 0.127021 -0.820901 -0.858749 1 0.127025 -0.820894 0.858761 6 1.632752 0.527182 -0.000003 1 1.718163 1.176460 0.875323 6 2.778302 -0.482165 -0.000000 1 2.736619 -1.125179 -0.880792 1 2.736623 -1.125170 0.880799 1 3.745086 0.020989 -0.000004 1 1.718160 1.176452 -0.875334	700.8163, 780.4966, 887.4962, 891.2703, 926.1719, 1034.4076, 1065.5998, 1114.2849, 1147.9493, 1237.0182, 1281.4425, 1323.1078, 1361.7626, 1396.2937, 1420.2587, 1428.2612, 1494.3379, 1500.9083, 1509.9075, 1560.8583, 2990.6098, 2996.2171, 3016.762, 3027.7137, 3044.8921, 3086.7411, 3095.499, 3159.215

Compound: *Syn*-nPrCHOO con 5	**Energy (Hartree)** -307.186732727465
Reaction Coordinates: 6 -0.205942 0.641897 -0.085374 6 0.590230 -0.557000 -0.380454 8 1.824682 -0.631311 -0.134533 8 2.418927 0.461411 0.440462 1 0.198132 -1.457442 -0.840990 1 0.274211 1.473455 -0.617889 1 -0.034583 0.893591 0.969095 6 -1.692408 0.511295 -0.420875 1 -1.806720 0.201905 -1.463399 6 -2.444352 -0.453842 0.495620 1 -2.381481 -0.132896 1.536793 1 -2.040316 -1.466844 0.440426 1 -3.499146 -0.508516 0.226356 1 -2.144142 1.501843 -0.351328	**Frequencies (cm^{-1}):** 66.391, 116.9869, 184.1646, 246.6209, 298.8611, 434.6715, 463.449, 681.6291, 728.2433, 785.0073, 874.0906, 891.423, 913.6468, 1004.7568, 1070.0682, 1097.643, 1144.8899, 1220.7339, 1285.0691, 1339.4048, 1374.5446, 1379.9094, 1419.9597, 1428.1661, 1493.5375, 1501.8971, 1508.0264, 1560.9653, 2994.014, 3000.9149, 3023.5939, 3026.2834, 3057.6537, 3084.2212, 3094.2295, 3161.356

S10.2.2 Aldehyde and Ketones

Compound: HCHO	**Energy (Hartree)** -114.386051813463
Reaction Coordinates: 6 -0.000000 -0.526970 -0.000000 8 0.000000 0.673271 0.000000 1 -0.000000 -1.112173 0.938294 1 -0.000000 -1.112173 -0.938294	**Frequencies (cm^{-1}):** 1198.1780, 1262.9587, 1530.2218, 1813.2454, 2885.3911, 2940.0951

Compound: CH_3CHO	**Energy (Hartree)** -153.656268371812
Reaction Coordinates: 6 -0.930255 -0.717875 -0.000000 6 -0.000000 0.459414 0.000000 8 1.202268 0.385569 0.000000 1 -0.496506 1.452140 0.000000 1 -0.376434 -1.653591 -0.000000 1 -1.581838 -0.666172 0.876235 1 -1.581838 -0.666172 -0.876235	**Frequencies (cm^{-1}):** 157.49, 509.7923, 774.8566, 886.2424, 1129.3368, 1135.746, 1379.3886, 1421.9604, 1459.9658, 1469.2145, 1805.3067, 2868.8104, 3021.8671, 3072.7019, 3134.3627

Compound: EtCHO con 1	**Energy (Hartree)** -192.913837029760
Reaction Coordinates: 6 -0.543174 0.724333 -0.000000 6 0.930840 0.419433 -0.000000 8 1.409880 -0.686094 0.000000 1 1.589155 1.313513 -0.000000 1 -0.730675 1.368894 0.867197 1 -0.730677 1.368896 -0.867194 6 -1.449528 -0.498268 -0.000000 1 -1.269156 -1.118012 -0.877396 1 -1.269148 -1.118018 0.877391 1 -2.497367 -0.199511 0.000006	**Frequencies (cm^{-1}):** 137.5718, 225.4743, 252.4946, 667.9491, 671.0327, 846.7328, 905.066, 1004.0188, 1110.2803, 1147.8003, 1282.794, 1365.2956, 1410.3368, 1424.1161, 1448.5397, 1494.3937, 1501.1112, 1800.8127, 2864.479, 3000.2219, 3017.4543, 3043.9519, 3106.2238, 3108.9258

Compound: EtCHO con 2	**Energy (Hartree)** -192.912338568899
Reaction Coordinates: 6 0.471414 0.591563 0.144443 6 -0.783366 -0.223964 0.305786 8 -1.809862 -0.045796 -0.298860 1 -0.710126 -1.048102 1.048532 1 0.303006 1.346400 -0.622882 1 0.640985 1.108503 1.095741 6 1.686869 -0.286831 -0.176400 1 1.828702 -1.060701 0.579780 1 1.571813 -0.777932 -1.142881 1 2.595014 0.313595 -0.210385	**Frequencies (cm^{-1}):** 77.0701, 211.6772, 328.3854, 508.5738, 759.2011, 873.8252, 921.0946, 1006.6118, 1133.4945, 1159.9478, 1273.7425, 1328.0464, 1410.4146, 1423.6601, 1467.8018, 1501.4797, 1505.8218, 1801.2012, 2850.7386, 3007.6748, 3032.5054, 3081.0494, 3099.782, 3103.2068

Compound: iPrCHO con 1	**Energy (Hartree)** -232.172228330803
Reaction Coordinates: 6 -0.424807 0.011130 0.411567 6 0.937214 -0.612380 0.203295 8 1.895814 -0.060080 -0.272802 1 1.009145 -1.672468 0.529672 6 -1.493645 -0.870458 -0.255268 1 -1.420692 -1.909310 0.070614 1 -2.491461 -0.511411 -0.004487 1 -1.391113 -0.848333 -1.341472 1 -0.591607 -0.042692 1.496286 6 -0.483246 1.465361 -0.041068 1 0.282622 2.063530 0.450349 1 -0.317857 1.543102 -1.116023 1 -1.458648 1.896299 0.186320	**Frequencies (cm^{-1}):** 94.38, 199.3595, 228.0336, 270.2049, 343.142, 400.1517, 638.9295, 791.9112, 913.8814, 925.7399, 945.4003, 974.5251, 1129.0298, 1154.3785, 1201.6496, 1304.4207, 1354.5164, 1404.0355, 1410.1452, 1431.8869, 1486.4235, 1490.7128, 1504.6756, 1509.354, 1798.0552, 2852.8215, 2972.8853, 3026.5846, 3037.3535, 3086.6913, 3095.4317, 3098.8093, 3108.0968

Compound: iPrCHO con 2	**Energy (Hartree)** -232.171466830656
Reaction Coordinates: 6 0.341720 0.000000 -0.340819 6 -0.997632 0.000023 0.357561 8 -2.071058 0.000007 -0.188449 1 -0.935722 0.000055 1.469066 6 1.115632 -1.269194 0.042815	**Frequencies (cm^{-1}):** 69.7947, 205.9689, 225.4671, 330.2493, 331.4338, 352.8203, 544.3316, 843.4077, 911.982, 931.9916, 958.9973, 981.0885, 1132.403, 1180.9634, 1183.6461,

1 0.585418 -2.169521 -0.268298 1 2.095803 -1.271210 -0.435015 1 1.273172 -1.323710 1.122300 1 0.142848 -0.000001 -1.413593 6 1.115677 1.269168 0.042806 1 0.585496 2.169513 -0.268310 1 1.273222 1.323684 1.122291 1 2.095848 1.271148 -0.435025	1320.7455, 1345.2516, 1398.9327, 1408.2364, 1426.0614, 1488.4443, 1491.9585, 1504.0805, 1511.3597, 1799.7755, 2838.1938, 3022.4608, 3025.208, 3052.1002, 3082.0856, 3089.2092, 3095.9544, 3096.6206

Compound: tBuCHO	**Energy (Hartree)** -271.432768566988
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.327863 0.027002 0.000000 6 -1.038328 -0.639844 0.000003 8 -2.101561 -0.075616 0.000001 1 -0.996024 -1.751482 0.000005 6 1.069906 -0.463705 1.258254 1 1.127500 -1.553428 1.290144 1 2.089773 -0.076452 1.262388 1 0.574689 -0.122370 2.168152 6 1.069897 -0.463701 -1.258260 1 0.574675 -0.122362 -2.168153 1 2.089765 -0.076449 -1.262399 1 1.127490 -1.553424 -1.290154 6 0.194291 1.549358 0.000003 1 -0.349217 1.895976 -0.878376 1 -0.349210 1.895974 0.878387 1 1.181275 2.014285 -0.000001	81.7708, 195.9456, 243.2167, 244.5766, 272.8523, 322.6699, 347.3042, 387.3488, 401.0632, 594.2683, 763.1273, 877.7581, 927.1989, 949.846, 961.6521, 968.464, 1056.6159, 1071.9643, 1226.8546, 1234.5254, 1290.9903, 1396.8823, 1403.7876, 1408.1713, 1436.9589, 1479.7446, 1486.5007, 1488.148, 1499.8075, 1506.854, 1519.3097, 1797.847, 2844.414, 3020.6027, 3023.7014, 3035.2588, 3082.3301, 3085.7412, 3090.5506, 3090.9174, 3097.7377, 3105.997

Compound: OCH-CHO con 1	**Energy (Hartree)** -266.852222733238
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.686244 -0.639816 0.000000 1 1.703444 -1.293431 -0.876216 1 2.564025 -0.000453 0.000000 1 1.703443 -1.293430 0.876217 6 0.432933 0.193453 -0.000001 6 -0.901455 -0.603806 -0.000000 8 -1.973369 -0.071325 0.000000 1 -0.799929 -1.708511 0.000001 8 0.413704 1.395930 0.000000	47.3713, 128.1887, 263.2023, 401.0914, 459.8692, 636.677, 798.6621, 875.4651, 969.6703, 1074.1133, 1175.5864, 1387.5164, 1401.8205, 1460.3017, 1467.9025, 1792.6692, 1827.3837, 2878.3114, 3022.7027, 3070.5679, 3146.1316

Compound: OCH-CHO con 2	**Energy (Hartree)** -266.860539824510
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.882013 1.273803 0.000000 1 -0.446243 1.763739 -0.872659 1 -1.961896 1.389470 0.000000 1 -0.446243 1.763737 0.872660 6 -0.521809 -0.181039 -0.000001 6 0.971192 -0.544801 0.000000 8 1.852626 0.271981 0.000000 1 1.154434 -1.635290 0.000001	83.9092, 120.9176, 247.4205, 467.0722, 483.6734, 568.3116, 777.5089, 907.5434, 1011.4438, 1081.1489, 1240.6326, 1360.532, 1393.964, 1456.9239, 1461.6638, 1778.9799, 1798.1316, 2932.8523, 3039.5034, 3090.9298, 3148.8663

8 -1.315661 -1.093160 0.000000	

Compound: $(CH_3)_2CO$	**Energy (Hartree)** -192.924334709876
Reaction Coordinates: 6 -1.287796 -0.611342 0.000009 6 -0.000000 0.184263 0.000001 8 0.000000 1.394544 -0.000000 6 1.287796 -0.611342 -0.000008 1 2.142292 0.059795 -0.000458 1 1.329612 -1.261732 -0.876460 1 1.329998 -1.260974 0.876992 1 -2.142291 0.059795 0.000470 1 -1.330002 -1.260963 -0.876999 1 -1.329607 -1.261743 0.876452	**Frequencies (cm^{-1}):** 27.6477, 131.5768, 380.6368, 490.9686, 535.2152, 782.9184, 886.7496, 887.4282, 1085.1731, 1120.8963, 1233.7118, 1387.5641, 1387.871, 1459.7874, 1465.7347, 1470.3334, 1488.1926, 1781.7479, 3025.4845, 3032.6623, 3076.7144, 3084.1624, 3137.7556, 3138.7532

Compound: CF_3CFO	**Energy (Hartree)** -550.398192942521
Reaction Coordinates: 6 -0.590884 0.016760 -0.000000 6 0.950258 0.161191 -0.000000 8 1.560686 1.164510 0.000000 9 1.511346 -1.053957 -0.000000 9 -0.986585 -0.656718 1.087722 9 -1.165035 1.213645 -0.000003 9 -0.986585 -0.656723 -1.087719	**Frequencies (cm^{-1}):** 43.7845, 226.0109, 238.7949, 378.7825, 419.3861,1. 512.0808, 584.7772, 688.3344, 765.2522, 800.0823, 1086.2930, 1167.3575, 1222.6180, ,1305.3726, 1935.9581

Compound: CF_3CF_2CHO con 1	**Energy (Hartree)** -688.812957684290
Reaction Coordinates: 6 -0.422322 0.474806 -0.007111 6 -1.578544 -0.376488 0.578734 8 -2.411136 -0.878783 -0.111479 1 -1.564497 -0.448302 1.679382 9 -0.698082 0.855351 -1.264304 9 -0.294172 1.582858 0.773134 6 0.938571 -0.268521 -0.002943 9 1.226271 -0.667494 1.247370 9 0.872605 -1.348671 -0.787048 9 1.918640 0.522377 -0.435778	**Frequencies (cm^{-1}):** 51.5838, 63.0683, 193.5618, 211.5132, 256.0864, 305.4401, 356.7146, 378.5992, 447.2778, 535.8368, 576.8438, 597.3911, 723.1946, 791.5991, 919.2348, 1072.488, 1137.8257, 1184.1741, 1198.6606, 1237.1088, 1317.8364, 1396.8437, 1843.4596, 2961.9338

Compound: CF_3CF_2CHO con 2	**Energy (Hartree)** -688.812777288418
Reaction Coordinates: 6 -0.437650 0.570319 0.000000 6 -1.776191 -0.200583 0.000000 8 -1.870643 -1.390064 -0.000000 1 -2.642222 0.486317 0.000000 9 -0.424425 1.368847 -1.097860 9 -0.424425 1.368847 1.097860 6 0.851157 -0.287979 0.000000	**Frequencies (cm^{-1}):** 69.26, 76.1892, 150.7349, 212.3416, 273.9584, 302.4093, 345.8929, 419.3262, 424.4234, 511.1899, 581.8153, 587.6043, 688.2018, 767.8071, 974.4221, 1102.9404, 1137.7221, 1174.2323, 1204.6731,

9 0.893553 -1.059323 1.088778 9 0.893553 -1.059323 -1.088778 9 1.926575 0.508024 0.000000	1208.8089, 1317.4186, 1420.6831, 1843.9034, 2940.2234

Compound: CF_3CHO	**Energy (Hartree)** -451.199957828211
Reaction Coordinates: 6 0.015009 0.360282 0.000000 6 0.501814 -1.106406 -0.000000 8 -0.245475 -2.035870 -0.000000 1 1.601864 -1.198064 -0.000000 9 0.501814 0.987869 1.088491 9 0.501814 0.987869 -1.088491 9 -1.307962 0.464459 0.000000	**Frequencies (cm^{-1}):** 73.5798, 250.7650, 307.2813, 422.6928, 518.9491, 524.0490, 701.8523, 834.5377, 974.2730, 1150.4161, 1174.8562, 1288.1325, 1403.3576, 1849.8517, 2955.8187

Compound: ClCHO	**Energy (Hartree)** -573.573415675277
Reaction Coordinates: 6 0.000000 0.806099 0.000000 17 -0.473506 -0.921812 0.000000 1 -0.898423 1.430438 0.000000 8 1.118503 1.175472 -0.000000	**Frequencies (cm^{-1}):** 445.4726, 717.2277, 947.4225, 1321.5214, 1845.7994, 3051.6439

Compound: FCHO	**Energy (Hartree)** -213.595002968390
Reaction Coordinates: 6 0.000000 0.400194 0.000000 9 -0.967389 -0.541739 0.000000 1 -0.464528 1.390119 0.000000 8 1.146378 0.135546 -0.000000	**Frequencies (cm^{-1}):** 661.6044, 1029.8624, 1055.9306, 1362.001, 1882.619, 3084.6994

Compound: nPrCHO con 1	**Energy (Hartree)** -232.170419945897
Reaction Coordinates: 6 -0.097122 0.733975 0.000001 6 -1.565367 0.404295 -0.000000 8 -2.028030 -0.708387 -0.000001 1 -2.238126 1.287813 0.000000 1 0.081540 1.382468 -0.867462 1 0.081539 1.382470 0.867462 6 0.841647 -0.466402 0.000003 1 0.624032 -1.088297 0.870079 1 0.624027 -1.088304 -0.870067 6 2.314355 -0.061509 -0.000002 1 2.563923 0.533617 -0.880971 1 2.563927 0.533624 0.880961 1 2.962296 -0.938444 0.000000	**Frequencies (cm^{-1}):** 79.0249, 171.9653, 191.8132, 244.2293, 344.4104, 666.0703, 692.8205, 790.8347, 852.1237, 951.5362, 961.9475, 1043.9681, 1133.3022, 1156.6431, 1256.8694, 1317.3106, 1325.6864, 1395.4313, 1415.1439, 1419.5698, 1447.599, 1491.6665, 1501.7294, 1508.6961, 1799.3454, 2861.5282, 2989.48, 3006.1864, 3020.0669, 3039.5484, 3058.8197, 3083.8279, 3087.8297

Compound: nPrCHO con 2	**Energy (Hartree)** -232.170348997214

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.199645 1.019758 0.141947 6 1.415581 0.135016 0.236253 8 1.523900 -0.957904 -0.259595 1 2.262649 0.575269 0.803554 1 -0.029844 1.367689 1.156366 1 0.531469 1.920463 -0.390414 6 -1.022395 0.397694 -0.529479 1 -1.724891 1.196104 -0.777518 1 -0.713996 -0.053718 -1.473928 6 -1.724791 -0.650424 0.334054 1 -1.059489 -1.481653 0.564841 1 -2.067959 -0.217559 1.276486 1 -2.597370 -1.055625 -0.179274	99.5657, 162.1953, 195.5618, 274.8177, 362.6911, 656.9668, 703.4042, 786.5623, 844.3608, 936.0297, 969.4128, 1057.1531, 1115.6621, 1146.5275, 1253.2475, 1297.9877, 1376.1737, 1381.507, 1413.563, 1419.1272, 1443.705, 1486.4416, 1500.17, 1510.136, 1799.5379, 2861.6032, 2993.2277, 3013.3291, 3024.6457, 3033.6785, 3062.7094, 3084.3356, 3103.6045

Compound: nPrCHO con 3	**Energy (Hartree)** -232.169370024577
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.118374 -0.465499 0.251195 6 1.458818 0.215512 0.288500 8 2.419405 -0.106593 -0.363825 1 1.521548 1.084936 0.978300 1 0.170448 -1.311078 -0.435125 1 -0.078575 -0.854737 1.257306 6 -1.009186 0.503603 -0.136768 1 -0.987093 1.370844 0.528866 1 -0.821525 0.883269 -1.143889 6 -2.389081 -0.148570 -0.081681 1 -2.616927 -0.504401 0.924822 1 -2.448282 -1.003756 -0.756908 1 -3.168382 0.557398 -0.370252	68.7684, 96.8771, 235.1684, 254.6435, 380.387, 515.9786, 746.7568, 805.7749, 901.2618, 953.5301, 1005.3719, 1041.2682, 1137.0209, 1165.6705, 1254.7152, 1290.5464, 1329.9931, 1379.6366, 1415.7718, 1421.7209, 1466.9131, 1494.153, 1500.1553, 1509.006, 1799.3304, 2852.6102, 2998.645, 3017.4256, 3024.9442, 3044.3664, 3080.8028, 3088.5077, 3090.2776

Compound: nPrCHO con 4	**Energy (Hartree)** -232.169477639287
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.155968 0.842209 -0.360288 6 -1.228391 0.075748 0.366894 8 -2.074188 -0.605771 -0.154061 1 -1.202106 0.180973 1.473895 1 -0.219596 0.615075 -1.425055 1 -0.390638 1.904968 -0.228506 6 1.248991 0.566634 0.197494 1 1.943330 1.283618 -0.243997 1 1.253859 0.764684 1.273298 6 1.737771 -0.856377 -0.069868 1 1.770445 -1.064835 -1.140641 1 1.083177 -1.600367 0.387544 1 2.740619 -1.007240 0.330553	68.4528, 118.7583, 216.731, 302.3159, 396.1621, 511.5794, 755.9297, 774.6293, 898.4108, 946.3573, 979.0731, 1056.5192, 1125.8027, 1160.8035, 1238.2905, 1281.6809, 1351.1196, 1376.0608, 1418.2633, 1422.1193, 1461.9924, 1492.0975, 1501.3307, 1505.2713, 1799.7486, 2845.5201, 3003.1553, 3017.902, 3026.1685, 3051.7702, 3079.617, 3086.974, 3091.144

Compound: nPrCHO con 5	**Energy (Hartree)** -232.167656622638
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.188305 0.723213 0.418471 6 -1.178795 -0.385544 0.184842 8 -2.274620 -0.231140 -0.295053 1 -0.847013 -1.401782 0.480098 1 -0.676292 1.665685 0.170991 1 0.055799 0.733347 1.486996 6 1.115237 0.558484 -0.389455 1 0.867846 0.473053 -1.450287 1 1.684892 1.483908 -0.285759 6 1.991488 -0.619543 0.038389 1 1.498318 -1.579572 -0.116221 1 2.256337 -0.549266 1.095310 1 2.919322 -0.635924 -0.534185	32.5075, 106.1833, 230.6751, 282.4868, 401.4827, 502.8874, 750.1966, 820.4108, 872.2837, 955.4863, 982.8532, 1050.0988, 1137.8552, 1149.2595, 1249.7828, 1288.7109, 1342.9645, 1376.2946, 1419.3167, 1427.9824, 1469.4841, 1495.2402, 1503.2179, 1509.413, 1794.2093, 2876.4281, 3003.0939, 3025.2069, 3028.2935, 3053.6752, 3085.6866, 3087.6659, 3092.9057

S10.2.3 Epoxide

Compound: MeCH(O)CH_2 epoxide	**Energy (Hartree)** -192.878663433749
Reaction Coordinates: 6 -1.508220 0.097295 -0.148746 6 -0.152958 -0.033618 0.484762 6 1.040045 0.616688 -0.061356 1 0.953858 1.210439 -0.965730 1 1.864601 0.879926 0.592659 8 0.828990 -0.789185 -0.238075 1 -0.153870 -0.247576 1.550743 1 -1.418683 0.319184 -1.211821 1 -2.074599 -0.828747 -0.037983 1 -2.076426 0.898071 0.328772	**Frequencies (cm^{-1}):** 206.9689, 367.2093, 410.1583, 770.2174, 842.076, 907.7501, 972.2655, 1042.6983, 1129.1516, 1156.8279, 1166.8292, 1189.2541, 1293.3958, 1406.7794, 1438.6459, 1483.164, 1496.9703, 1529.0015, 3027.8395, 3080.6169, 3084.617, 3087.9567, 3109.3484, 3163.9921

Compound: MVK epoxide 1	**Energy (Hartree)** -306.085253261747
Reaction Coordinates: 6 2.038053 -0.662345 0.054704 6 0.786358 0.178150 -0.014888 6 -0.509862 -0.589469 -0.125013 6 -1.672912 -0.147652 0.669190 1 -2.400258 -0.885087 0.991096 1 -1.563704 0.737727 1.285160 8 -1.610151 0.085568 -0.727499 1 -0.429169 -1.641442 -0.381104 8 0.799777 1.384927 0.028628 1 2.178921 -1.190621 -0.891664 1 1.946886 -1.424690 0.831905 1 2.900495 -0.031953 0.251609	**Frequencies (cm^{-1}):** 59.3766, 128.7536, 238.073, 266.2238, 374.635, 593.4428, 611.4556, 763.4566, 866.6265, 891.2063, 956.7035, 995.5147, 1058.3488, 1100.7998, 1161.1896, 1165.9146, 1197.2407, 1276.3587, 1384.3475, 1413.5506, 1463.6677, 1473.9134, 1508.1708, 1789.418, 3025.4932, 3076.2812, 3088.1766, 3116.7276, 3142.22, 3183.5725

Compound: MVK epoxide 2	**Energy (Hartree)** -306.088513722259
Reaction Coordinates: 6 1.189939 1.271715 0.081328 6 0.866183 -0.196251 -0.021157 6 -0.566270 -0.592823 -0.248650 6 -1.635483 -0.142820 0.660098	**Frequencies (cm^{-1}):** 91.8198, 110.1739, 234.6262, 263.4874, 478.3598, 506.3708, 595.9417, 739.7356, 858.0709, 896.9919, 931.2284, 1011.6297, 1065.5649, 1097.0453, 1154.8359,

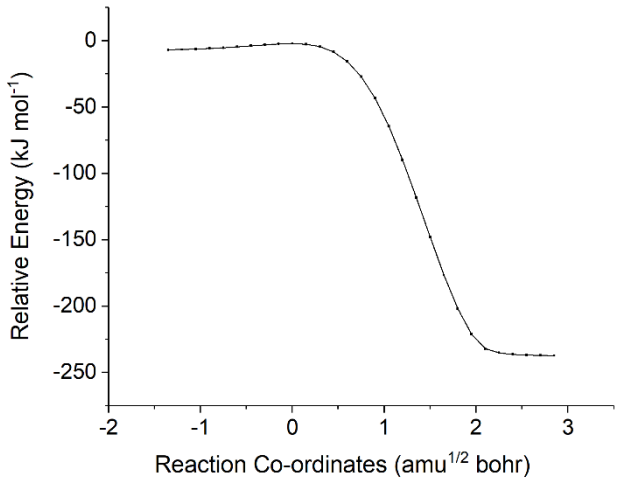
1 -2.496959 -0.785349 0.802985 1 -1.398787 0.519029 1.486012 8 -1.497983 0.422872 -0.636579 1 -0.682880 -1.550471 -0.744110 8 1.706168 -1.065329 0.055880 1 0.517612 1.787253 0.767438 1 1.047793 1.737605 -0.896035 1 2.221528 1.392670 0.399584	1165.8901, 1249.4673, 1272.1889, 1387.5027, 1393.4862, 1457.9142, 1469.6452, 1524.813, 1772.6261, 3040.1397, 3090.4468, 3094.1255, 3138.5166, 3144.7729, 3178.0915

S10.2.4 Oxygen

Compound: O_2	**Energy (Hartree)** -150.147598743643
Reaction Coordinates: 8 0.000000 0.000000 0.602585 8 0.000000 0.000000 -0.602585	**Frequencies (cm^{-1}):** 1614.3238

S10.3 Ozonolysis of Propene (Alkene 1)

Compound: $MeCHCH_2 + O_3$ PRC1	**Energy (Hartree)** -342.973340622844
Reaction Coordinates: 6 2.046171 -0.757081 0.514567 6 1.408907 0.107682 -0.521617 6 0.971533 1.353841 -0.316182 1 0.531213 1.938242 -1.112426 1 1.068868 1.835740 0.648039 1 1.323959 -0.317086 -1.516737 1 2.105661 -0.251830 1.477924 1 1.478727 -1.680958 0.645647 1 3.055910 -1.045358 0.210847 8 -1.512327 0.661928 0.752210 8 -1.842990 -0.098257 -0.199497 8 -1.160183 -1.151847 -0.354451	**Frequencies (cm^{-1}):** 38.8907, 70.1551, 90.066, 100.3661, 129.2045, 212.2132, 276.861, 427.6039, 602.623, 741.8813, 925.1872, 952.2453, 956.0315, 1008.9446, 1069.5981, 1163.1981, 1192.1138, 1196.8335, 1325.778, 1407.2116, 1449.5641, 1477.8939, 1493.0218, 1667.0177, 3019.2457, 3064.5642, 3098.9453, 3134.0848, 3139.2265, 3220.6033

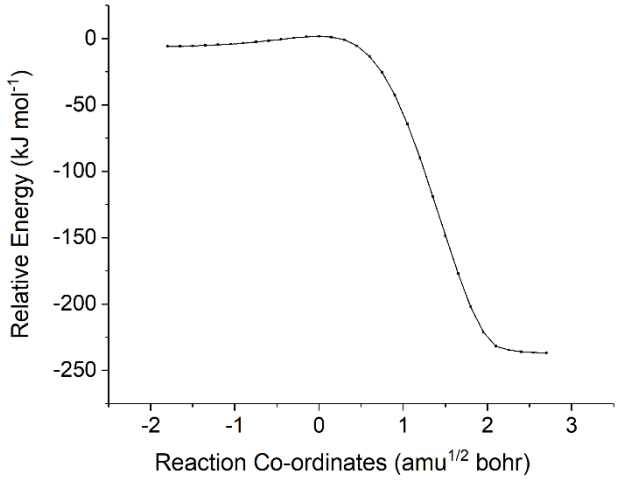
Compound: $MeCHCH_2 + O_3$ TS_{OZO} 1	**Energy (Hartree)** -342.964246608645
Reaction Coordinates: 6 -2.033369 -0.503898 -0.421156 6 -1.110850 0.185356 0.526972 6 -0.481983 1.364071 0.249512 1 0.044756 1.912973 1.015219 1 -0.647546 1.872572 -0.689368 1 -1.080407 -0.191077 1.541692 1 -1.849166 -1.578058 -0.436073 1 -1.924197 -0.119125 -1.434144 1 -3.071437 -0.358797 -0.108116 8 1.461418 0.617093 -0.613638 8 1.635810 -0.360818 0.205516 8 0.688422 -1.232732 0.155476	**Frequencies (cm^{-1}):** -195.1873, 83.5637, 131.979, 180.8475, 224.0039, 352.6094, 427.7067, 456.8352, 682.3138, 743.3604, 919.2146, 949.3388, 962.0258, 990.9226, 1054.6825, 1085.5173, 1117.2666, 1199.1591, 1300.8936, 1407.9286, 1445.1137, 1476.5941, 1492.8063, 1591.4831, 3019.9589, 3076.4735, 3109.7043, 3154.1064, 3165.2523, 3245.1805
IRC:  	

Compound: $MeCHCH_2 + O_3$ POZ1	**Energy (Hartree)** -343.063267068713

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.050387 0.025192 -0.245438 6 -0.701157 -0.038194 0.438893 6 0.246523 1.167424 0.181761 1 -0.151447 1.870719 -0.548496 1 0.491174 1.681784 1.113020 8 1.410517 0.590862 -0.404377 8 1.391085 -0.754568 0.128139 8 0.032978 -1.138922 -0.110778 1 -0.811837 -0.188223 1.515612 1 -1.931064 0.181911 -1.317147 1 -2.637065 0.846341 0.167823 1 -2.606274 -0.898030 -0.085981	75.1327, 229.9592, 316.7004, 364.9438, 462.5479, 667.3721, 717.3333, 743.3922, 839.0161, 906.0755, 933.0356, 962.7378, 994.9027, 1078.8553, 1146.0166, 1166.3657, 1235.2029, 1332.5979, 1351.3282, 1390.4342, 1416.348, 1486.5674, 1500.2498, 1512.1843, 3023.4868, 3037.8377, 3039.6458, 3100.108, 3104.1246, 3113.6936

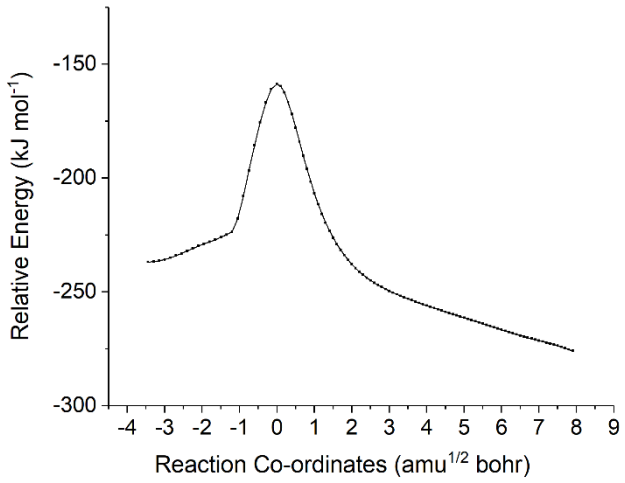
Compound: MeCHCH$_2$ + O$_3$ PRC 2	**Energy (Hartree)** -342.973281732246
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.122525 -0.742209 -0.531744 6 1.459586 0.116335 0.496454 6 0.975341 1.340484 0.275489 1 1.047800 1.810920 -0.697473 1 0.511754 1.915285 1.063783 1 1.389971 -0.298113 1.496664 1 3.146442 -0.982935 -0.233810 1 1.600609 -1.696077 -0.641658 1 2.155223 -0.253003 -1.505010 8 -1.736533 0.801348 -0.451900 8 -1.633209 -0.454117 -0.385960 8 -1.279821 -0.945198 0.722399	35.9939, 49.1724, 78.4193, 94.9363, 117.9646, 211.3654, 257.3273, 427.3409, 603.4208, 742.7204, 924.135, 951.236, 959.3925, 1011.0515, 1069.5952, 1168.0601, 1194.718, 1197.6079, 1326.2731, 1408.371, 1451.0589, 1477.7041, 1494.3744, 1672.3857, 3015.9712, 3057.2143, 3094.5576, 3136.0295, 3141.2178, 3226.5704

Compound: MeCHCH$_2$ + O$_3$ TS$_{OZO}$ 2	**Energy (Hartree)** -342.962560927001
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.926380 -0.562291 -0.477319 6 -1.129988 0.244089 0.497661 6 -0.475375 1.395306 0.162784 1 -0.050295 2.032662 0.921434 1 -0.529152 1.793872 -0.840672 1 -1.234267 -0.003310 1.545558 1 -1.872560 -1.626643 -0.255180 1 -1.589302 -0.398940 -1.501043 1 -2.980842 -0.273298 -0.426744 8 1.594726 0.664324 -0.303132 8 1.327607 -0.592512 -0.409856 8 0.758526 -1.070183 0.645224	-214.9837, 83.3289, 117.0989, 184.5561, 203.7508, 365.4669, 433.7475, 476.5627, 688.6408, 742.19, 916.1274, 952.9509, 955.9557, 989.4269, 1054.6929, 1079.7675, 1111.3577, 1196.1878, 1295.6607, 1406.6303, 1442.8075, 1479.0257, 1493.3283, 1586.1367, 3015.0671, 3074.3987, 3111.8664, 3155.4298, 3174.4678, 3251.3228
IRC:	



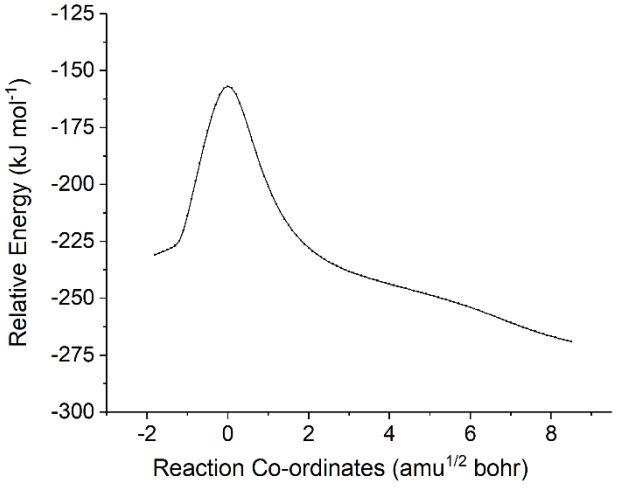
Compound: $MeCHCH_2 + O_3$ POZ 2	**Energy (Hartree)** -343.063413011835
Reaction Coordinates: 6 1.938333 0.041783 -0.397501 6 0.719003 0.104400 0.503272 6 -0.319630 1.177145 0.070401 1 -0.487873 1.944716 0.823288 1 -0.031970 1.631370 -0.880474 8 -1.539167 0.459373 -0.060512 8 -1.069230 -0.827669 -0.500997 8 -0.047318 -1.110899 0.476472 1 1.003755 0.228290 1.548449 1 2.474743 0.992813 -0.375366 1 1.641410 -0.162621 -1.426001 1 2.619423 -0.740974 -0.066630	**Frequencies (cm^{-1}):** 91.6591, 236.5009, 316.9286, 387.176, 478.9595, 671.8908, 711.1444, 742.0023, 835.0898, 904.9102, 934.1492, 954.7888, 1002.126, 1062.4926, 1110.8867, 1165.6292, 1241.2155, 1308.3908, 1345.076, 1380.989, 1411.275, 1486.8762, 1496.3555, 1506.9092, 3029.3811, 3033.4412, 3063.3112, 3095.2046, 3110.6938, 3116.8918

Compound: $MeCHCH_2 + O_3$ TS_{ANTI}	**Energy (Hartree)** -343.031950106195
Reaction Coordinates: 6 2.108980 0.187069 -0.056931 6 0.704892 -0.095474 0.369695 6 -0.497599 1.290475 -0.095848 1 -0.181191 1.950361 0.727608 1 -0.106096 1.573175 -1.084563 1 0.465767 -0.120182 1.427646 1 2.797103 -0.533157 0.389879 1 2.404011 1.180431 0.278889 1 2.204504 0.138218 -1.140033 8 -1.642531 0.750919 -0.019875 8 -1.134302 -1.261881 0.114900 8 0.091617 -1.049195 -0.332642	**Frequencies (cm^{-1}):** -435.5564, 159.8915, 162.7443, 243.3816, 337.013, 364.1606, 493.2648, 518.3261, 616.5203, 856.7676, 907.117, 994.0697, 1017.6363, 1120.2254, 1153.7143, 1182.835, 1220.6793, 1270.1363, 1389.7569, 1392.5438, 1423.9989, 1479.9475, 1492.2612, 1544.0705, 2907.356, 2969.0715, 3037.5842, 3097.7653, 3121.9158, 3139.4026
IRC:	



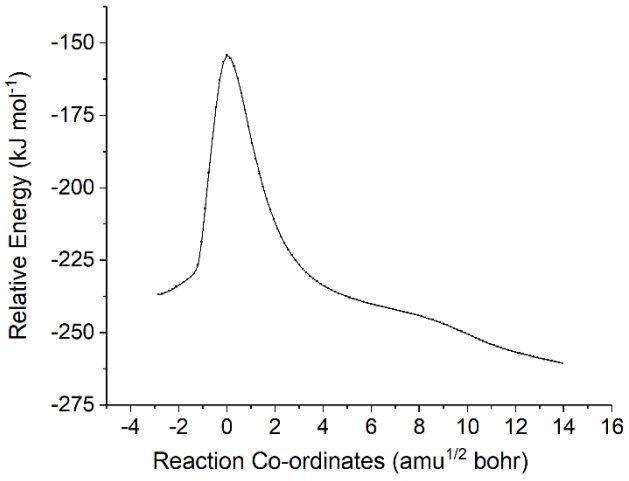
Compound: $MeCHCH_2 + O_3$ C_{ANTI}	**Energy (Hartree)** -343.070570907990
Reaction Coordinates: 6 2.197640 -0.529115 0.098610 6 0.958332 0.105026 -0.385106 1 0.536037 -0.090929 -1.361383 8 0.400476 0.976339 0.330402 8 -0.826700 1.434854 -0.130168 1 3.011534 -0.346947 -0.607012 1 2.037337 -1.608719 0.138469 1 2.469683 -0.163904 1.085429 6 -1.874516 -0.546271 0.078546 1 -2.271882 -0.198727 1.040808 1 -2.454921 -0.266176 -0.810583 8 -0.950841 -1.348998 0.020012	**Frequencies (cm^{-1}):** 62.1318, 97.2317, 140.2578, 151.4405, 304.1128, 314.8473, 337.3339, 380.8651, 561.4254, 573.6272, 866.8006, 897.8345, 973.5133, 1066.902, 1149.0758, 1168.9578, 1251.1705, 1351.7798, 1408.3246, 1454.1633, 1464.0759, 1508.2848, 1579.4701, 1689.4636, 2956.3467, 3020.7985, 3031.2656, 3081.6618, 3140.6488, 3197.8733

Compound: $MeCHCH_2 + O_3$ TS_{FO} 1	**Energy (Hartree)** -343.029736721201
Reaction Coordinates: 6 -1.863419 0.325251 -0.555472 6 -0.900294 -0.214589 0.490774 6 0.531012 0.992746 0.625922 1 0.176450 2.014223 0.558547 1 0.967698 0.645722 1.554058 1 -1.203517 -0.031654 1.537554 1 -2.730821 -0.335153 -0.601855 1 -2.213169 1.328091 -0.307063 1 -1.396042 0.333887 -1.538607 8 1.170957 0.617530 -0.477435 8 1.591772 -0.629740 -0.367051 8 -0.288279 -1.309736 0.273239	**Frequencies (cm^{-1}):** -441.1182, 130.408, 178.8658, 265.1302, 306.2098, 476.8837, 494.434, 566.6192, 606.6314, 848.6613, 897.3717, 947.7903, 1017.5617, 1051.8142, 1112.7448, 1170.13, 1222.4076, 1267.6481, 1317.82, 1398.6733, 1451.4804, 1477.7491, 1481.9663, 1499.9064, 2891.6285, 3032.5107, 3092.4971, 3106.4542, 3118.8222, 3224.4608
IRC:	



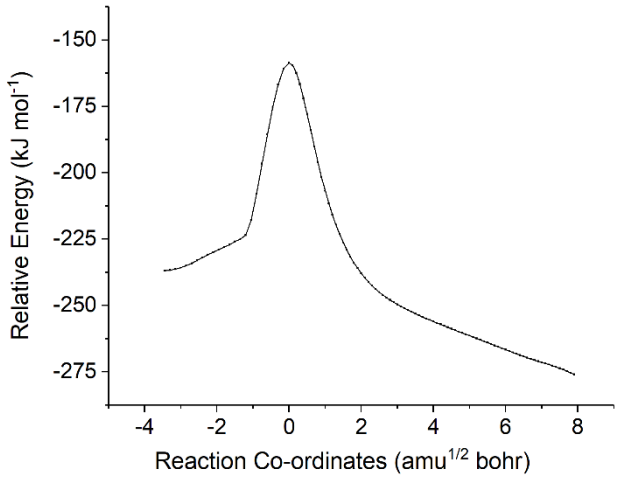
Compound: $MeCHCH_2 + O_3$ CPr_{FO} 1	**Energy (Hartree)** -343.066723044814
Reaction Coordinates: 6 -1.628628 1.178988 0.019416 6 -2.014980 -0.263196 0.043493 1 -3.099230 -0.463665 0.154371 8 -1.252698 -1.199519 -0.046059 1 -2.182262 1.678699 -0.780919 1 -1.959522 1.646138 0.951932 1 -0.555607 1.321104 -0.111564 6 1.459277 -1.055111 -0.183656 1 1.514456 -1.979499 0.373492 1 1.142293 -0.980298 -1.214471 8 1.809286 -0.028010 0.433852 8 1.724144 1.179208 -0.218837	**Frequencies (cm^{-1}):** 51.0945, 82.2432, 90.2483, 109.0794, 128.3928, 181.0936, 202.4777, 519.0435, 532.8399, 678.8141, 782.7034, 865.1322, 896.3788, 992.8464, 1143.6419, 1149.8444, 1235.5433, 1389.7419, 1413.674, 1423.7214, 1467.8134, 1478.4089, 1567.3742, 1779.2423, 2890.1717, 3004.4732, 3062.778, 3101.2363, 3132.8648, 3276.8435

Compound: $MeCHCH_2 + O_3$ TS_{FO} 2	**Energy (Hartree)** -343.028828640250
Reaction Coordinates: 6 -2.095277 0.231115 0.315259 6 -0.856701 -0.188307 -0.474101 6 0.400100 1.129165 0.043748 1 0.272014 2.028118 -0.546933 1 0.150824 1.152906 1.097425 1 -0.899090 0.060505 -1.547828 1 -1.950961 0.042396 1.377925 1 -2.938163 -0.371555 -0.025995 1 -2.345793 1.281110 0.155790 8 1.515835 0.486568 -0.264913 8 1.626155 -0.617773 0.450336 8 -0.264186 -1.271960 -0.162900	**Frequencies (cm^{-1}):** -447.2867, 92.3351, 208.7885, 274.9778, 337.672, 466.7115, 477.8343, 529.6582, 599.4037, 873.647, 884.7108, 988.5419, 989.6916, 1062.2058, 1090.5631, 1182.0517, 1229.8464, 1265.8517, 1351.3143, 1392.0788, 1451.3561, 1479.2682, 1483.454, 1501.2031, 2912.5449, 3028.9988, 3091.7495, 3104.8768, 3115.7515, 3224.0316
IRC	



Compound: $MeCHCH_2 + O_3$ CPr_{FO} 2	**Energy (Hartree)** -343.064735066772
Reaction Coordinates: 6 -2.019621 -1.247414 -0.000007 6 -2.440784 0.188467 0.000015 1 -3.534865 0.363110 0.000049 8 -1.686882 1.132770 -0.000001 1 -2.444380 -1.746527 -0.875108 1 -2.444331 -1.746540 0.875111 1 -0.937189 -1.348876 -0.000038 6 1.565528 1.042583 -0.000006 1 2.454020 1.663367 0.000053 1 0.539327 1.388502 -0.000047 8 1.702666 -0.203437 -0.000027 8 2.951301 -0.738689 0.000024	**Frequencies (cm^{-1}):** 28.4229, 38.0975, 54.7174, 62.5817, 92.6413, 123.3914, 164.5267, 515.2057, 531.0457, 712.471, 778.0505, 891.4224, 901.1816, 997.4803, 1137.4001, 1140.1854, 1255.8368, 1384.2757, 1409.2608, 1426.4191, 1461.2988, 1469.9073, 1544.7324, 1792.4954, 2893.9688, 3022.6592, 3072.2478, 3098.3098, 3137.99, 3251.0177

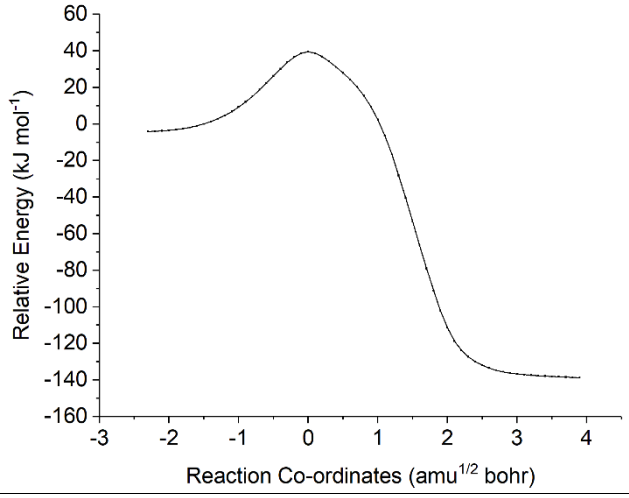
Compound: $MeCHCH_2 + O_3$ TS_{SYN}	**Energy (Hartree)** -343.031540552877
Reaction Coordinates: 6 1.547685 -0.613374 -0.584216 6 0.726375 -0.220193 0.609068 6 -0.947402 -1.023218 0.365839 1 -0.525956 -1.999100 0.078884 1 -1.371198 -0.992132 1.379130 1 1.095816 -0.499901 1.591394 1 0.965329 -0.573860 -1.499174 1 1.942306 -1.617141 -0.438116 1 2.387497 0.079938 -0.677500 8 -1.491250 -0.326126 -0.549136 8 -0.299553 1.391748 -0.474450 8 0.234086 1.027242 0.676240	**Frequencies (cm^{-1}):** -444.8601, 156.655, 188.4216, 296.5703, 306.3347, 344.3532, 527.3134, 563.6148, 702.2926, 871.6034, 883.8925, 939.2037, 1020.9308, 1086.1398, 1147.213, 1186.0746, 1222.8821, 1223.6026, 1375.6538, 1398.5207, 1429.4044, 1471.5763, 1495.3352, 1539.1968, 2919.339, 2983.6402, 3034.7282, 3105.2349, 3132.4762, 3154.7314
IRC	



Compound: $MeCHCH_2 + O_3$ CPr_{SYN}	**Energy (Hartree)** -343.071168900871
Reaction Coordinates: 6 -1.491663 1.023885 -0.580865 6 -1.291439 0.196594 0.612757 1 -1.657196 0.454777 1.600228 8 -0.704673 -0.916383 0.595860 8 -0.164546 -1.328994 -0.604524 1 -0.524243 1.411419 -0.910582 1 -2.169283 1.847171 -0.372369 1 -1.860722 0.392913 -1.393197 6 2.029503 -0.043452 -0.167678 1 2.334801 -0.918443 0.427315 1 2.130582 -0.146991 -1.259248 8 1.652675 0.982500 0.348985	**Frequencies (cm^{-1}):** 77.6957, 91.1998, 96.0059, 126.0497, 167.3703, 210.1412, 301.7889, 345.5066, 454.0568, 670.0869, 770.7042, 884.7781, 980.147, 1062.5706, 1116.0221, 1173.9362, 1259.687, 1354.4061, 1396.7133, 1442.0159, 1468.6435, 1527.8804, 1576.3099, 1770.6073, 2929.3797, 2990.1892, 3027.6469, 3074.0465, 3139.4954, 3172.2283

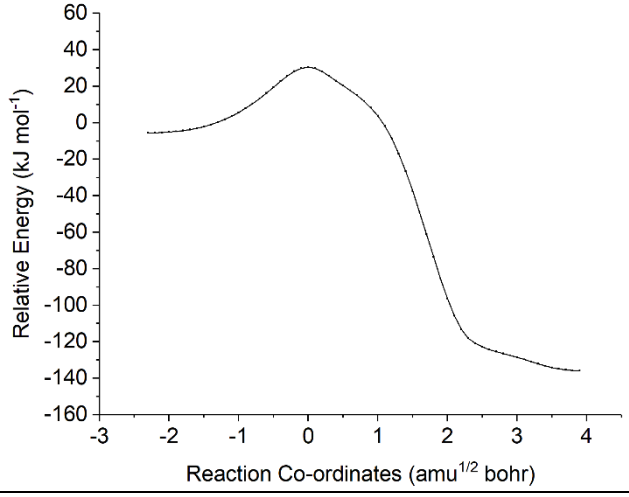
Compound: $MeCHCH_2 + O_3$ TS_{POZ} 1	**Energy (Hartree)** -343.058289489220
Reaction Coordinates: 6 -1.770030 0.021830 -0.574846 1 -2.452965 0.862794 -0.443128 6 0.294413 1.112429 0.491275 1 -0.105029 2.071086 0.164575 1 0.824696 1.213039 1.441433 1 -1.216489 -0.057506 1.527534 1 -1.282974 0.115213 -1.544233 1 -2.354401 -0.897134 -0.567872 6 -0.743636 -0.003946 0.545064 8 1.155342 0.668945 -0.541954 8 0.106216 -1.149527 0.497977 8 1.226277 -0.780590 -0.374431	**Frequencies (cm^{-1}):** -148.4636, 205.8173, 210.8383, 355.8478, 435.069, 679.0243, 730.9869, 792.7407, 825.3244, 857.8566, 940.0433, 963.0335, 1010.6141, 1058.0101, 1108.7303, 1166.2742, 1238.0158, 1289.3759, 1346.913, 1371.4596, 1412.9007, 1485.8917, 1496.2793, 1499.0454, 3028.4694, 3038.0729, 3061.594, 3102.2062, 3113.0063, 3121.4633
IRC To low a barrier for IRC to be done	

Compound: MeCHCH$_2$ + O$_3$ TS$_{POZ}$ 2	**Energy (Hartree)** -343.058489104847
Reaction Coordinates: 6 2.106630 0.013743 0.107061 1 2.638281 0.896363 -0.249638 6 -0.219517 1.125932 0.180945 1 -0.061519 1.244385 1.257219 1 -0.133667 2.081572 -0.334133 1 0.636947 0.072052 -1.487915 1 2.136289 -0.003363 1.195784 1 2.625909 -0.866339 -0.268922 6 0.677520 0.040398 -0.394185 8 -1.511611 0.632049 -0.109715 8 0.018055 -1.131655 0.081309 8 -1.410199 -0.813532 0.093991	**Frequencies (cm^{-1}):** -156.0534, 207.4398, 217.9388, 304.7319, 474.3486, 588.3768, 687.9952, 796.7495, 854.3928, 882.1112, 929.957, 973.3332, 1026.6192, 1098.1578, 1154.8162, 1172.7298, 1231.7007, 1320.6615, 1350.6856, 1399.1551, 1415.5187, 1485.3536, 1489.7797, 1502.139, 3004.8346, 3019.348, 3042.6493, 3106.7355, 3109.9472, 3117.9724
IRC To low a barrier for IRC to be done	

Compound: MeCHCH$_2$ + O$_3$ TS$_{EPOX}$ 1.1	**Energy (Hartree)** -342.948262646173
Reaction Coordinates: 6 -2.740752 0.144761 0.021832 6 -1.391132 -0.185457 -0.483571 6 -0.353293 -0.702617 0.286337 1 0.429019 -1.316895 -0.170983 1 -0.570496 -0.983558 1.309457 1 -1.167316 0.073903 -1.512007 1 -2.889008 -0.180268 1.050220 1 -2.919873 1.225437 -0.031890 1 -3.512534 -0.310908 -0.607440 8 0.604187 0.688710 0.497098 8 1.729170 0.590012 -0.273224 8 2.359302 -0.534701 -0.096993	**Frequencies (cm^{-1}):** -382.1614, 101.4164, 108.0224, 135.5877, 254.3742, 279.205, 398.7884, 482.7397, 690.1105, 757.4164, 829.2432, 914.079, 939.2783, 1025.804, 1082.0467, 1101.5531, 1173.6473, 1211.9429, 1282.641, 1395.4896, 1428.4528, 1461.2645, 1489.0598, 1554.2961, 2989.9711, 2995.3128, 3023.6044, 3105.4394, 3155.2867, 3173.0738
IRC  	

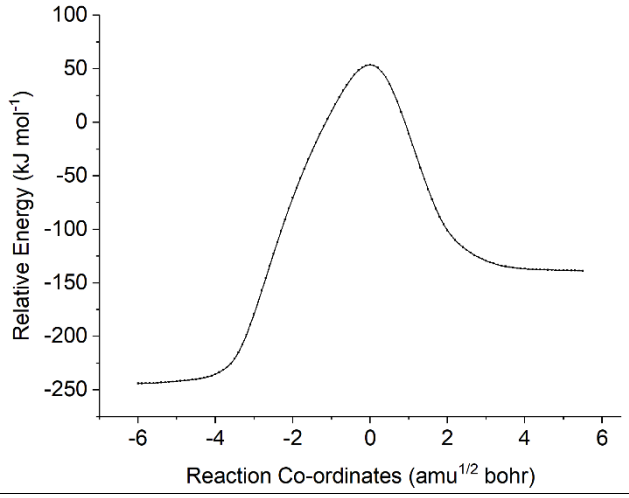
Compound: MeCHCH$_2$ + O$_3$ C$_{EPOX}$ 1.1	**Energy (Hartree)** -343.028197768054
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.468762 -0.455772 -0.212769 6 1.008149 -0.149538 -0.361990 6 0.417189 1.137867 0.005508 1 -0.495557 1.467169 -0.488777 1 1.034580 1.929810 0.415405 1 0.472611 -0.732859 -1.105092 1 2.923340 0.172896 0.552033 1 2.615225 -1.500105 0.065859 1 2.985959 -0.284690 -1.158719 8 0.255585 0.005407 0.860174 8 -1.992246 -0.669045 0.307241 8 -2.375935 0.132694 -0.525565	44.7431, 88.8489, 110.1613, 139.1573, 204.1164, 226.2105, 388.693, 414.3471, 765.5782, 835.097, 898.2627, 975.6358, 1045.4723, 1127.4202, 1159.6756, 1167.79, 1189.7997, 1292.8954, 1408.9358, 1440.3971, 1482.727, 1496.9486, 1509.1175, 1532.2595, 3031.7441, 3055.2511, 3090.019, 3101.4133, 3121.2395, 3154.7858

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 1.2	**Energy (Hartree)** -342.951372446173
Reaction Coordinates: 6 -1.579663 -1.108916 -0.032929 6 -1.594030 0.357591 0.017869 6 -0.518118 1.052013 0.571927 1 0.050748 0.587741 1.375602 1 -0.545260 2.132299 0.592692 1 -2.357344 0.903858 -0.521367 1 -0.736611 -1.423102 -0.679896 1 -1.339462 -1.547748 0.940208 1 -2.497742 -1.537360 -0.426263 8 0.642833 0.816537 -0.688149 8 1.256242 -0.388099 -0.532121 8 1.797992 -0.543415 0.642497	**Frequencies (cm^{-1}):** -372.8165, 91.0412, 209.2279, 218.0342, 269.3696, 312.015, 417.7306, 459.9832, 661.5842, 734.0844, 823.6845, 937.4342, 976.3175, 1012.6483, 1070.9918, 1088.3252, 1155.4584, 1189.5664, 1274.4453, 1380.0642, 1435.6745, 1444.0909, 1482.1532, 1541.6648, 2879.1075, 3025.6445, 3074.3884, 3125.3923, 3171.6796, 3206.1311
IRC  	

Compound: $MeCHCH_2 + O_3$ C_{EPOX} 1.2	**Energy (Hartree)** -343.029307044133
Reaction Coordinates: 6 1.376762 1.351779 0.177650 6 1.500104 -0.120290 -0.087224 6 0.669838 -1.120100 0.588975 1 -0.080770 -0.784239 1.302479 1 1.023592 -2.134735 0.734062	**Frequencies (cm^{-1}):** 50.9066, 85.4481, 94.5183, 136.9927, 190.4257, 221.3491, 375.9241, 415.1245, 762.5352, 826.4749, 911.1214, 974.7285, 1045.134, 1127.4185, 1154.2868, 1172.3421, 1191.6762, 1293.661,

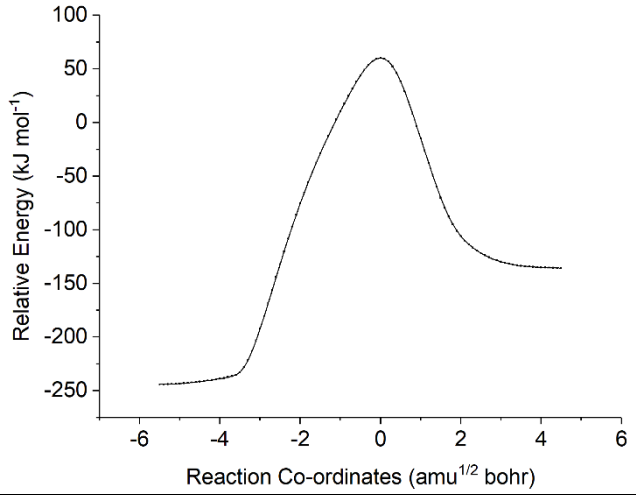
1 2.464399 -0.448757 -0.464688 1 2.123888 1.660795 0.911168 1 1.549837 1.919557 -0.737509 1 0.388328 1.603503 0.557108 8 0.401585 -0.764709 -0.767803 8 -1.828064 0.313752 -0.591601 8 -2.167209 0.140399 0.562027	1410.1606, 1438.9188, 1484.0048, 1497.8489, 1520.1165, 1541.095, 3033.594, 3058.9607, 3088.6311, 3100.8575, 3124.0406, 3156.8632

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.1	**Energy (Hartree)** -342.928960564643
Reaction Coordinates: 6 2.307968 -0.223449 0.009537 6 0.849810 0.012745 0.359857 6 0.242926 1.285914 -0.020434 1 0.445718 1.664840 -1.011123 1 -0.455477 1.823400 0.599345 1 0.629809 -0.280291 1.386818 1 2.507648 0.054573 -1.024486 1 2.957659 0.359086 0.664014 1 2.536428 -1.280825 0.137433 8 -0.010822 -0.690193 -0.550564 8 -1.505744 -0.721235 0.291598 8 -2.111686 0.312422 -0.096755	**Frequencies (cm^{-1}):** -570.1874, 128.0702, 137.9225, 225.4772, 319.844, 334.1269, 368.2555, 458.78, 526.1414, 621.5262, 822.399, 861.2638, 916.7975, 948.0967, 1066.1151, 1163.5387, 1214.8922, 1229.5672, 1291.2611, 1367.1173, 1403.3944, 1481.5273, 1488.0138, 1501.7066, 3036.926, 3061.6297, 3105.6648, 3117.5296, 3173.9609, 3290.3376
IRC  	

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.2	**Energy (Hartree)** -342.925694536270
Reaction Coordinates: 6 1.682531 -0.794664 -0.476267 6 1.059805 0.340558 0.303264 6 0.304998 1.364428 -0.406042 1 -0.117171 1.199946 -1.385016 1 0.072890 2.288173 0.100559 1 1.764245 0.755207 1.028041 1 0.986512 -1.208694 -1.200915 1 2.563276 -0.425932 -1.004781 1 1.995727 -1.586447 0.203116 8 -0.127945 0.014087 1.084656	**Frequencies (cm^{-1}):** -598.1671, 102.2364, 146.5392, 213.2375, 280.9727, 319.1854, 392.2809, 484.7764, 541.5084, 590.46, 770.9612, 868.9008, 926.4686, 933.3537, 1072.1183, 1183.7133, 1194.7462, 1208.365, 1254.3455, 1384.9941, 1415.4801, 1481.0829, 1495.1666, 1507.3114, 3034.5635, 3042.9244, 3104.0708, 3136.5178, 3174.9153, 3286.5389

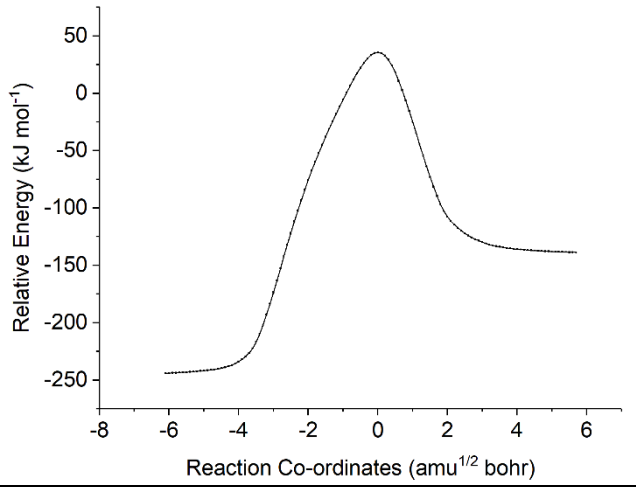
8 -1.150903 -0.845288 0.076444 8 -1.914837 0.020678 -0.444441	

IRC



Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.3	**Energy (Hartree)** -342.931620239017
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.947490 -0.728760 -0.290679 6 0.931486 -0.131639 0.584130 6 0.418762 1.227928 0.388197 1 1.172716 1.960499 0.085628 1 -0.183677 1.622359 1.205815 1 0.502315 -0.755781 1.354848 1 2.263195 -0.061581 -1.088696 1 2.815531 -0.997095 0.326883 1 1.585413 -1.666660 -0.718523 8 -0.369994 0.854890 -0.735818 8 -1.727811 0.035347 0.006916 8 -1.394935 -1.178601 0.071921	-543.7565, 115.8676, 145.0436, 170.7617, 255.7417, 306.5185, 372.0354, 402.9876, 493.3588, 776.0273, 869.0121, 930.3549, 941.6226, 1011.6996, 1133.6489, 1190.1843, 1224.7159, 1241.3858, 1309.7704, 1382.3611, 1413.7772, 1449.889, 1479.3643, 1502.6432, 2985.7553, 3014.4114, 3051.191, 3084.796, 3128.7091, 3209.2065

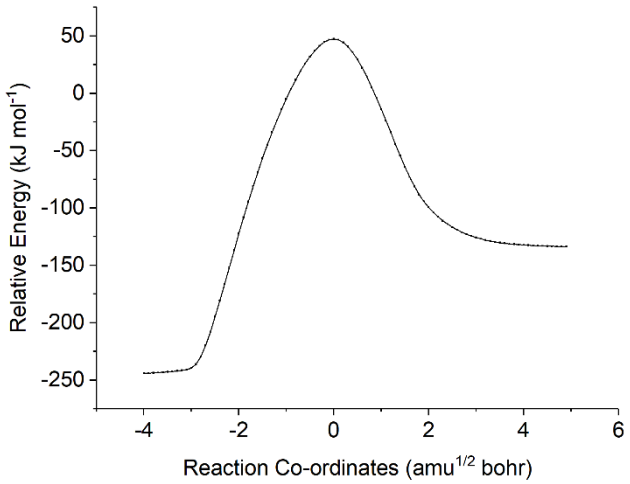
IRC



Compound: MeCHCH$_2$ + O$_3$ C$_{EPOX}$ 2.3	**Energy (Hartree)** -343.028240894697
Reaction Coordinates: 6 -2.203837 -0.830412 0.110700 6 -0.870121 -0.241187 -0.247402 6 -0.662937 1.176457 -0.546883 1 -1.495972 1.868095 -0.489852 1 0.159729 1.474456 -1.186470 1 -0.155688 -0.936753 -0.690347 1 -2.863513 -0.072392 0.531355 1 -2.676804 -1.253652 -0.777018 1 -2.083937 -1.630028 0.842587 8 -0.265318 0.622207 0.720320 8 2.081622 0.103362 0.447648 8 2.125890 -0.735429 -0.434062	**Frequencies (cm^{-1}):** 49.8264, 85.1125, 94.1088, 145.019, 202.2485, 233.9425, 372.4427, 416.6181, 769.7162, 841.9186, 901.5127, 967.7652, 1046.2344, 1129.1427, 1156.9692, 1169.5062, 1192.3677, 1295.4624, 1408.8841, 1438.239, 1483.4503, 1496.6679, 1515.101, 1531.9835, 3032.8811, 3048.3083, 3092.9898, 3094.901, 3110.0811, 3183.2719

Compound: MeCHCH$_2$ + O$_3$ TS$_{EPOX}$ 2.4	**Energy (Hartree)** -342.928697425059
Reaction Coordinates: 6 -1.666830 -0.989808 0.197115 6 -1.098744 0.196731 -0.450311 6 -0.485261 1.314852 0.272052 1 -0.483094 1.193098 1.359517 1 -0.907821 2.295956 0.023029 1 -1.136147 0.298970 -1.526126 1 -1.137526 -1.237058 1.116400 1 -2.692684 -0.710039 0.499230 1 -1.727998 -1.856055 -0.454462 8 0.790343 1.169754 -0.297898 8 1.449696 -0.320871 0.486130 8 1.208745 -1.238324 -0.329571	**Frequencies (cm^{-1}):** -443.6144, 65.4392, 137.6475, 218.3967, 247.7296, 351.5253, 382.7625, 407.8247, 475.0785, 699.9707, 881.1373, 927.2014, 958.212, 1032.4886, 1122.6276, 1184.4346, 1238.1183, 1280.1881, 1297.0164, 1369.8806, 1418.1876, 1440.5792, 1458.7186, 1483.9871, 2917.021, 2979.2809, 3032.3658, 3075.2598, 3144.9878, 3202.5677

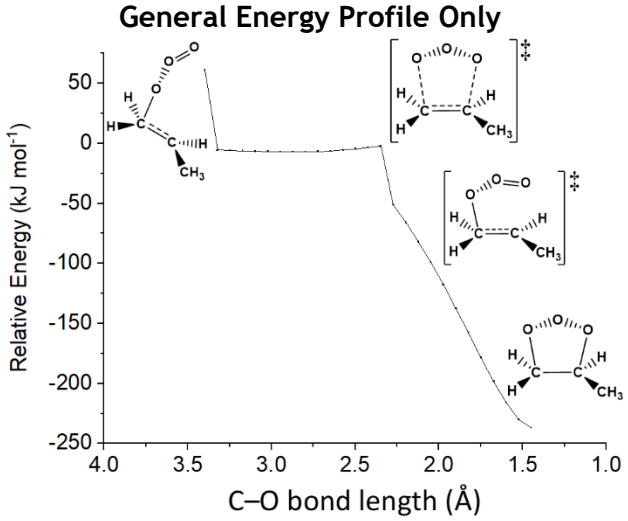
IRC



Compound: MeCHCH$_2$ + O$_3$ C$_{EPOX}$ 2.4	**Energy (Hartree)** -343.029307044133
Reaction Coordinates: 6 1.433661 1.420098 0.157776 6 1.575944 0.003105 -0.316831	**Frequencies (cm^{-1}):** 17.8645, 47.078, 59.583, 85.3431, 148.5701, 207.7645, 368.7, 411.5208,

6 1.165124 -1.148303 0.489058 1 0.721361 -0.981024 1.464760 1 1.644825 -2.111088 0.351837 1 2.352034 -0.166597 -1.058609 1 0.630995 1.505919 0.888676 1 2.365153 1.759272 0.615041 1 1.208914 2.083680 -0.678487 8 0.363265 -0.711534 -0.616745 8 -1.866126 0.021292 0.488935 8 -2.743595 0.222797 -0.317594	763.5696, 836.1884, 908.1741, 971.1267, 1043.617, 1127.3473, 1156.0878, 1168.4814, 1191.6137, 1292.7872, 1407.3048, 1437.8474, 1482.9579, 1498.0797, 1526.5915, 1576.3728, 3030.8861, 3086.7625, 3087.1007, 3094.0738, 3116.7155, 3171.8456

Compound: $MeCHCH_2 + O_3$ DeMore Potential Energy Profile	**Energy (Hartree):** -342.948262646173



Compound: $MeCHCH_2 + O_3$ ONB-FO Peroxide 1	**Energy (Hartree):** -343.484193141
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.272126 0.103385 0.041429 6 -0.801456 -0.021298 0.395647 6 0.143048 0.989285 -0.194926 1 0.583852 1.754296 0.435642 1 -0.123550 1.351130 -1.184855 1 -0.680586 -0.070549 1.484057 1 -2.706443 0.987324 0.513103 1 -2.405091 0.170662 -1.038323 1 -2.813498 -0.770329 0.402688 8 -0.191959 -1.138666 -0.231869 8 1.258843 -0.043907 -0.472310 8 2.149181 -0.048773 0.446028	80.5836, 222.7457, 235.6853, 322.2538, 423.0561, 469.4196, 542.105, 608.9869, 740.4712, 870.1395, 920.8792, 939.3966, 1071.2455, 1118.7094, 1148.9278, 1186.7389, 1214.8742, 1310.1261, 1337.3771, 1402.5353, 1407.8932, 1474.9867, 1484.5924, 1497.7261, 2987.9746, 3028.9085, 3090.5242, 3094.2853, 3110.0487, 3174.0136

Compound: $MeCHCH_2 + O_3$ ONB-FO Peroxide 2	**Energy (Hartree):** -343.487149953

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.230125 0.143640 0.367330 6 0.940214 -0.028777 -0.418443 6 -0.167345 0.957387 -0.122563 1 -0.372388 1.804083 -0.774406 1 -0.244257 1.212215 0.929767 8 -1.259318 -0.073053 -0.365743 8 -2.223506 -0.008518 0.464589 1 1.157917 -0.063203 -1.493896 8 0.204902 -1.159812 -0.010567 1 2.751428 1.050071 0.053098 1 2.023752 0.198946 1.435731 1 2.888954 -0.704551 0.185528	100.0591, 203.1911, 245.0323, 350.8402, 449.8442, 487.8751, 504.9341, 574.9146, 782.1075, 889.188, 906.6207, 945.8169, 1087.8725, 1122.0522, 1138.3857, 1192.8166, 1237.5262, 1315.5609, 1337.5866, 1400.4855, 1403.5146, 1481.0941, 1487.7448, 1499.6147, 2969.1949, 3030.9021, 3081.0559, 3097.2239, 3113.574, 3163.7853

Compound: MeCHCH$_2$ + O$_3$ ONB-syn Peroxide 1	**Energy (Hartree):** -343.486142163
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.845629 -0.386311 -0.103463 6 0.469359 -0.552448 0.443581 6 -0.631533 -1.182025 -0.358818 1 -0.861538 -2.213538 -0.069463 1 -0.426996 -1.150250 -1.435535 8 -1.656351 -0.298536 0.027054 1 0.427466 -0.808074 1.498791 8 -0.333671 0.861171 0.490263 8 0.011989 1.687041 -0.409939 1 2.262391 -1.383084 -0.269447 1 1.821466 0.137849 -1.056686 1 2.500749 0.144405 0.585512	111.5593, 153.1257, 274.1986, 285.9033, 363.2266, 475.3843, 541.3792, 565.6826, 662.8582, 908.379, 942.9607, 999.1782, 1029.9506, 1127.6079, 1158.1658, 1169.4811, 1217.2385, 1293.2675, 1323.622, 1390.2367, 1423.4972, 1472.2741, 1496.3418, 1510.8412, 2981.6085, 3018.5759, 3035.3879, 3096.8591, 3115.6971, 3134.524

Compound: MeCHCH$_2$ + O$_3$ ONB-anti Peroxide 1	**Energy (Hartree):** -343.490023154
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.941309 -0.266641 -0.131932 6 -0.589171 0.130192 0.377354 6 0.053943 1.459130 0.047312 1 -0.033001 2.197915 0.850597 1 -0.335743 1.891483 -0.882993 8 1.362831 0.976172 -0.078066 1 -0.398835 -0.163523 1.405496 8 0.519542 -0.636524 -0.402115 8 0.931039 -1.688814 0.181559 1 -2.698820 0.302572 0.411502 1 -2.047208 -0.046761 -1.193514 1 -2.134464 -1.324441 0.041490	123.17, 185.9303, 242.7556, 304.1067, 366.5118, 498.2052, 541.4021, 578.8512, 709.3819, 884.4297, 951.9928, 1009.4578, 1042.4612, 1150.4249, 1155.5849, 1209.0507, 1237.3383, 1281.3085, 1326.4396, 1391.3792, 1413.2324, 1481.6456, 1494.789, 1513.4168, 2973.9092, 3021.791, 3036.1841, 3095.5976, 3113.997, 3131.0685

Compound: MeCHCH$_2$ + O$_3$ **TS$_{ONB-FO}$ 1**	**Energy (Hartree)** -343.028828640250

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.836062 -0.653290 -0.491019 6 0.991365 0.257836 0.446741 6 -0.310749 -0.448929 0.854963 1 -0.226416 -1.506097 1.115032 1 -0.883089 0.115193 1.584714 8 -1.067349 -0.392056 -0.401600 8 -2.244445 0.074888 -0.278585 8 0.592432 1.387904 -0.163235 1 1.642940 0.471596 1.316352 1 1.266054 -0.912924 -1.380984 1 2.128610 -1.560616 0.039973 1 2.726735 -0.106742 -0.791838	-631.9261, 63.6094, 187.5917, 245.6075, 320.3171, 428.3492, 498.8722, 634.9112, 713.5036, 810.3263, 896.9373, 933.0906, 1014.7758, 1077.856, 1103.3776, 1176.7174, 1233.5094, 1268.6714, 1290.5878, 1339.8197, 1381.4014, 1460.8918, 1471.4111, 1497.731, 2856.7224, 3033.2576, 3043.4068, 3112.799, 3133.7409, 3149.5452

Compound: $MeCHCH_2 + O_3$ $TS_{ONB\text{-}FO}$ **2**	**Energy (Hartree)** -343.472849788
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.297080 -0.353429 0.161578 6 0.905310 0.093489 -0.296014 6 -0.268610 -0.824878 0.107910 1 -0.280442 -1.809835 -0.359637 1 -0.424067 -0.865781 1.182916 8 -1.382439 -0.071000 -0.458035 8 -2.379056 0.064742 0.322852 8 0.546209 1.315990 0.124744 1 0.898831 0.064118 -1.408224 1 2.556880 -1.329740 -0.250733 1 2.333879 -0.402687 1.250068 1 3.034525 0.374977 -0.171718	-631.7117, 57.6964, 178.6302, 202.2871, 329.4188, 449.8084, 491.7163, 522.7637, 691.822, 847.2595, 915.1299, 928.7476, 1057.7195, 1084.0355, 1127.5552, 1180.923, 1234.0681, 1245.9581, 1277.6069, 1322.4269, 1391.0264, 1461.5473, 1476.5502, 1491.5158, 2795.601, 3030.5572, 3053.4778, 3098.6155, 3114.6912, 3142.5354

Compound: $MeCHCH_2 + O_3$ $TS_{ONB\text{-}ANTI}$	**Energy (Hartree)** -343.476275701
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.595226 -1.003440 -0.148809 6 -0.363214 -0.433209 0.502384 6 -0.267462 1.083393 0.608364 1 -0.982367 1.636090 1.240683 1 0.730975 1.250680 1.092911 8 -0.264064 1.494679 -0.672773 8 1.895066 -0.510308 0.113972 8 0.787318 -0.526156 -0.513200 1 -0.012220 -0.999957 1.361532 1 -1.874911 -0.411658 -1.016865 1 -2.411269 -0.982017 0.575394 1 -1.441359 -2.039318 -0.449279	-429.1565, 172.5596, 196.7804, 264.7994, 310.8541, 398.1918, 524.5804, 608.9871, 727.8918, 843.1469, 866.865, 994.5698, 1052.1192, 1078.6788, 1132.5854, 1207.5335, 1233.8279, 1283.7425, 1319.5505, 1365.5829, 1400.9976, 1417.0333, 1480.1083, 1500.7955, 2694.5164, 2929.7592, 3042.0388, 3101.0357, 3101.8741, 3137.209

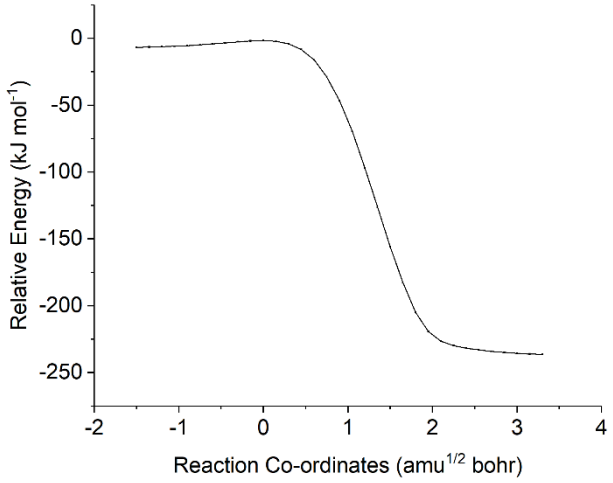
Compound: $MeCHCH_2 + O_3$ $TS_{ONB\text{-}SYN}$	**Energy (Hartree)** -343.475746656
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.678203 0.881525 -0.047781 6 -0.288687 0.560083 0.423280 6 0.917733 0.762015 -0.479685 1 0.626907 0.214961 -1.419294 1 1.188318 1.775253 -0.821622 8 1.914442 0.134413 0.166098 8 -0.533094 -1.555473 -0.471390 8 -0.052196 -0.961119 0.544831 1 -0.074209 0.892011 1.435818 1 -1.867917 0.486020 -1.042372 1 -1.777339 1.967942 -0.081837 1 -2.434035 0.499496 0.638112	-446.364, 154.2305, 180.1837, 289.4486, 296.6983, 416.3057, 514.4708, 606.4215, 638.0309, 854.6356, 882.3178, 1004.0609, 1061.347, 1118.0441, 1144.3939, 1173.0339, 1215.3353, 1273.0876, 1311.7197, 1367.226, 1397.9574, 1413.5593, 1480.2705, 1498.155, 2668.7287, 2928.3512, 3042.6308, 3099.253, 3114.0453, 3135.229

S10.4 Ozonolysis of 1-butene (Alkene 2)

Compound: $EtCHCH_2 + O_3$ PRC1.1	**Energy (Hartree)** -382.230525502064
Reaction Coordinates: 6 -1.630533 -0.283798 -0.487614 6 -0.817910 0.450015 0.531206 6 -0.158363 1.591715 0.313309 1 0.397505 2.085402 1.098787 1 -0.177762 2.080236 -0.652450 1 -0.802016 0.018866 1.528307 1 -1.573144 0.236659 -1.445564 1 -1.186508 -1.271775 -0.640964 6 -3.095701 -0.455801 -0.065475 1 -3.587170 0.510387 0.054068 1 -3.172059 -0.988424 0.884063 1 -3.648243 -1.026577 -0.812353 8 2.158409 0.444344 -0.765220 8 2.348457 -0.356707 0.191122 8 1.488688 -1.269832 0.353793	**Frequencies (cm^{-1}):** 34.8339, 52.3655, 65.9584, 83.5563, 92.9886, 161.968, 227.1799, 266.4111, 335.1609, 436.6102, 656.9583, 741.9062, 795.9895, 859.8372, 957.6317, 991.829, 1012.5774, 1024.1559, 1093.5321, 1164.0568, 1193.1405, 1203.3832, 1288.523, 1321.5176, 1343.3053, 1410.0117, 1459.5007, 1484.6247, 1498.7092, 1507.23, 1663.4004, 3016.5505, 3026.5198, 3053.5385, 3088.1504, 3093.1286, 3123.3646, 3135.6188, 3218.3977

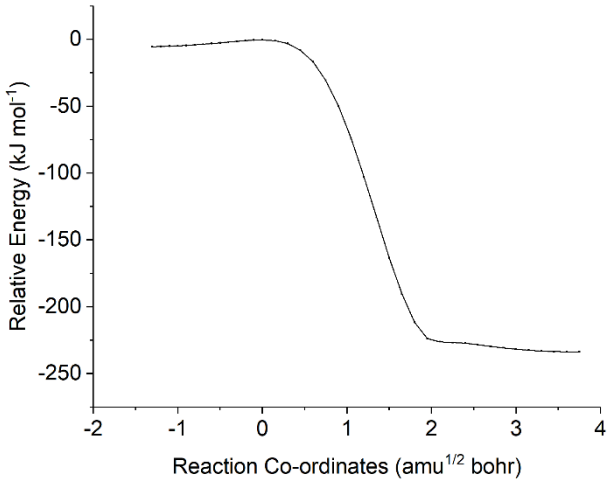
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.1	**Energy (Hartree)** -382.221047574187
Reaction Coordinates: 6 -1.538579 -0.373826 -0.433901 6 -0.569324 0.255682 0.514995 6 0.122688 1.400418 0.244280 1 0.674544 1.920171 1.012754 1 -0.011181 1.918302 -0.694751 1 -0.566953 -0.124072 1.529990 1 -1.361180 0.007638 -1.440851 1 -1.357647 -1.449767 -0.466709 6 -2.997624 -0.121693 -0.023701 1 -3.232361 0.943128 -0.027567	**Frequencies (cm^{-1}):** -186.9921, 54.9005, 76.5792, 142.2443, 210.6562, 232.5778, 262.8272, 411.6885, 432.19, 478.1984, 714.0718, 747.067, 794.6543, 861.8132, 955.4058, 987.4069, 1002.5004, 1015.5685, 1082.7432, 1087.4429, 1114.8814, 1203.9886, 1284.0831, 1304.8381, 1339.2164, 1409.0095, 1455.9482, 1489.2505, 1498.4093, 1509.5707, 1586.0963,

1 -3.197435 -0.504462 0.978389 1 -3.678318 -0.621194 -0.713484 8 2.033050 0.557152 -0.602040 8 2.143735 -0.434807 0.211468 8 1.151660 -1.253999 0.142095	3027.8581, 3034.8293, 3065.9934, 3092.126, 3096.2226, 3151.4553, 3155.197, 3243.0157
IRC:  	

Compound: $EtCHCH_2 + O_3$ POZ1.1	**Energy (Hartree)** -382.319943476474
Reaction Coordinates: 6 -1.504470 -0.525361 -0.399433 6 -0.230572 -0.245440 0.381137 6 0.440859 1.133954 0.123839 1 0.533128 1.709240 1.046655 1 -0.069143 1.719758 -0.639727 8 1.723752 0.812806 -0.405419 8 1.992878 -0.467463 0.207223 8 0.771985 -1.172593 -0.052943 1 -0.396593 -0.373982 1.454649 1 -1.316340 -0.328687 -1.456880 1 -1.731671 -1.589510 -0.311050 6 -2.692381 0.297014 0.100263 1 -2.514752 1.369409 0.001653 1 -3.589153 0.060618 -0.471490 1 -2.905019 0.090152 1.150457	**Frequencies (cm^{-1}):** 68.6128, 108.3092, 198.6264, 238.6002, 373.725, 400.4181, 438.3137, 687.4325, 714.0783, 740.3368, 798.552, 849.5255, 926.8129, 963.3562, 980.875, 991.108, 1015.8819, 1066.249, 1146.141, 1176.6836, 1234.4693, 1289.8072, 1317.1576, 1350.708, 1365.2287, 1402.6174, 1420.9226, 1492.1014, 1503.5637, 1507.7334, 1512.2073, 3012.9544, 3027.309, 3034.9297, 3039.3954, 3064.1211, 3088.5102, 3098.2701, 3101.9917

Compound: $EtCHCH_2 + O_3$ PRC1.2	**Energy (Hartree)** -382.230906391601
Reaction Coordinates: 6 1.767471 -0.594112 -0.456608 6 0.846397 0.471600 -0.967277 6 0.427271 1.550464 -0.297606 1 -0.227650 2.275577 -0.760757 1 0.743788 1.760789 0.714088 1 0.519284 0.344256 -1.994507 1 1.256026 -1.556009 -0.564209 1 2.624080 -0.652528 -1.137801 6 2.256393 -0.430501 0.978654	**Frequencies (cm^{-1}):** 35.6908, 48.5383, 74.4002, 89.8883, 105.4143, 203.3659, 256.2881, 271.5581, 288.8633, 547.3533, 572.4638, 741.9925, 800.6366, 838.3618, 954.8439, 998.1469, 1019.4682, 1033.0241, 1107.0148, 1147.9657, 1163.3939, 1191.5189, 1294.2422, 1329.206, 1382.8584, 1412.5565, 1453.5151, 1469.1815,

1 1.423014 -0.419772 1.681525 1 2.818708 0.495485 1.108062 1 2.912644 -1.256634 1.252351 8 -1.702680 0.339272 1.064797 8 -2.222647 -0.160325 0.028660 8 -1.556559 -1.050931 -0.573674	1500.7741, 1510.7445, 1661.5009, 2998.8943, 3020.446, 3031.8002, 3089.8524, 3096.7225, 3130.3167, 3147.8487, 3227.611

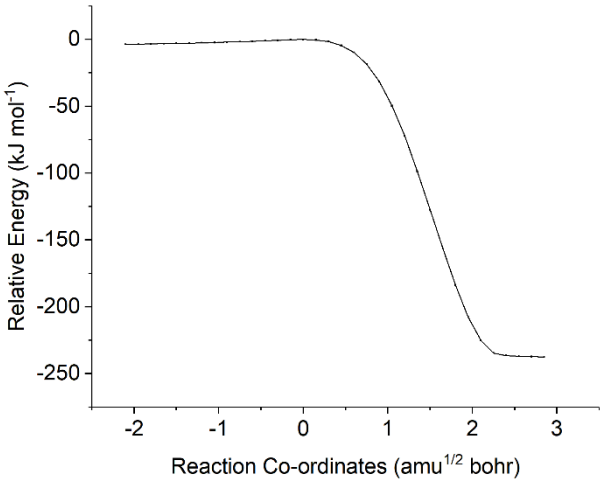
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.2	**Energy (Hartree)** -382.221276651576
Reaction Coordinates: 6 -1.712962 -0.533934 0.383261 6 -0.536592 0.149186 1.011613 6 -0.001738 1.339207 0.605554 1 0.732251 1.849827 1.209861 1 -0.423885 1.896673 -0.216067 1 -0.208465 -0.259898 1.959088 1 -1.473913 -1.596028 0.288575 1 -2.539491 -0.490237 1.102413 6 -2.167224 0.015088 -0.965669 1 -1.357160 -0.014443 -1.694061 1 -2.517082 1.045457 -0.887553 1 -2.992067 -0.580889 -1.355624 8 1.600670 0.643595 -0.803980 8 1.996373 -0.365597 -0.106980 8 1.064320 -1.236466 0.084062	**Frequencies (cm^{-1}):** -201.5674, 68.1783, 75.7968, 171.7182, 217.2814, 264.1829, 282.1966, 360.9185, 454.9815, 549.9239, 662.3059, 741.6828, 799.7036, 836.2231, 956.5864, 991.1374, 1005.9099, 1030.4454, 1080.9974, 1097.9025, 1117.3764, 1149.1535, 1290.9145, 1306.2081, 1384.2254, 1412.8333, 1449.7188, 1467.687, 1502.4339, 1511.2094, 1584.0667, 2996.9013, 3033.3241, 3039.7643, 3091.504, 3103.3231, 3159.5234, 3166.6355, 3252.5972
IRC:  	

Compound: $EtCHCH_2 + O_3$ POZ1.2	**Energy (Hartree)** -382.319409856411
Reaction Coordinates: 6 -1.671383 -0.182012 0.556324 6 -0.164756 -0.219936 0.788165 6 0.628399 1.087394 0.502234 1 1.180480 1.407435 1.387717 1 0.007863 1.899676 0.129414 8 1.518475 0.741033 -0.552767 8 1.755705 -0.659398 -0.293450 8 0.418696 -1.154957 -0.128843	**Frequencies (cm^{-1}):** 65.1323, 98.7274, 200.7239, 263.5289, 320.1656, 390.3531, 544.6024, 677.8918, 725.6788, 741.3978, 780.5397, 818.4099, 925.8984, 942.846, 962.1285, 996.4387, 1010.3064, 1096.9266, 1126.9136, 1156.0492, 1228.1477, 1298.0739, 1338.4963, 1354.7237, 1366.2583,

1 0.045874 -0.545944 1.809935 1 -2.067838 -1.172352 0.790852 1 -2.094352 0.494503 1.304166 6 -2.112007 0.230650 -0.847219 1 -1.715061 -0.448552 -1.599170 1 -3.199695 0.217004 -0.917000 1 -1.781807 1.238230 -1.102464	1400.8007, 1425.8291, 1484.1072, 1495.1786, 1507.9826, 1514.3224, 3015.519, 3028.5272, 3038.9265, 3043.2625, 3054.2167, 3092.8109, 3111.6942, 3115.7622

Compound: $EtCHCH_2 + O_3$ PRC1.3	**Energy (Hartree)** -382.228599800530
Reaction Coordinates: 6 -2.130347 0.202561 -0.259217 6 -1.068762 0.848588 0.576226 6 -0.227477 1.795396 0.158017 1 0.493447 2.249035 0.824237 1 -0.253661 2.168164 -0.858187 1 -1.016379 0.523041 1.611897 1 -3.106984 0.538012 0.108359 1 -2.049004 0.554764 -1.289562 6 -2.094436 -1.329642 -0.217914 1 -2.196083 -1.696756 0.804883 1 -1.153952 -1.708552 -0.615361 1 -2.911121 -1.750322 -0.805266 8 2.052280 0.360976 -0.814691 8 2.222685 -0.342675 0.215684 8 1.390019 -1.265652 0.433548	**Frequencies (cm^{-1}):** 23.0789, 43.8839, 49.2668, 59.765, 84.0331, 149.3418, 213.395, 231.6386, 318.2882, 439.6973, 649.9411, 742.7602, 797.2015, 857.7105, 956.8765, 994.2985, 1016.1967, 1029.7659, 1095.4383, 1172.6715, 1202.4061, 1204.4995, 1291.3919, 1323.8675, 1344.3324, 1411.4945, 1459.5393, 1479.6798, 1498.2473, 1508.1073, 1672.1468, 2993.2549, 3030.2285, 3048.7193, 3087.9893, 3107.3691, 3118.4952, 3134.2576, 3216.6013

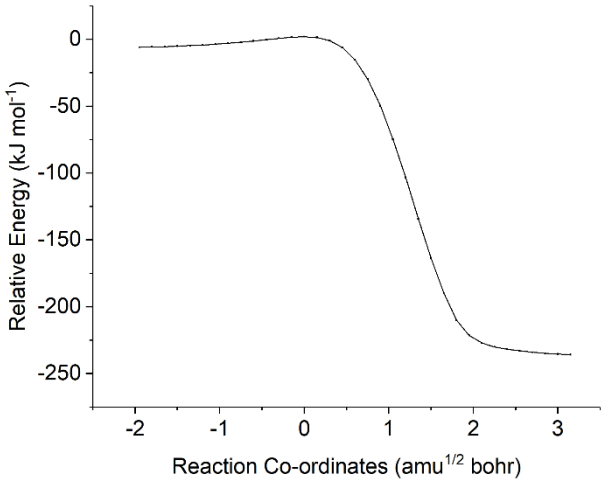
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (Hartree)** -382.220877506051
Reaction Coordinates: 6 -1.649715 0.465644 -0.434184 6 -0.537339 0.773639 0.522467 6 0.496938 1.610163 0.236390 1 1.190992 1.926638 1.000131 1 0.557914 2.116167 -0.716831 1 -0.651302 0.421193 1.541098 1 -2.281738 1.357365 -0.517668 1 -1.224181 0.305159 -1.427546 6 -2.513638 -0.724773 -0.023055 1 -2.968880 -0.559415 0.955277 1 -1.922368 -1.637756 0.031829 1 -3.318922 -0.884845 -0.739860 8 2.037598 0.144752 -0.598616 8 1.819320 -0.825642 0.213165 8 0.623207 -1.293178 0.143433	**Frequencies (cm^{-1}):** -151.4348, 66.5451, 72.7259, 135.018, 184.6745, 231.8333, 299.451, 336.152, 443.7817, 466.5845, 641.355, 740.5878, 794.0563, 854.1417, 959.481, 986.8413, 1001.663, 1048.5826, 1093.4344, 1095.0729, 1120.7129, 1189.02, 1289.7741, 1307.1898, 1340.1493, 1417.2828, 1458.2862, 1462.7855, 1500.0279, 1506.4582, 1593.2837, 2995.0998, 3031.3143, 3044.8711, 3089.5667, 3108.3985, 3149.9663, 3153.2702, 3241.6098
IRC:	



Compound: $EtCHCH_2 + O_3$ POZ1.3	**Energy (Hartree)** -382.320341440266
Reaction Coordinates: 6 -1.508790 0.629419 -0.257676 6 -0.221171 0.211465 0.431242 6 1.001698 1.137758 0.183797 1 1.361927 1.572940 1.117838 1 0.798603 1.919519 -0.546997 8 1.986854 0.287469 -0.397164 8 1.624374 -1.010790 0.128621 8 0.214659 -1.039123 -0.117651 1 -0.375765 0.090394 1.507336 1 -1.767424 1.626656 0.108450 1 -1.311502 0.724308 -1.327945 6 -2.671807 -0.330536 -0.011437 1 -2.884976 -0.425536 1.054865 1 -3.577316 0.027236 -0.501398 1 -2.450214 -1.324605 -0.398156	**Frequencies (cm^{-1}):** 65.2954, 115.3709, 199.6292, 237.2257, 358.9284, 388.1195, 460.5116, 671.0041, 727.5271, 748.2662, 780.3189, 850.9964, 928.8021, 952.2661, 985.2885, 999.3279, 1014.839, 1078.7281, 1134.1059, 1173.6122, 1230.9585, 1303.126, 1332.7172, 1338.3592, 1362.5094, 1408.7121, 1419.7459, 1478.2041, 1500.0585, 1507.1522, 1511.7475, 3012.9483, 3022.6369, 3031.6265, 3037.112, 3058.7669, 3091.3823, 3099.8501, 3105.2803

Compound: $EtCHCH_2 + O_3$ PRC 2.1	**Energy (Hartree)** -382.229766660375
Reaction Coordinates: 6 1.685301 -0.305632 -0.496591 6 0.861220 0.432571 0.512355 6 0.184925 1.559275 0.278125 1 0.196250 2.033770 -0.695621 1 -0.384317 2.049707 1.054293 1 0.846041 0.012981 1.513944 6 3.155354 -0.439892 -0.076511 1 3.718331 -1.012405 -0.814241 1 3.624553 0.539327 0.023644 1 3.244660 -0.952350 0.882759 1 1.268379 -1.309131 -0.631056 1 1.617010 0.195583 -1.464413 8 -2.399302 0.574651 -0.482150 8 -2.096428 -0.646445 -0.392639	**Frequencies (cm^{-1}):** 30.6697, 43.3188, 54.7551, 77.1034, 86.5672, 155.6428, 227.1418, 249.883, 333.6375, 435.6802, 659.5907, 742.7863, 797.815, 859.5351, 960.8561, 992.822, 1013.1985, 1024.2658, 1093.0287, 1168.7283, 1198.3471, 1202.9182, 1291.6098, 1321.6709, 1344.4412, 1409.6733, 1459.7266, 1483.9957, 1498.3309, 1506.7607, 1668.6475, 3005.0352, 3027.4241, 3048.3987, 3089.2462, 3094.1611, 3128.4813, 3135.03, 3224.5733

8 -1.685734 -1.057633 0.728093	

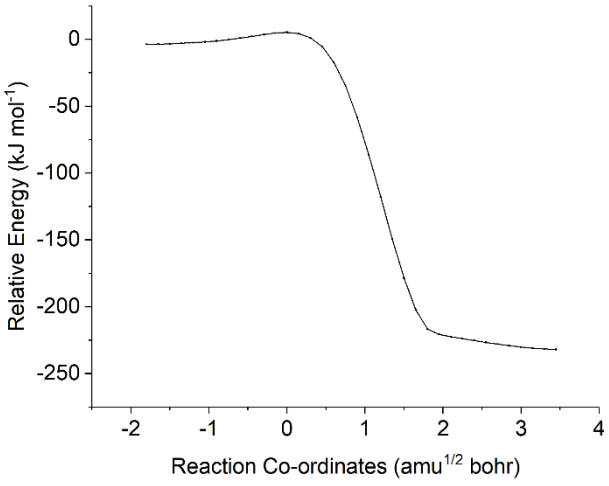
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.1	**Energy (Hartree)** -382.219503800034
Reaction Coordinates: 6 -1.462939 -0.494091 -0.325934 6 -0.566078 0.285518 0.586995 6 0.100146 1.414625 0.201979 1 0.588999 2.047408 0.925351 1 -0.002763 1.804812 -0.801195 1 -0.615149 0.049662 1.642512 1 -1.151867 -0.341502 -1.361697 1 -1.362830 -1.558946 -0.113835 6 -2.937108 -0.086645 -0.166508 1 -3.086262 0.963423 -0.419242 1 -3.277366 -0.235338 0.859314 1 -3.570312 -0.687515 -0.819889 8 2.120045 0.621501 -0.367062 8 1.808891 -0.626026 -0.462951 8 1.280243 -1.090280 0.618698	**Frequencies (cm^{-1}):** -204.3484, 54.9709, 76.6521, 138.6429, 201.8572, 231.9775, 269.5435, 420.3311, 438.2748, 497.5519, 724.8427, 743.4985, 797.3091, 860.6013, 953.6243, 982.6006, 1003.3736, 1012.3355, 1078.8743, 1084.6019, 1109.3998, 1202.4471, 1282.6618, 1303.051, 1341.1662, 1407.4473, 1451.4457, 1491.5665, 1497.3453, 1510.6323, 1581.3824, 3028.0308, 3032.9149, 3069.6986, 3092.601, 3098.1658, 3153.276, 3164.6213, 3249.0501
IRC:  	

Compound: $EtCHCH_2 + O_3$ POZ 2.1	**Energy (Hartree)** -382.320300568466
Reaction Coordinates: 6 -1.434055 -0.592551 -0.314644 6 -0.231647 -0.199059 0.532914 6 0.432006 1.142453 0.112456 1 0.004090 1.510330 -0.822798 1 0.384944 1.911811 0.880344 8 1.805368 0.819846 -0.057236 8 1.721955 -0.527475 -0.551667 8 0.849333 -1.139157 0.421901 1 -0.490778 -0.195338 1.593421 1 -1.704203 -1.618325 -0.058681 1 -1.136431 -0.594912 -1.365442 6 -2.635931 0.327860 -0.097814 1 -2.953581 0.324298 0.946782	**Frequencies (cm^{-1}):** 82.5702, 118.0096, 203.5935, 237.0846, 358.3483, 418.328, 468.0392, 674.8196, 716.5394, 751.948, 795.5835, 847.7329, 918.1178, 950.7069, 979.6512, 990.3533, 1012.1364, 1057.8407, 1125.6752, 1176.028, 1238.8846, 1279.2342, 1312.0312, 1343.0749, 1356.7101, 1393.5814, 1419.1277, 1490.7329, 1503.3503, 1505.3105, 1509.5686, 3024.9742, 3031.4673, 3034.1999,

1 -3.483486 0.003596 -0.700886 1 -2.416036 1.360614 -0.374202	3048.4558, 3066.0854, 3087.8796, 3096.0377, 3114.5574

Compound: $EtCHCH_2 + O_3$ PRC 2.2	**Energy (Hartree)** -382.229362194436
Reaction Coordinates: 6 -1.854147 -0.561921 0.487839 6 -0.896901 0.510766 0.916176 6 -0.446851 1.522350 0.169942 1 0.239654 2.250643 0.575869 1 -0.759969 1.668612 -0.854877 1 -0.561703 0.443682 1.946111 1 -1.373886 -1.532644 0.653537 1 -2.701616 -0.552449 1.182586 6 -2.365624 -0.478324 -0.946845 1 -1.549527 -0.536688 -1.668271 1 -2.902263 0.454360 -1.125737 1 -3.050568 -1.300214 -1.155002 8 2.008382 0.479814 -0.921559 8 1.912518 -0.653404 -0.376326 8 1.834228 -0.682977 0.883274	**Frequencies (cm^{-1}):** 30.9161, 36.703, 68.0854, 73.3323, 92.3649, 195.1418, 241.5331, 265.5029, 279.191, 547.9026, 574.4011, 742.4574, 801.4713, 837.1697, 957.7929, 999.0433, 1022.663, 1032.4371, 1106.6463, 1147.2995, 1169.2825, 1198.5046, 1291.7927, 1330.4384, 1381.0894, 1414.1438, 1455.4124, 1472.9456, 1500.424, 1509.1558, 1668.3891, 2997.8741, 3010.6237, 3031.0017, 3089.0505, 3094.0824, 3135.1185, 3149.6993

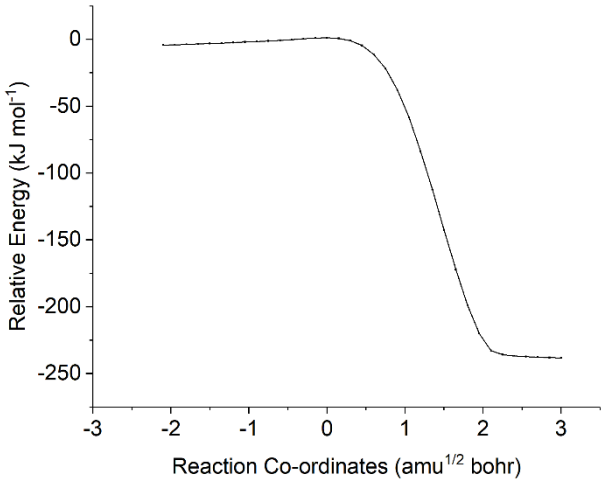
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (Hartree)** -382.218900812696
Reaction Coordinates: 6 -1.700854 -0.267542 0.541592 6 -0.537533 0.628918 0.857918 6 0.052496 1.499472 -0.019713 1 0.744061 2.245718 0.336053 1 -0.301979 1.607511 -1.033395 1 -0.295233 0.728926 1.907732 1 -1.525354 -1.239065 1.007379 1 -2.572874 0.144704 1.063725 6 -2.032566 -0.449937 -0.937745 1 -1.184956 -0.852350 -1.492778 1 -2.326632 0.490000 -1.406418 1 -2.863355 -1.145779 -1.052250 8 1.812373 0.368266 -0.757857 8 1.451309 -0.811979 -0.377848 8 1.190951 -0.861929 0.887911	**Frequencies (cm^{-1}):** -235.593, 55.1677, 79.6926, 172.9339, 203.8574, 257.8951, 284.5879, 383.6153, 471.2708, 557.969, 680.7842, 741.3744, 800.658, 831.2277, 952.4826, 987.3973, 1010.9764, 1029.0652, 1072.7843, 1094.9067, 1113.4809, 1148.7725, 1288.3515, 1301.8287, 1381.368, 1414.1937, 1447.0297, 1471.9504, 1503.1831, 1508.9876, 1576.4679, 2992.2243, 3034.4174, 3050.2089, 3093.6289, 3099.8519, 3167.942, 3170.4636, 3258.7538
IRC:	



Compound: $EtCHCH_2 + O_3$ POZ 2.2	**Energy (Hartree)** -382.319190983776
Reaction Coordinates: 6 1.636123 0.462232 0.356338 6 0.151317 0.554586 0.703371 6 -0.758631 1.089353 -0.434513 1 -0.218881 1.147799 -1.381044 1 -1.211852 2.050003 -0.198233 8 -1.819804 0.147330 -0.513469 8 -1.139392 -1.077104 -0.193864 8 -0.439136 -0.718170 1.019424 1 0.020095 1.150096 1.607856 1 1.973745 1.471127 0.096330 1 2.172025 0.190794 1.268171 6 1.997444 -0.522261 -0.754937 1 1.546792 -0.255221 -1.710826 1 3.078082 -0.544915 -0.896658 1 1.669138 -1.529590 -0.503886	**Frequencies (cm^{-1}):** 84.6723, 107.9295, 209.6912, 261.2108, 320.3458, 403.9985, 555.3593, 665.3836, 714.7415, 749.1073, 789.2843, 816.6065, 915.1655, 941.9277, 958.0387, 1003.6401, 1013.0747, 1090.8281, 1117.156, 1150.3434, 1233.0562, 1280.2428, 1335.004, 1342.314, 1360.5873, 1398.1213, 1424.6931, 1482.7604, 1495.8028, 1506.0249, 1512.4485, 3009.8762, 3038.9152, 3044.8776, 3049.2336, 3059.6143, 3095.1818, 3110.9134, 3114.273

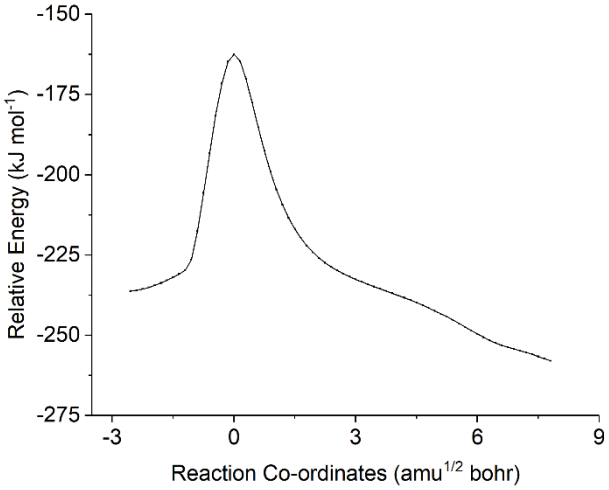
Compound: $EtCHCH_2 + O_3$ PRC 2.3	**Energy (Hartree)** -382.228988543684
Reaction Coordinates: 6 -2.131443 0.231655 -0.280235 6 -1.049453 0.870700 0.534898 6 -0.185370 1.785553 0.092271 1 0.553197 2.228362 0.744144 1 -0.207099 2.135666 -0.932855 1 -0.998164 0.567888 1.576912 1 -3.098605 0.588003 0.092141 1 -2.056910 0.566625 -1.317073 6 -2.123682 -1.300570 -0.214677 1 -2.216344 -1.649370 0.815015 1 -1.197151 -1.708807 -0.618202 1 -2.955083 -1.716447 -0.784484 8 2.354289 0.442990 -0.468242 8 1.899856 -0.726071 -0.343496	**Frequencies (cm^{-1}):** 22.6626, 35.4936, 53.5445, 64.8888, 88.374, 149.874, 218.031, 228.4202, 321.2589, 439.4355, 651.1886, 742.4998, 796.6083, 857.3987, 959.5339, 993.9451, 1016.2569, 1029.1111, 1094.0636, 1173.2198, 1201.7851, 1204.4696, 1290.3604, 1323.7089, 1343.7175, 1412.3911, 1460.481, 1480.1734, 1499.0118, 1504.5769, 1671.9808, 2995.1495, 3030.171, 3045.9941, 3090.4018, 3098.006, 3125.2871, 3133.9174, 3225.082

8 1.385335 -1.033911 0.765595	

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.3	**Energy (Hartree)** -382.220139501245
Reaction Coordinates: 6 -1.534308 0.433568 -0.513878 6 -0.507377 0.858345 0.492953 6 0.577161 1.620722 0.180637 1 1.224681 2.008935 0.950634 1 0.724259 2.000392 -0.821133 1 -0.722783 0.666394 1.536637 1 -2.116223 1.317975 -0.799207 1 -1.024252 0.116216 -1.428897 6 -2.480144 -0.659891 -0.024807 1 -3.018908 -0.340810 0.869317 1 -1.928168 -1.566415 0.221028 1 -3.219255 -0.904402 -0.787543 8 2.149087 0.055625 -0.316026 8 1.378618 -0.970535 -0.410096 8 0.690877 -1.186934 0.657339	**Frequencies (cm^{-1}):** -168.2698, 58.7495, 76.7611, 136.5375, 185.055, 236.4693, 290.742, 358.0783, 461.7294, 477.0377, 647.9795, 739.97, 794.9847, 854.4728, 955.3336, 984.3293, 1001.6007, 1049.8064, 1086.0975, 1093.3256, 1113.4519, 1189.4787, 1285.358, 1299.7608, 1338.7952, 1416.4246, 1455.5804, 1465.169, 1498.3143, 1508.3509, 1589.0042, 2991.8327, 3020.5171, 3031.9198, 3089.5066, 3106.1029, 3152.9313, 3162.6447, 3248.0556
IRC:  	

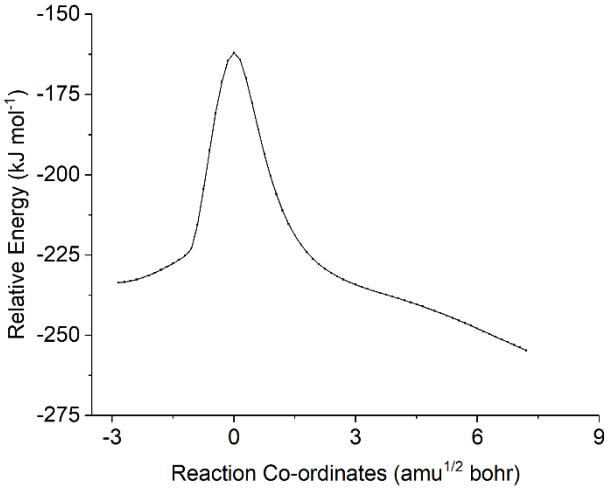
Compound: $EtCHCH_2 + O_3$ POZ 2.3	**Energy (Hartree)** -382.320843504655
Reaction Coordinates: 6 1.408035 0.534175 -0.433196 6 0.217196 0.312940 0.488041 6 -1.039479 1.131011 0.081841 1 -0.873489 1.648517 -0.865698 1 -1.363769 1.833508 0.847062 8 -2.071410 0.161535 -0.045729 8 -1.333186 -0.987149 -0.501395 8 -0.262413 -1.042222 0.462805 1 0.489293 0.488747 1.530378 1 1.111022 0.256084 -1.447162 1 1.622627 1.607498 -0.453342 6 2.652953 -0.240665 -0.009066 1 2.456984 -1.312432 0.009838	**Frequencies (cm^{-1}):** 77.9942, 120.7532, 201.9758, 243.3015, 357.8386, 389.9929, 493.3642, 683.9226, 709.8102, 736.2562, 798.7846, 845.2126, 917.3025, 951.4054, 969.1676, 1008.2779, 1014.6077, 1067.6618, 1114.4308, 1171.2805, 1238.0894, 1288.0406, 1300.1652, 1342.4949, 1360.94, 1399.2376, 1417.3, 1477.7868, 1499.8086, 1505.8782, 1508.0937, 3011.6614, 3028.7019, 3032.2436, 3044.6618,

1 3.476830 -0.061680 -0.699891 1 2.984349 0.057675 0.987653	3061.7501, 3088.8055, 3102.6517, 3112.0209

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 1	**Energy (Hartree)** -382.288435179066
Reaction Coordinates: 6 1.587555 -0.637953 -0.270134 6 0.212007 -0.388776 0.277428 6 -0.517248 1.298246 -0.207860 1 -0.154166 1.380884 -1.243624 1 0.071282 1.862109 0.531919 1 0.086226 -0.273544 1.350028 1 1.898083 -1.634092 0.060435 1 1.537484 -0.670872 -1.359333 6 2.617885 0.391514 0.196232 1 2.658544 0.448510 1.284864 1 3.609766 0.113804 -0.157132 1 2.396951 1.387143 -0.186792 8 -1.761525 1.170027 -0.001130 8 -1.927157 -0.880085 0.263091 8 -0.749489 -1.113958 -0.293756	**Frequencies (cm^{-1}):** -434.0304, 75.6953, 147.5764, 183.594, 224.0216, 292.1293, 353.3707, 419.8875, 490.1163, 523.8618, 605.4591, 783.5479, 852.3054, 927.0852, 1003.563, 1029.483, 1055.1412, 1116.9828, 1161.7934, 1181.4548, 1224.4051, 1252.5473, 1302.1954, 1332.5051, 1393.2667, 1414.6061, 1427.3964, 1481.6291, 1504.2286, 1508.2415, 1543.6663, 2910.6113, 2972.0186, 3015.5485, 3038.2162, 3067.72, 3100.3525, 3108.6845, 3124.3699
IRC:  	

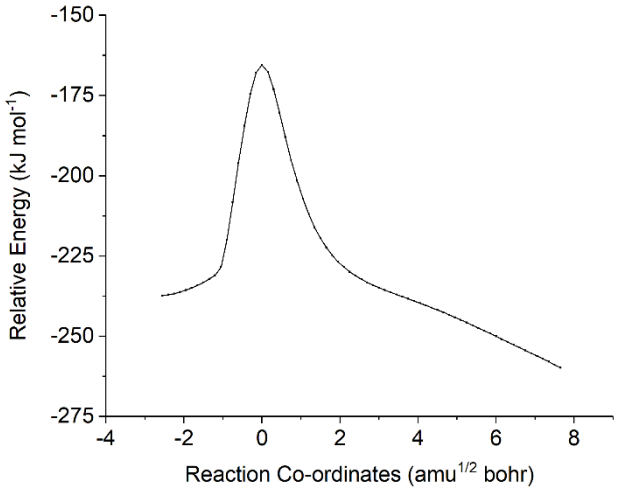
Compound: $EtCHCH_2 + O_3$ C_{ANTI} 1	**Energy (Hartree)** -382.327414870490
Reaction Coordinates: 6 1.843116 -0.591495 -0.106239 6 0.444781 -0.643042 0.373716 1 0.139883 -0.271908 1.344490 8 -0.425720 -1.210164 -0.333197 8 -1.729254 -1.160568 0.144151 1 2.424929 -1.275924 0.522807 1 1.883765 -0.969697 -1.127010 6 2.439931 0.820739 -0.002034 1 2.412401 1.185460 1.024438 1 3.478628 0.802260 -0.328420	**Frequencies (cm^{-1}):** 53.1664, 78.9036, 95.3849, 127.9186, 199.3209, 225.5953, 301.9227, 329.7278, 355.6831, 435.7429, 541.6656, 557.1088, 779.185, 916.4365, 922.6306, 936.7791, 1024.1576, 1095.0425, 1151.2462, 1184.8295, 1252.3289, 1274.1252, 1326.8585, 1372.4759, 1420.4265, 1466.6476, 1496.2997, 1505.7345, 1511.6516, 1570.3404, 1699.5236,

1 1.883143 1.520213 -0.620722 6 -1.963460 1.088778 -0.082899 1 -2.610212 1.038337 0.803492 1 -2.453896 0.898097 -1.046584 8 -0.813132 1.498643 -0.019425	2953.0824, 2998.9893, 3016.5501, 3047.2738, 3088.2774, 3111.2552, 3132.6541, 3182.4676

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -382.288487214481
Reaction Coordinates: 6 1.659253 0.181981 0.651277 6 0.182166 -0.094199 0.672300 6 -0.864046 1.292519 -0.066820 1 -0.231108 1.605286 -0.909508 1 -0.796177 1.940074 0.821030 1 -0.318812 -0.118208 1.634803 1 1.801261 1.196201 1.031760 1 2.129537 -0.477073 1.388228 6 2.341100 0.017274 -0.706474 1 1.897220 0.666523 -1.460604 1 3.396781 0.272644 -0.623856 1 2.268595 -1.007603 -1.066062 8 -1.982312 0.743625 -0.318351 8 -1.539077 -1.250146 -0.038180 8 -0.235878 -1.051391 -0.158154	**Frequencies (cm^{-1}):** -437.1696, 87.1471, 131.7377, 194.8405, 220.1672, 268.7754, 364.1744, 419.2462, 512.0625, 555.544, 642.733, 780.7455, 859.0935, 906.5766, 985.9784, 1037.189, 1059.6134, 1110.0781, 1139.7597, 1183.368, 1219.7462, 1262.7138, 1293.3588, 1377.5272, 1386.2681, 1398.4668, 1430.0063, 1478.4616, 1500.0669, 1507.1304, 1543.9012, 2914.596, 2977.6132, 3013.7009, 3045.7768, 3050.3427, 3106.0962, 3115.1249, 3129.1534
IRC:  	

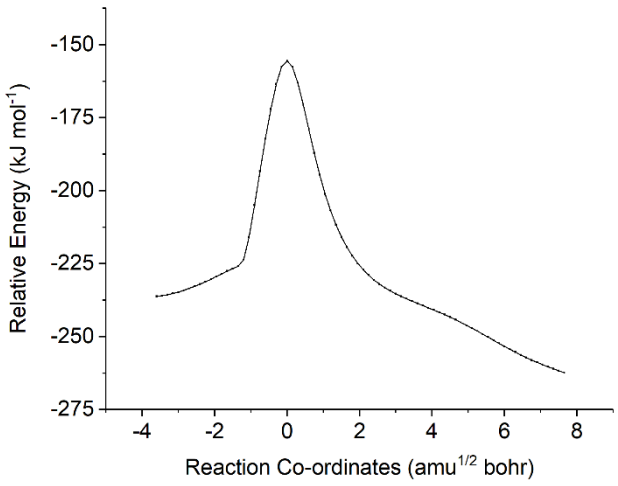
Compound: $EtCHCH_2 + O_3$ C_{ANTI} 2	**Energy (Hartree)** -382.328011970473
Reaction Coordinates: 6 -1.755577 -0.445704 0.572883 6 -0.420233 0.171306 0.724077 1 0.202463 -0.003937 1.591673 8 -0.007795 0.991083 -0.134147 8 1.303864 1.426479 0.030106 1 -1.593733 -1.523630 0.678597 1 -2.342470 -0.159618 1.454188	**Frequencies (cm^{-1}):** 50.0336, 82.8265, 98.5641, 139.8074, 195.5855, 219.4728, 312.8821, 322.6917, 353.1724, 447.2378, 565.8749, 626.9306, 739.932, 897.8154, 928.2548, 931.7204, 1027.8774, 1105.2947, 1125.4762, 1151.0374, 1251.5156, 1278.9729,

6 -2.496093 -0.121325 -0.719737 1 -1.922202 -0.441577 -1.587747 1 -3.455146 -0.636532 -0.734751 1 -2.682059 0.947404 -0.815607 6 2.234231 -0.597799 -0.325639 1 3.000035 -0.305728 0.405386 1 2.419669 -0.291318 -1.363267 8 1.328865 -1.370554 -0.038206	1350.4671, 1392.6685, 1423.7201, 1440.7971, 1499.9997, 1504.8281, 1509.239, 1572.3312, 1692.315, 2954.8476, 3002.3246, 3018.4074, 3031.757, 3049.2372, 3113.5535, 3117.2996, 3190.2494

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 3	**Energy (Hartree)** -382.289183739601
Reaction Coordinates: 6 -1.545335 -0.609861 -0.286742 6 -0.255296 -0.069809 0.251718 6 1.212363 -1.226087 -0.030727 1 0.976700 -1.609793 -1.034609 1 0.942455 -1.905010 0.793582 1 -0.135030 0.032524 1.326185 1 -1.502398 -0.601549 -1.376635 1 -1.624653 -1.653921 0.022398 6 -2.768403 0.172136 0.209604 1 -2.728957 1.210393 -0.118345 1 -3.683810 -0.272204 -0.180487 1 -2.829451 0.163127 1.298494 8 2.231101 -0.484774 0.118844 8 1.363557 1.404732 0.115508 8 0.245988 0.959812 -0.433565	**Frequencies (cm^{-1}):** -426.1407, 72.9101, 138.5843, 183.0661, 219.8746, 268.0899, 346.7494, 459.651, 508.2332, 523.3521, 608.4241, 777.8767, 857.5223, 922.2455, 989.5744, 1023.7985, 1053.4144, 1129.407, 1159.8942, 1175.5114, 1220.2794, 1247.9129, 1308.0359, 1345.6354, 1391.6902, 1409.0356, 1427.4596, 1478.9227, 1499.4702, 1506.0657, 1543.4644, 2908.3518, 2969.9697, 3035.1435, 3042.1514, 3076.1155, 3099.8787, 3107.8007, 3125.5084
IRC:  	

Compound: $EtCHCH_2 + O_3$ C_{ANTI} 3	**Energy (Hartree)** -382.326871850469
Reaction Coordinates: 6 1.682958 -0.376258 0.480233 6 0.478414 0.168596 -0.181204 1 0.202695 -0.081213 -1.197907 8 -0.218075 1.026178 0.419951	**Frequencies (cm^{-1}):** 51.1515, 66.648, 92.4584, 130.9317, 194.017, 208.92, 301.0918, 341.8677, 380.6756, 450.7932, 551.7221, 568.1698, 771.8888, 904.0266, 922.2135, 945.5875,

8 -1.395417 1.400440 -0.215688 1 1.766417 0.049307 1.479484 1 1.508398 -1.450676 0.592772 6 2.958300 -0.143078 -0.344184 1 3.173608 0.919880 -0.447576 1 3.807066 -0.614721 0.148639 1 2.869657 -0.572464 -1.342310 6 -2.363237 -0.631119 -0.075880 1 -2.836350 -0.404181 -1.040674 1 -2.897077 -0.277371 0.815657 8 -1.403136 -1.386295 0.010503	1022.4017, 1090.9935, 1150.018, 1184.417, 1251.413, 1272.135, 1327.7774, 1372.5887, 1418.121, 1468.3447, 1501.0234, 1505.4013, 1509.1729, 1568.4794, 1691.7973, 2954.917, 3018.8271, 3028.4212, 3040.1328, 3089.064, 3109.3343, 3111.5661, 3186.394

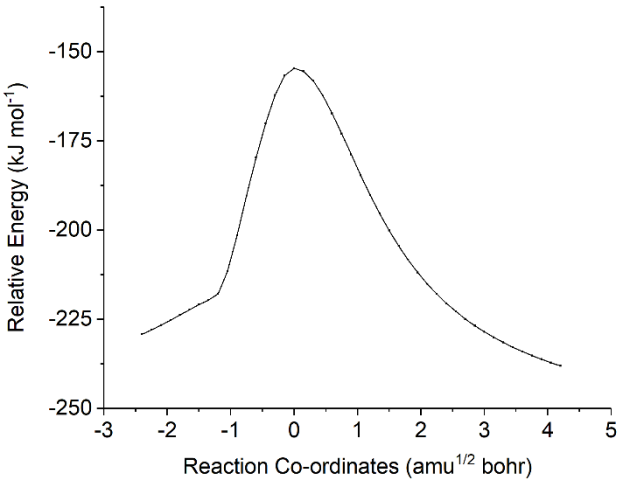
Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.1	**Energy (Hartree)** -382.286715066888
Reaction Coordinates: 6 1.430273 0.428141 -0.530970 6 0.313174 0.606204 0.496953 6 -0.634902 -1.014463 0.644438 1 0.035500 -1.863800 0.607104 1 -1.176311 -0.810951 1.559690 1 0.645912 0.547928 1.551081 1 0.998266 0.069531 -1.466329 1 1.805312 1.433304 -0.737928 6 2.578517 -0.464086 -0.067641 1 2.988791 -0.119827 0.884153 1 3.390562 -0.457095 -0.794199 1 2.272042 -1.503845 0.060999 8 -1.342866 -0.893243 -0.473810 8 -2.159319 0.142811 -0.396169 8 -0.633122 1.421680 0.254823	**Frequencies (cm^{-1}):** -439.9642, 73.5107, 123.9199, 197.9683, 238.1236, 296.9909, 335.888, 478.116, 506.3905, 581.9165, 606.1546, 780.8548, 842.1224, 893.1091, 953.5894, 1027.9135, 1048.2043, 1070.4783, 1124.7923, 1168.9999, 1222.7028, 1265.3405, 1283.8069, 1314.4639, 1346.4603, 1419.469, 1461.539, 1478.6197, 1481.5675, 1501.4491, 1504.7972, 2873.6851, 3024.9481, 3036.4129, 3064.2374, 3085.6938, 3094.9348, 3112.2787, 3230.1392
IRC:  	

Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (Hartree)** -382.322960896800

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.494273 -0.344190 -0.523841 6 1.422253 1.097645 -0.123270 1 2.404034 1.595192 0.019096 8 0.409876 1.737145 0.055801 1 1.983726 -0.368340 -1.505034 1 0.489418 -0.755936 -0.630550 6 2.332601 -1.162023 0.469615 1 1.850120 -1.202299 1.446027 1 2.443377 -2.183987 0.111109 1 3.331545 -0.741677 0.599234 6 -2.119883 0.748437 0.053993 1 -2.363421 1.499628 0.791643 1 -1.945866 0.953429 -0.993139 8 -2.060711 -0.425791 0.474275 8 -1.720215 -1.415757 -0.417246	34.4786, 46.0728, 85.1184, 93.0153, 104.2227, 118.4669, 195.5732, 213.3356, 335.6695, 518.6634, 525.2046, 678.9695, 772.7089, 864.2354, 882.4815, 926.1092, 992.1537, 1005.1802, 1135.3161, 1171.588, 1235.5085, 1281.3139, 1348.2432, 1410.5303, 1413.6336, 1426.4816, 1479.1031, 1501.1103, 1505.8132, 1566.9118, 1773.7664, 2874.6532, 2995.7611, 3032.0021, 3066.2573, 3094.3015, 3109.391, 3132.972, 3276.9654

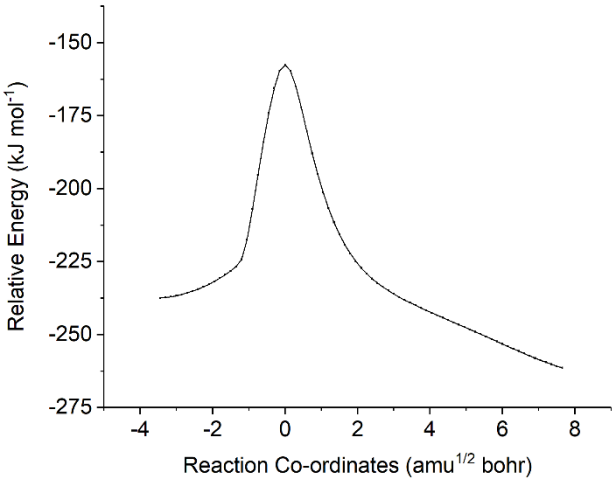
Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.2	**Energy (Hartree)** -382.286633762054
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.669419 -0.390400 0.329076 6 -0.327425 -1.002909 -0.084376 6 1.001530 -0.411284 1.082840 1 0.609067 -0.304648 2.087097 1 1.750780 -1.169851 0.892977 1 -0.210568 -2.052340 0.245868 1 -1.804013 -0.507487 1.407643 1 -2.432180 -1.023162 -0.136648 6 -1.878597 1.057735 -0.101288 1 -1.192284 1.733355 0.408864 1 -2.895563 1.378306 0.125182 1 -1.713752 1.167345 -1.171700 8 1.243552 0.770668 0.519786 8 1.715580 0.608773 -0.702705 8 0.182366 -0.721986 -1.219180	-431.625, 72.6385, 113.6497, 197.6924, 245.8676, 283.2265, 333.528, 494.8075, 519.3491, 599.6621, 675.4146, 789.6207, 798.1682, 904.8531, 958.3955, 1023.7223, 1046.5755, 1071.4018, 1104.8068, 1178.6738, 1220.4895, 1268.8971, 1291.6494, 1316.9868, 1349.2776, 1412.0758, 1462.3548, 1479.2253, 1488.4552, 1496.3595, 1508.5396, 2874.8741, 3008.9864, 3037.5066, 3042.1086, 3098.02, 3105.0916, 3114.9436, 3221.3521

IRC:



Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (Hartree)** -382.323347312587
Reaction Coordinates: 6 -2.143370 0.450045 0.362502 6 -1.676271 -0.975116 0.392088 1 -2.228098 -1.628750 1.097833 8 -0.781336 -1.439385 -0.275327 1 -2.076685 0.816305 1.394341 1 -3.220804 0.412340 0.157199 6 -1.409309 1.366318 -0.605344 1 -1.477623 0.989585 -1.626070 1 -1.846835 2.364064 -0.584346 1 -0.354608 1.453491 -0.343643 6 1.927570 -0.812155 -0.549178 1 2.088213 -1.873144 -0.423573 1 1.541445 -0.351449 -1.448276 8 2.206846 -0.102471 0.440087 8 1.997400 1.247232 0.357256	**Frequencies (cm^{-1}):** 27.7695, 46.0962, 56.3463, 84.5413, 97.9148, 139.1692, 167.3712, 247.6305, 261.9927, 521.5857, 662.647, 671.4475, 675.0085, 848.2526, 876.4525, 913.0698, 987.0925, 1009.638, 1115.4177, 1150.9914, 1238.9928, 1284.4164, 1369.5373, 1413.9423, 1415.5243, 1427.4129, 1444.7288, 1500.2482, 1516.5709, 1564.1745, 1783.0075, 2880.5873, 2995.9452, 3013.5071, 3032.9964, 3098.8361, 3101.6314, 3131.6207, 3276.7604

Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.3	**Energy (Hartree)** -382.286982119882
Reaction Coordinates: 6 -1.384973 0.562988 -0.352627 6 -0.377448 -0.032768 0.625844 6 1.192010 0.993598 0.525410 1 0.953416 2.043977 0.410791 1 1.676826 0.658206 1.433644 1 -0.545509 0.245664 1.683675 1 -0.995771 0.447263 -1.364893 1 -1.500774 1.632356 -0.157284 6 -2.740661 -0.138092 -0.230040 1 -3.152188 -0.033546 0.775867 1 -3.460668 0.286794 -0.929765 1 -2.641004 -1.201781 -0.443789 8 1.668326 0.468690 -0.598820 8 1.951950 -0.810120 -0.430387 8 0.071236 -1.207732 0.426736	**Frequencies (cm^{-1}):** -424.932, 77.4893, 119.7766, 191.7724, 237.2637, 298.5403, 322.8331, 489.0463, 505.4911, 580.9748, 633.1193, 788.9526, 838.7947, 897.2929, 957.1657, 1009.0628, 1048.0401, 1076.4676, 1134.5701, 1165.2999, 1223.5572, 1267.8332, 1288.9107, 1311.1114, 1355.2908, 1408.5138, 1467.9994, 1477.9073, 1481.9822, 1498.0798, 1505.6619, 2875.1948, 3022.0107, 3027.4968, 3071.0723, 3089.9051, 3105.1015, 3107.5291, 3225.5746
IRC:	

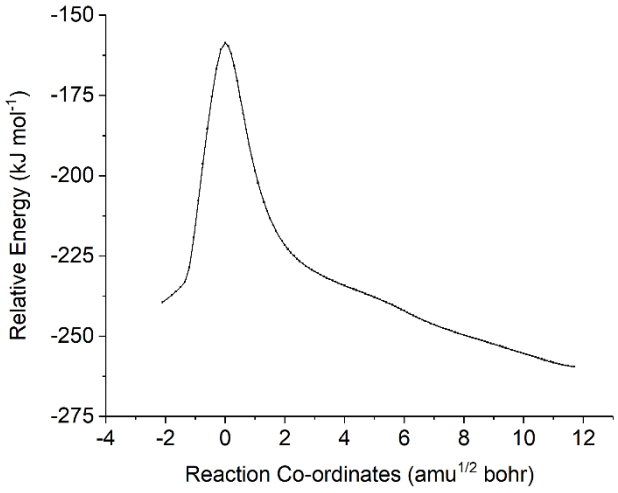


Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.3	**Energy (Hartree)** -382.324741015052
Reaction Coordinates: 6 1.690299 -0.271686 -0.499951 6 0.717208 0.406541 0.422288 1 0.658832 -0.023362 1.438769 8 0.074983 1.399255 0.144480 1 1.639784 0.205032 -1.478686 1 1.367481 -1.309750 -0.605386 6 3.115162 -0.228054 0.069823 1 3.159076 -0.679739 1.062176 1 3.799203 -0.779180 -0.574592 1 3.479119 0.796760 0.149273 6 -2.412001 0.558882 -0.414034 1 -3.165813 1.266421 -0.096921 1 -1.817787 0.654924 -1.311459 8 -2.260816 -0.429976 0.335637 8 -1.287156 -1.334929 0.013392	**Frequencies (cm^{-1}):** 30.1604, 45.954, 81.5336, 95.3035, 147.8648, 188.3603, 214.9774, 217.4755, 363.5651, 509.4182, 524.9259, 676.2711, 776.3402, 876.5636, 889.8252, 921.666, 990.6525, 1002.4105, 1123.8642, 1162.4648, 1241.0283, 1270.7939, 1326.749, 1409.0759, 1415.1813, 1426.0621, 1473.3976, 1501.6345, 1505.7828, 1565.3267, 1751.1933, 2921.5946, 3030.7455, 3040.648, 3080.0986, 3099.3125, 3101.7129, 3132.2871, 3277.322

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.1	**Energy (Hartree)** -382.285727858044
Reaction Coordinates: 6 -1.618514 0.557145 -0.349981 6 -0.316079 0.542469 0.462769 6 0.505089 -1.097080 -0.057941 1 0.123052 -1.926393 0.523542 1 0.263850 -1.036333 -1.112195 1 -0.456725 0.295517 1.530484 1 -2.080925 1.524470 -0.138895 1 -1.370482 0.564587 -1.412577 6 -2.598471 -0.560825 -0.004392 1 -2.791455 -0.598416 1.069596 1 -3.554966 -0.400594 -0.501329 1 -2.236929 -1.543321 -0.312432 8 1.756841 -0.809148 0.259922 8 2.190552 0.221640 -0.441849	**Frequencies (cm^{-1}):** -448.8384, 78.4755, 95.2102, 209.1631, 230.6325, 301.357, 379.0108, 463.2562, 495.4682, 541.6127, 599.2368, 770.3083, 863.1983, 886.8491, 973.744, 1022.3731, 1043.7217, 1062.7042, 1109.8577, 1180.2242, 1234.2499, 1264.8443, 1282.1637, 1332.1159, 1358.1025, 1418.3983, 1458.126, 1482.4169, 1485.6258, 1502.4556, 1506.1168, 2893.5197, 3026.2583, 3031.9729, 3062.6604, 3086.0261, 3094.0449, 3105.9157, 3227.6936

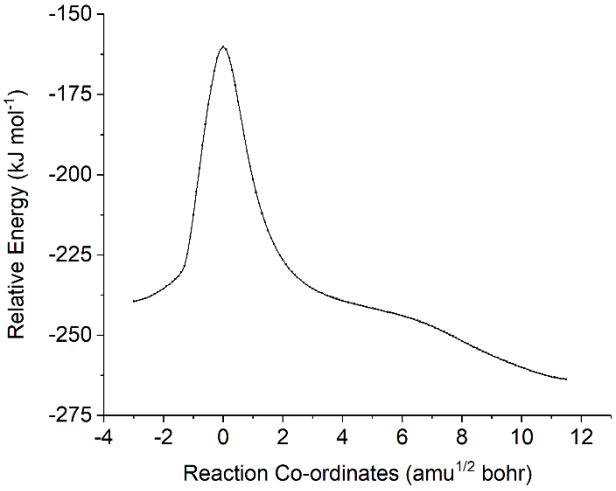
8 0.586661 1.396287 0.188311	

IRC:



Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.1	**Energy (Hartree)** -382.319882014753
Reaction Coordinates: 6 3.100135 0.334385 -0.321039 6 1.626375 0.050355 -0.328125 1 1.339533 -0.938687 -0.740989 8 0.773504 0.803979 0.077677 1 3.417142 0.387282 -1.368841 1 3.269702 1.310668 0.131445 6 3.891702 -0.771625 0.389330 1 3.694880 -1.749138 -0.053250 1 3.633856 -0.821695 1.447183 1 4.961152 -0.581744 0.312327 6 -2.499820 0.672071 0.291620 1 -1.420404 0.748633 0.232645 1 -3.170302 1.439262 0.662170 8 -2.990701 -0.408999 -0.110362 8 -4.337292 -0.583192 -0.068991	**Frequencies (cm^{-1}):** 8.574, 14.6458, 29.6453, 57.9778, 68.5375, 91.1792, 100.5617, 212.5462, 329.69, 513.4695, 534.6844, 716.2997, 761.5634, 876.8402, 901.0774, 925.3868, 1000.3357, 1006.8919, 1136.6527, 1164.0504, 1252.4723, 1273.8152, 1329.2202, 1412.5385, 1416.8349, 1428.0329, 1466.8784, 1501.7927, 1506.0223, 1554.0107, 1788.3676, 2880.2464, 3008.2946, 3035.4159, 3084.2167, 3090.1533, 3102.8332, 3107.5848, 3241.9038

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.2	**Energy (Hartree)** -382.286060556534
Reaction Coordinates: 6 -1.724202 0.481397 -0.356216 6 -0.314432 0.124543 -0.865086 6 0.798931 1.085288 0.300072 1 0.883801 2.114736 -0.026101 1 0.272036 0.871095 1.221654 1 -0.042473 0.650639 -1.796374 1 -1.781128 1.554233 -0.151653 1 -2.389409 0.304097 -1.206541 6 -2.192805 -0.338010 0.839238 1 -1.572489 -0.173978 1.722045 1 -2.157064 -1.402075 0.614987	**Frequencies (cm^{-1}):** -439.3855, 81.5282, 103.8601, 185.656, 249.9298, 291.3336, 352.1234, 465.8166, 519.5706, 596.2634, 628.1544, 786.5274, 822.6682, 901.607, 974.009, 1019.9214, 1042.4958, 1068.4654, 1098.145, 1180.6734, 1229.7018, 1264.0493, 1288.2701, 1329.2497, 1351.6901, 1414.9754, 1465.6484, 1479.2756, 1491.4379, 1495.3083, 1502.3192, 2903.0416, 3013.7327, 3033.7897,

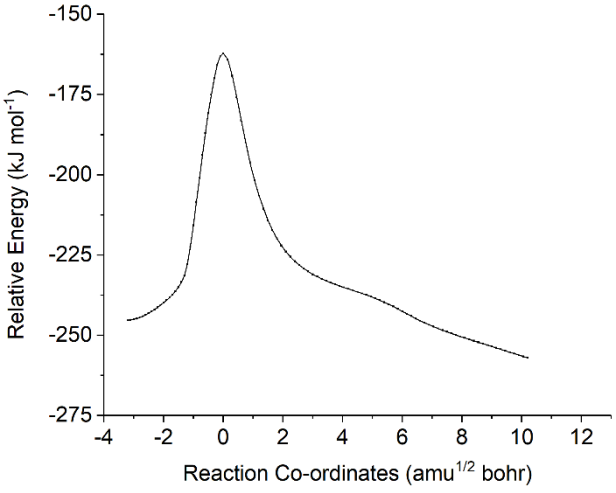
1 -3.216043 -0.070814 1.103436 8 1.929386 0.416122 0.122558 8 1.784203 -0.841753 0.497432 8 0.111138 -1.070274 -0.743678	3041.2551, 3088.0703, 3105.446, 3118.2012, 3222.6824
IRC:  	

Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.2	**Energy (Hartree)** -382.322073512602
Reaction Coordinates: 6 2.633058 0.616289 -0.148968 6 2.342748 -0.856848 -0.175731 1 3.203424 -1.496240 -0.458344 8 1.277338 -1.363825 0.079930 1 3.005686 0.877513 -1.147139 1 3.500133 0.751900 0.508843 6 1.465181 1.499497 0.265979 1 1.758797 2.548438 0.262072 1 0.619458 1.382485 -0.410106 1 1.120852 1.247634 1.268438 6 -1.972442 -0.946911 0.241183 1 -2.781141 -1.620219 0.500213 1 -0.915803 -1.179874 0.266588 8 -2.261166 0.218933 -0.126858 8 -3.556507 0.596918 -0.188739	**Frequencies (cm^{-1}):** 17.4864, 24.5871, 38.4025, 52.8191, 79.9849, 109.927, 154.131, 235.7045, 254.1316, 537.152, 665.3932, 673.6723, 712.6024, 849.8849, 908.0474, 921.9476, 976.6018, 1007.0634, 1111.6093, 1149.4799, 1252.8649, 1283.2775, 1369.5684, 1409.9663, 1415.4914, 1427.9099, 1448.2734, 1498.4471, 1504.5696, 1544.9548, 1798.5572, 2886.0564, 3002.6774, 3019.1633, 3047.959, 3103.8004, 3110.2835, 3114.4077, 3259.3132

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.3	**Energy (Hartree)** -382.286281629323
Reaction Coordinates: 6 -1.550578 0.506450 0.377655 6 -0.378433 -0.064813 -0.429539 6 1.019875 1.115235 0.039352 1 0.962627 2.019681 -0.553893 1 0.811665 1.167467 1.100901 1 -0.424881 0.166520 -1.508926 1 -1.356405 0.326843 1.436055 1 -1.619062 1.586881 0.222499	**Frequencies (cm^{-1}):** -427.6269, 76.2639, 104.8845, 195.3002, 234.7553, 311.1044, 339.9104, 467.8435, 488.8197, 562.6578, 598.8786, 789.7228, 864.3865, 897.2137, 983.946, 1006.6296, 1054.1284, 1070.5482, 1120.9523, 1171.0366, 1231.0101, 1265.9809, 1290.7426, 1334.0374, 1362.9572,

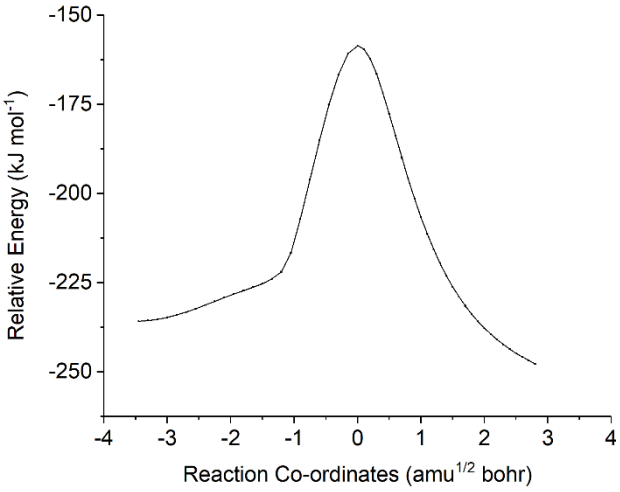
6 -2.863586 -0.160003 -0.038879 1 -2.828558 -1.231588 0.154590 1 -3.061167 -0.015177 -1.102511 1 -3.701968 0.263051 0.515418 8 2.052595 0.361364 -0.303770 8 2.082635 -0.743032 0.418888 8 0.096530 -1.201443 -0.109577	1409.4332, 1459.9018, 1477.9161, 1483.4163, 1496.147, 1503.807, 2894.3577, 3016.0586, 3029.0684, 3068.197, 3089.5138, 3104.7318, 3105.673, 3224.62

IRC:



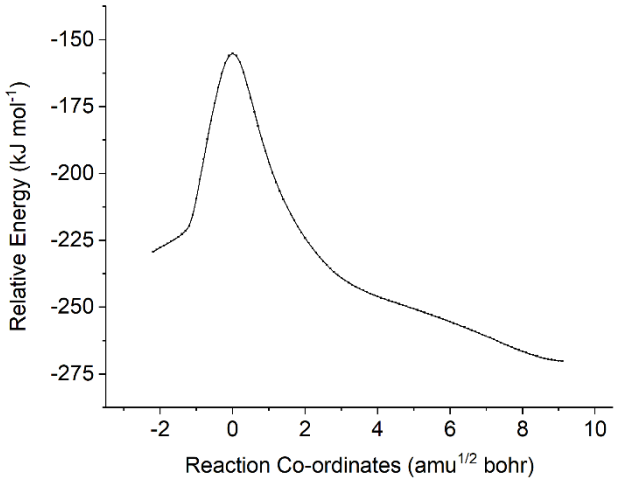
Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (Hartree)** -382.319253491307
Reaction Coordinates: 6 3.103895 -0.666554 0.000001 6 1.603232 -0.690025 -0.000060 1 1.150470 -1.701332 -0.000125 8 0.895512 0.289627 -0.000049 1 3.424521 -1.257896 -0.866269 1 3.424447 -1.257951 0.866260 6 3.728040 0.721365 0.000072 1 4.815026 0.651035 0.000117 1 3.421694 1.288371 -0.877987 1 3.421618 1.288315 0.878142 6 -2.352945 0.755007 -0.000071 1 -2.884957 1.699684 -0.000159 1 -1.275884 0.634474 -0.000052 8 -3.018767 -0.307060 0.000050 8 -4.375528 -0.240499 0.000052	**Frequencies (cm^{-1}):** 37.3724, 54.0953, 76.03, 86.588, 103.4856, 117.3332, 197.9561, 210.566, 335.3409, 518.5461, 522.1436, 677.9979, 759.5761, 865.3737, 882.7833, 925.194, 991.7934, 1008.9756, 1135.769, 1168.654, 1235.3345, 1282.2624, 1355.5913, 1411.607, 1413.5132, 1427.5967, 1472.7195, 1500.9884, 1506.0778, 1566.9298, 1773.9166, 2873.5664, 2994.791, 3031.4022, 3064.6244, 3092.3966, 3107.6809, 3133.3849, 3277.3626

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 1	**Energy (Hartree)** -382.288517541471
Reaction Coordinates: 6 -1.212418 -0.416797 -0.456320 6 -0.214385 -0.290017 0.668319 6 0.684875 1.321298 0.402284	**Frequencies (cm^{-1}):** -440.1427, 89.2366, 158.5907, 198.5178, 239.5251, 291.054, 343.1318, 383.717, 523.8873,

1 -0.233412 1.897168 0.208361 1 1.133265 1.505873 1.388296 1 -0.603923 -0.295303 1.683584 1 -0.797639 0.010420 -1.366138 1 -1.323258 -1.489798 -0.645931 6 -2.563646 0.203725 -0.112345 1 -3.002224 -0.251537 0.777236 1 -2.483662 1.277510 0.064459 1 -3.262638 0.062516 -0.935736 8 1.450887 1.087897 -0.587106 8 1.449732 -1.003507 -0.568325 8 0.900248 -1.037652 0.632211	567.0281, 708.8541, 786.3762, 871.0614, 905.1493, 950.24, 1021.9987, 1068.6957, 1080.919, 1150.3101, 1185.3924, 1214.2464, 1223.5968, 1283.3211, 1333.3493, 1378.3889, 1420.1614, 1431.9697, 1481.527, 1503.2818, 1504.4665, 1537.9293, 2919.6449, 2983.2082, 3016.75, 3029.4161, 3080.6706, 3100.0278, 3109.4595, 3122.3869
IRC  	

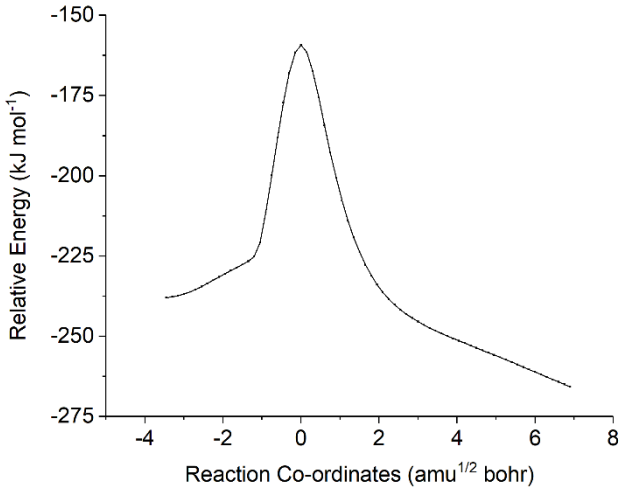
Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 1	**Energy (Hartree)** -382.327479598047
Reaction Coordinates: 6 -1.366405 0.090136 -0.469928 6 -0.726726 -0.590966 0.664619 1 -1.118208 -0.569233 1.677127 8 0.309198 -1.297525 0.566207 8 0.910221 -1.367103 -0.675054 1 -1.472711 -0.656888 -1.265588 1 -0.635787 0.801151 -0.867360 6 -2.685367 0.767733 -0.109194 1 -2.540772 1.536816 0.649970 1 -3.113514 1.247834 -0.987415 1 -3.417293 0.051275 0.265856 6 2.290668 0.765309 -0.203290 1 2.984526 0.095552 0.328432 1 2.380067 0.774490 -1.300849 8 1.513166 1.480344 0.384670	**Frequencies (cm^{-1}):** 51.2029, 74.5323, 90.7015, 93.9644, 138.2429, 201.8235, 207.701, 228.4531, 345.0508, 360.9387, 457.2332, 683.5288, 703.9688, 853.768, 876.7399, 936.3311, 1046.6932, 1107.6506, 1140.6115, 1173.3573, 1258.7894, 1259.6906, 1326.5811, 1378.6696, 1424.2028, 1426.1182, 1503.612, 1506.1109, 1527.7859, 1576.3443, 1770.4676, 2928.9124, 2989.5063, 3009.8623, 3036.4438, 3041.6298, 3095.7188, 3109.9274, 3154.0723

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 2	**Energy (Hartree)** -382.284033260298
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.463028 -0.418751 0.461912 6 -0.012774 -0.611109 0.860403 6 0.880302 1.042595 0.789515 1 0.037766 1.613062 1.213075 1 1.704849 0.863277 1.493561 1 0.135755 -1.005138 1.862567 1 -1.993303 -0.197948 1.390964 1 -1.798326 -1.414906 0.148796 6 -1.856807 0.601481 -0.605375 1 -1.392434 0.378302 -1.559994 1 -2.940828 0.581779 -0.724686 1 -1.573083 1.613913 -0.322723 8 1.150850 1.207571 -0.440199 8 0.817054 -0.737034 -1.174707 8 0.848777 -1.235242 0.047370	-429.0211, 57.4673, 168.6678, 231.4167, 257.9251, 267.8266, 312.4284, 416.121, 525.4244, 557.9337, 728.7221, 768.1373, 850.7435, 881.7869, 945.6776, 1011.9977, 1058.2694, 1111.4014, 1132.2061, 1177.0797, 1223.3155, 1233.8927, 1308.7506, 1372.9293, 1388.0543, 1417.0395, 1436.8388, 1462.5505, 1494.2816, 1501.1403, 1544.8087, 2909.8646, 2975.6213, 2998.2539, 3045.2036, 3051.5429, 3101.6442, 3123.1774, 3152.6663
IRC  	

Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 2	**Energy (Hartree)** -382.323026652093
Reaction Coordinates: 6 -2.016923 0.354860 0.074549 6 -1.121475 -0.483278 0.889383 1 -1.102244 -0.471635 1.973869 8 -0.286670 -1.292411 0.407348 8 -0.186366 -1.389047 -0.963281 1 -2.861941 0.659539 0.692118 1 -2.368595 -0.261301 -0.755869 6 -1.298244 1.598465 -0.496807 1 -2.004980 2.172619 -1.094329 1 -0.918953 2.237271 0.298997 1 -0.467315 1.296316 -1.127522 6 2.713775 0.100237 -0.251127 1 2.082873 -0.610473 -0.809624 1 3.801216 0.084397 -0.457502 8 2.245178 0.865404 0.553917	**Frequencies (cm^{-1}):** 25.67, 35.5123, 54.897, 64.6087, 102.8399, 120.797, 143.9543, 189.5781, 241.717, 322.8617, 535.5147, 648.8954, 811.6442, 846.5712, 875.0535, 906.311, 1008.992, 1084.7894, 1149.0123, 1223.5346, 1281.7979, 1289.4245, 1330.4292, 1374.8344, 1405.1727, 1462.3773, 1493.8901, 1506.6287, 1536.2747, 1570.837, 1789.1101, 2878.2978, 2980.1146, 3035.9277, 3050.436, 3088.4127, 3113.4934, 3143.8816, 3163.6244

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 3	**Energy (Hartree)** -382.288986821508

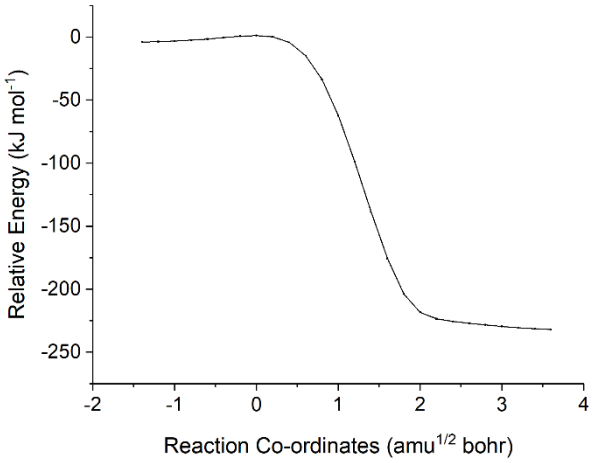
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.139313 -0.745949 -0.329732 6 0.172070 -0.295269 0.735179 6 -1.504407 -0.968989 0.223426 1 -1.113331 -1.962499 -0.044429 1 -2.058965 -0.938720 1.171780 1 0.370240 -0.614656 1.755274 1 1.289484 -1.818239 -0.196371 1 0.696430 -0.588587 -1.309695 6 2.479814 -0.008289 -0.220679 1 2.351457 1.062006 -0.374359 1 2.946394 -0.162551 0.753285 1 3.165822 -0.377177 -0.982965 8 -1.870266 -0.204811 -0.725008 8 -0.569809 1.409392 -0.440604 8 -0.230959 0.984343 0.762901	-435.4487, 81.4339, 152.4647, 200.2964, 228.8993, 290.6216, 342.778, 398.4184, 534.4638, 588.1708, 675.5289, 798.6774, 864.0052, 892.7892, 949.2167, 990.8005, 1058.7695, 1092.8118, 1149.2529, 1183.6557, 1216.0403, 1222.2684, 1305.3248, 1348.4056, 1382.9338, 1408.586, 1436.0844, 1482.362, 1498.3042, 1505.8137, 1540.0255, 2919.412, 2982.1101, 3035.0546, 3053.7511, 3091.8497, 3109.9608, 3118.1835, 3131.0544
IRC  	

Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 3	**Energy (Hartree)** -382.326620083051
Reaction Coordinates: 6 1.240436 -0.873423 0.020622 6 0.647868 0.047219 1.006383 1 0.781998 -0.058283 2.078085 8 -0.011375 1.079072 0.715751 8 -0.282347 1.323265 -0.615623 1 1.456734 -1.817970 0.518154 1 0.506553 -1.042357 -0.764945 6 2.526805 -0.276690 -0.594626 1 2.305978 0.663203 -1.094832 1 3.290437 -0.105371 0.163736 1 2.927957 -0.975581 -1.327084 6 -2.363545 -0.185175 -0.509072 1 -2.878130 0.713776 -0.135671 1 -2.227962 -0.240608 -1.600904 8 -2.015396 -1.078386 0.227824	**Frequencies (cm^{-1}):** 56.3724, 73.1273, 74.5611, 101.6324, 133.5406, 198.5728, 216.2526, 257.3288, 323.2996, 357.0709, 529.8793, 649.6167, 808.4707, 863.1902, 874.6502, 907.0196, 1002.4159, 1083.5403, 1153.3104, 1171.6386, 1259.2095, 1281.1752, 1327.9208, 1377.8934, 1403.7791, 1470.1403, 1496.2481, 1510.2691, 1527.5009, 1573.782, 1768.4684, 2927.9084, 2988.0762, 3044.3065, 3065.7932, 3103.6046, 3119.7448, 3133.2652, 3161.4318

S10.5 Ozonolysis of 3-methyl-1-butene (Alkene 3)

Compound: $iPrCHCH_2 + O_3$ PRC1.1	**Energy (Hartree)** -421.489482849833
Reaction Coordinates: 6 -1.464524 -0.250101 -0.288012 6 -0.543113 -0.161743 0.896637 6 0.084766 0.927362 1.351486 1 0.709616 0.883281 2.233069 1 -0.023164 1.895646 0.884024 1 -0.416960 -1.091856 1.443445 6 -1.623909 1.058531 -1.059926 1 -2.264037 0.907006 -1.929654 1 -0.663617 1.434471 -1.412564 1 -2.086010 1.830781 -0.441284 1 -1.016377 -0.986134 -0.965576 6 -2.827884 -0.813797 0.149671 1 -3.337708 -0.119516 0.820236 1 -2.717008 -1.764800 0.672722 1 -3.469632 -0.980115 -0.716525 8 2.324840 0.819733 -0.337556 8 2.600682 -0.383656 -0.075361 8 1.766089 -1.257362 -0.447961	**Frequencies (cm^{-1}):** 31.8282, 40.3334, 59.0657, 79.6143, 90.6047, 168.1063, 234.1535, 259.437, 265.9682, 295.3763, 359.1346, 389.732, 541.3701, 675.5503, 742.1642, 782.7728, 922.8119, 933.3482, 957.4492, 969.8111, 1021.1703, 1037.3617, 1115.7058, 1155.0823, 1164.0818, 1192.662, 1208.7715, 1312.9152, 1335.6855, 1370.9888, 1400.7006, 1416.6564, 1457.0657, 1491.1988, 1494.4483, 1504.9377, 1515.5425, 1658.5015, 2990.882, 3021.3132, 3026.5971, 3081.4837, 3085.2655, 3088.6269, 3097.0735, 3122.1312, 3147.1755, 3227.1471

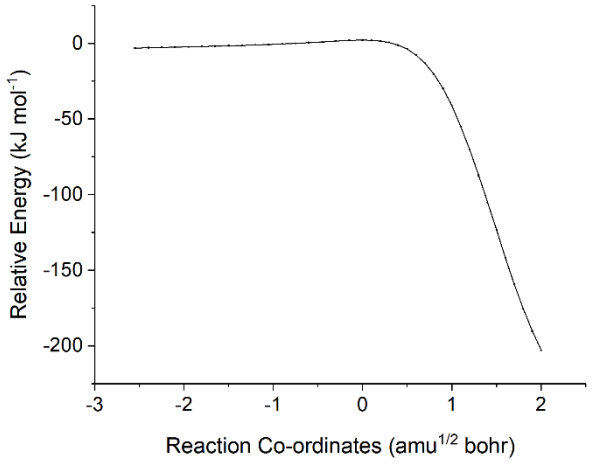
Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 1.1	**Energy (Hartree)** -421.480904807623
Reaction Coordinates: 6 1.395496 -0.224617 -0.309478 6 0.306054 -0.376163 0.716460 6 -0.379908 0.644519 1.311611 1 -1.011382 0.460564 2.167365 1 -0.172852 1.677178 1.077564 1 0.201415 -1.369883 1.135674 6 1.463594 1.160607 -0.951080 1 2.206610 1.166038 -1.749002 1 1.757875 1.924058 -0.227828 1 0.504127 1.446575 -1.380744 1 1.176074 -0.949591 -1.098764 6 2.746701 -0.626864 0.310450 1 3.034858 0.065581 1.103359 1 3.529001 -0.614223 -0.449503 1 2.709158 -1.630348 0.736616 8 -2.187929 0.795484 -0.013669 8 -2.356716 -0.469075 -0.194481 8 -1.346169 -1.031516 -0.764664	**Frequencies (cm^{-1}):** -191.7729, 49.3077, 72.7606, 131.1261, 211.5504, 232.2945, 257.3244, 270.3991, 297.5703, 371.878, 425.2393, 493.2796, 553.5254, 715.1305, 748.2884, 785.4731, 916.636, 935.7704, 957.7554, 969.3069, 1003.2055, 1036.1649, 1082.1979, 1108.9408, 1117.1182, 1151.7946, 1208.3295, 1299.2855, 1326.6037, 1374.6047, 1401.6084, 1415.1188, 1453.35, 1490.8505, 1495.5015, 1505.3806, 1515.3757, 1580.6629, 3013.2154, 3022.5412, 3028.1943, 3082.3569, 3087.4696, 3090.2022, 3103.6931, 3152.5397, 3165.2434, 3251.58
IRC:	



Compound: $iPrCHCH_2 + O_3$ POZ1.1	**Energy (Hartree)** -421.578518282609
Reaction Coordinates: 6 -1.373590 -0.294526 -0.338568 6 0.022147 0.279030 -0.604937 6 0.712833 1.061071 0.549343 1 0.997808 2.063216 0.224943 1 0.118949 1.113812 1.459153 8 1.863488 0.285214 0.864043 8 2.194230 -0.285855 -0.418350 8 0.924485 -0.810179 -0.839074 1 -0.006938 0.913115 -1.495319 6 -1.442787 -1.185493 0.903538 1 -2.425834 -1.652824 0.971136 1 -1.292767 -0.614742 1.821971 1 -0.692771 -1.973223 0.869670 1 -1.604156 -0.915792 -1.209279 6 -2.405779 0.836861 -0.288955 1 -2.234398 1.497455 0.564091 1 -3.411478 0.428946 -0.187063 1 -2.382979 1.444930 -1.194787	**Frequencies (cm^{-1}):** 64.6972, 83.1839, 204.8846, 212.2893, 240.7958, 274.7452, 342.4752, 391.9514, 444.1586, 542.0804, 688.6748, 731.5728, 735.8208, 802.8704, 890.2946, 926.1251, 937.3681, 965.1475, 983.2844, 991.0528, 1030.0028, 1036.6958, 1141.2549, 1166.0392, 1208.5972, 1234.4773, 1314.2187, 1347.5183, 1353.0846, 1365.8611, 1400.4929, 1407.5437, 1430.06, 1490.5894, 1492.6218, 1504.3786, 1512.5968, 1514.603, 3008.9786, 3018.5681, 3021.6055, 3032.3006, 3043.8503, 3077.7207, 3084.7376, 3093.2585, 3114.4672, 3116.0706

Compound: $iPrCHCH_2 + O_3$ PRC1.2	**Energy (Hartree)** -421.487640851647
Reaction Coordinates: 6 1.709232 0.043070 0.339030 6 0.716612 -0.705227 -0.503268 6 -0.045677 -1.715989 -0.085947 1 -0.005051 -2.072478 0.935787 1 -0.715903 -2.236939 -0.756136 1 0.657578 -0.397324 -1.544796 6 1.424593 1.551735 0.328983 1 2.147577 2.081189 0.951582 1 0.424313 1.768029 0.700564 1 1.499905 1.953904 -0.683958 1 1.618127 -0.318440 1.367236 6 3.140419 -0.243750 -0.145424 1 3.273782 0.081845 -1.179564	**Frequencies (cm^{-1}):** 24.0644, 29.3215, 42.8574, 51.9733, 73.3551, 137.7397, 203.5513, 223.3737, 241.1009, 316.3551, 332.7771, 348.8893, 503.7519, 701.5887, 742.9039, 801.7848, 929.4988, 934.9146, 956.9629, 965.0306, 1007.7716, 1025.228, 1110.6505, 1174.1137, 1184.7875, 1207.1399, 1219.8865, 1321.8451, 1335.5437, 1340.6646, 1397.5499, 1416.7347, 1461.5641, 1489.3117, 1490.0097, 1501.8104, 1511.8733, 1672.3498,

1 3.370043 -1.308259 -0.096533 1 3.866731 0.291806 0.468225 8 -2.467492 -0.440328 0.842535 8 -2.734464 0.135847 -0.244433 8 -2.024066 1.126685 -0.568434	3013.9647, 3018.8397, 3024.1292, 3075.7117, 3082.1764, 3092.6219, 3107.8281, 3110.5178, 3132.1775, 3214.0095

Compound: iPrCHCH$_2$ + O$_3$ TS$_{OZO}$ 1.2	**Energy (Hartree)** -421.477477773765
Reaction Coordinates: 6 1.383613 0.069998 -0.290670 6 0.302309 -0.434735 0.625615 6 -0.474409 -1.519811 0.352818 1 -1.110048 -1.960187 1.105829 1 -0.347954 -2.079743 -0.563065 1 0.266601 -0.009842 1.622575 6 1.773708 1.517508 0.017802 1 2.166706 1.603550 1.033809 1 0.922406 2.188965 -0.073392 1 2.551535 1.858130 -0.666436 1 0.995642 0.019690 -1.312085 6 2.617519 -0.851120 -0.208379 1 2.369722 -1.877923 -0.476169 1 3.032748 -0.857686 0.801378 1 3.394836 -0.498647 -0.888065 8 -2.288794 -0.573860 -0.625463 8 -2.366177 0.466716 0.124415 8 -1.327358 1.222477 0.055111	**Frequencies (cm^{-1}):** -155.6518, 44.7862, 70.8365, 130.7102, 187.6012, 221.8311, 241.6815, 268.1595, 320.9395, 368.9074, 407.5938, 465.3902, 492.7118, 713.3698, 745.9637, 801.2743, 922.0225, 937.5032, 960.0778, 967.5409, 996.7537, 1016.4088, 1092.3878, 1112.8757, 1116.8791, 1185.9805, 1209.1299, 1303.6601, 1317.3723, 1339.7409, 1399.0018, 1419.979, 1457.607, 1489.1537, 1491.0063, 1503.5512, 1512.3702, 1588.4372, 3015.9815, 3021.8266, 3027.5657, 3079.7276, 3086.359, 3096.3688, 3116.3783, 3146.4653, 3152.1784, 3241.2519
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ POZ1.2	**Energy (Hartree)** -421.579433158252
Reaction Coordinates: 6 -1.318544 0.027796 -0.327615 6 0.025972 0.016434 0.395519 6 0.995057 1.184109 0.054426 1 1.211392 1.790185 0.935932 1 0.633659 1.812138 -0.758538 8 2.174623 0.545869 -0.427571	**Frequencies (cm^{-1}):** 67.067, 97.6952, 183.5727, 218.8699, 237.4027, 312.5247, 328.4754, 411.2599, 421.8582, 461.2679, 690.5704, 732.4875, 745.6522, 829.7053, 896.7526, 929.6827, 937.8114, 967.3374, 986.7387, 1003.3089, 1024.1176, 1044.4486, 1144.78,

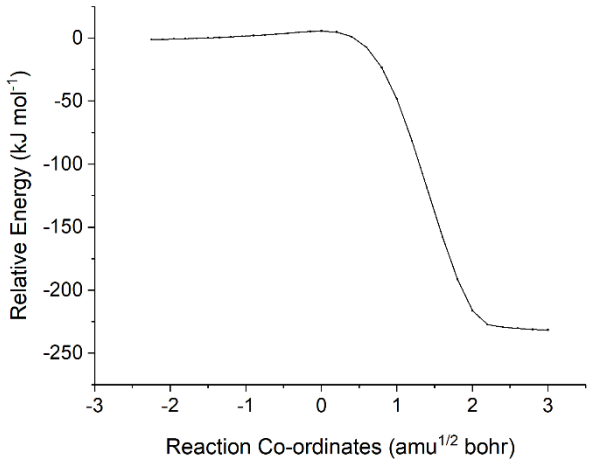
8 2.122436 -0.740952 0.230515 8 0.769749 -1.136855 -0.017407 1 -0.124678 -0.028228 1.478942 6 -2.147353 1.238645 0.114334 1 -3.097640 1.260012 -0.419338 1 -2.370310 1.191432 1.182578 1 -1.639529 2.184155 -0.081022 1 -1.104556 0.117847 -1.396948 6 -2.085743 -1.276585 -0.092353 1 -2.300641 -1.415488 0.969830 1 -3.037795 -1.258114 -0.624162 1 -1.520704 -2.140838 -0.437439	1183.8341, 1197.3571, 1238.3924, 1317.9712, 1333.5507, 1346.8571, 1354.0138, 1403.2977, 1406.3155, 1428.5174, 1489.8272, 1493.9072, 1507.0454, 1511.0334, 1513.5464, 3002.0141, 3017.4191, 3022.472, 3027.9418, 3038.5592, 3079.8884, 3084.2202, 3093.3431, 3101.5292, 3109.0159

Compound: $iPrCHCH_2 + O_3$ PRC1.3	**Energy (Hartree)** -421.487419417331
Reaction Coordinates: 6 -1.881925 0.096932 0.246370 6 -0.752279 -0.500656 1.040881 6 -0.044907 -1.592418 0.746041 1 -0.226171 -2.179427 -0.143297 1 0.729840 -1.950572 1.410060 1 -0.523639 0.023508 1.965052 6 -2.162944 -0.612629 -1.077328 1 -3.011569 -0.148906 -1.581227 1 -2.400812 -1.666584 -0.929812 1 -1.302935 -0.549977 -1.746437 1 -2.775829 -0.002316 0.876952 6 -1.656847 1.603895 0.037488 1 -0.786389 1.779329 -0.595009 1 -1.488851 2.114894 0.986662 1 -2.526141 2.058269 -0.439637 8 2.195983 -0.661616 -0.817313 8 2.581242 0.216253 -0.001302 8 1.886015 1.264243 0.098113	**Frequencies (cm^{-1}):** 18.6081, 31.3964, 40.847, 53.1454, 80.6257, 153.4446, 203.8197, 235.448, 256.719, 287.8633, 359.7377, 389.4496, 533.0584, 678.1061, 742.935, 781.3382, 923.514, 933.9275, 956.0575, 971.2865, 1027.0128, 1037.846, 1113.807, 1157.7633, 1174.0399, 1205.8223, 1209.0919, 1315.1434, 1335.3552, 1366.213, 1401.6822, 1417.3702, 1456.9933, 1491.5292, 1494.2689, 1504.7235, 1515.4136, 1668.8334, 2963.1433, 3025.4874, 3028.9973, 3086.1546, 3088.1527, 3090.3695, 3098.7163, 3116.7035, 3145.7298, 3224.0228

Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (Hartree)** -421.478853556703
Reaction Coordinates: 6 1.585337 -0.274088 0.238839 6 0.275998 -0.371233 0.978534 6 -0.652685 -1.360599 0.830804 1 -1.447282 -1.482178 1.550663 1 -0.521256 -2.160607 0.118569 1 0.172495 0.293214 1.828488 6 1.555998 -0.880248 -1.167070 1 0.830297 -0.364071 -1.794541 1 1.301022 -1.939944 -1.153926 1 2.538060 -0.788715 -1.631877 1 2.289713 -0.866380 0.840654 6 2.125262 1.161709 0.226137 1 2.158713 1.580429 1.233197 1 1.500269 1.809261 -0.387096 1 3.137624 1.182670 -0.178328 8 -2.143908 -0.431698 -0.570572 8 -2.092706 0.765250 -0.101292	**Frequencies (cm^{-1}):** -182.6792, 57.3358, 74.8137, 133.533, 187.7176, 215.7944, 235.1529, 286.8336, 333.5935, 366.6959, 411.9175, 478.5036, 523.4547, 709.5612, 741.668, 780.7328, 926.1582, 931.4445, 958.0195, 973.2032, 998.8914, 1043.986, 1086.1847, 1099.4574, 1117.365, 1167.5873, 1209.1177, 1306.3356, 1322.3109, 1347.7984, 1403.0918, 1417.4109, 1453.9285, 1491.5591, 1494.6521, 1506.8973, 1515.1754, 1581.7822, 2950.4076, 3031.5388, 3036.9535, 3088.2036, 3091.8749, 3107.1981, 3110.3428, 3150.3316, 3164.3506, 3250.2012

8 -0.925776 1.301833 -0.211795	

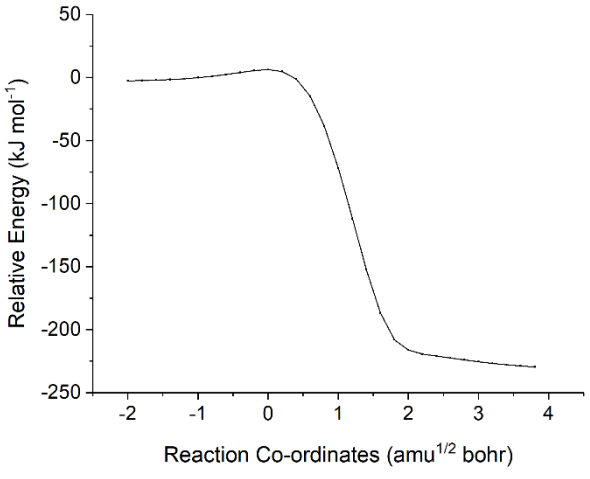
IRC:



Compound: $iPrCHCH_2 + O_3$ POZ1.3	**Energy (Hartree)** -421.578348006076
Reaction Coordinates: 6 1.377131 0.280261 0.355442 6 -0.023540 -0.285670 0.611541 6 -1.156018 0.743486 0.886773 1 -1.638234 0.542207 1.845046 1 -0.823094 1.778336 0.841416 8 -2.070795 0.563434 -0.187855 8 -1.913265 -0.841576 -0.475932 8 -0.485220 -0.963894 -0.565012 1 0.014893 -0.999198 1.439498 6 2.399688 -0.852621 0.210373 1 3.408403 -0.449279 0.116584 1 2.194444 -1.451478 -0.677745 1 2.383432 -1.517797 1.075315 1 1.626968 0.840681 1.263416 6 1.437008 1.238518 -0.837675 1 1.220887 0.715686 -1.768229 1 2.434234 1.672601 -0.915565 1 0.726700 2.060694 -0.748068	**Frequencies (cm^{-1}):** 61.6595, 83.8675, 202.8082, 204.169, 249.8785, 272.2855, 341.7976, 390.5216, 432.3574, 566.7256, 679.3514, 738.2273, 743.4427, 795.1247, 895.7239, 927.7753, 935.7532, 965.329, 968.2765, 1001.2376, 1032.006, 1048.3324, 1136.7663, 1158.4649, 1206.165, 1230.0199, 1324.2179, 1332.9331, 1346.4274, 1375.9762, 1390.7964, 1408.0304, 1430.9027, 1488.4539, 1493.2623, 1503.5889, 1512.7592, 1515.2632, 2994.1971, 3013.7958, 3027.5007, 3037.5209, 3041.5696, 3087.6979, 3091.8076, 3095.0245, 3108.4168, 3112.2936

Compound: $iPrCHCH_2 + O_3$ PRC 2.1	**Energy (Hartree)** -421.488119294631
Reaction Coordinates: 6 1.529544 -0.202130 0.336244 6 0.579810 -0.283115 -0.828452 6 -0.059663 0.727687 -1.421317 1 -0.712682 0.553825 -2.264049 1 0.057681 1.754485 -1.102957 1 0.433419 -1.283416 -1.224899 6 1.734500 1.208371 0.887193 1 2.397229 1.183081 1.752738	**Frequencies (cm^{-1}):** 28.9197, 35.6144, 43.2668, 73.194, 84.5012, 159.5007, 233.9537, 240.4621, 260.4736, 292.9114, 358.7737, 389.2604, 540.9129, 677.0492, 742.6851, 782.5319, 921.6178, 933.4301, 960.3162, 969.8545, 1024.2714, 1038.3023, 1114.6272, 1154.753, 1169.789, 1199.6556, 1207.3639,

1 0.794198 1.662285 1.201529 1 2.190408 1.861675 0.140581 1 1.092914 -0.815316 1.134674 6 2.871968 -0.855283 -0.037119 1 3.372962 -0.286147 -0.822319 1 2.731157 -1.874432 -0.399599 1 3.534643 -0.894687 0.828424 8 -2.600096 0.780385 -0.047218 8 -2.337657 -0.175570 0.732233 8 -2.040857 -1.284132 0.207059	1315.8098, 1336.4725, 1367.6129, 1401.3587, 1417.5024, 1458.2759, 1490.5952, 1494.1826, 1504.6191, 1514.1995, 1665.1274, 2976.1106, 3022.0546, 3026.9234, 3082.824, 3087.1324, 3088.7391, 3092.1121, 3127.1823, 3149.7378, 3230.526

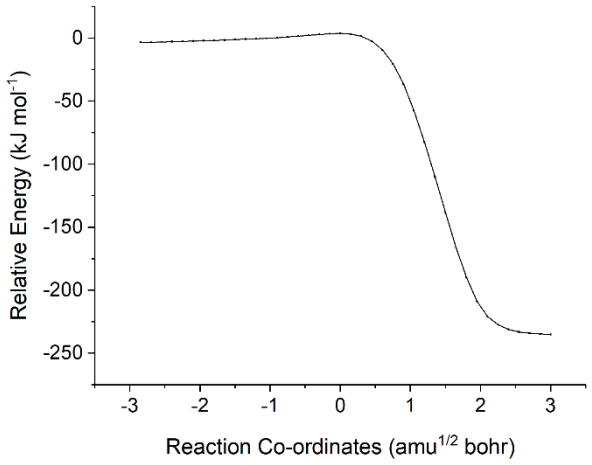
Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 2.1	**Energy (Hartree)** -421.478267576213
Reaction Coordinates: 6 1.368332 0.233744 0.318267 6 0.320906 -0.841820 0.177528 6 -0.380220 -1.130003 -0.962773 1 -0.943087 -2.046146 -1.039296 1 -0.233800 -0.571583 -1.874761 1 0.292732 -1.566924 0.981013 6 2.761446 -0.422983 0.362488 1 2.993625 -0.909375 -0.586586 1 2.824870 -1.174209 1.150711 1 3.527276 0.330017 0.553664 1 1.207422 0.706538 1.290203 6 1.304749 1.320760 -0.755709 1 0.320264 1.785659 -0.805759 1 1.544183 0.923371 -1.743963 1 2.030950 2.103715 -0.535894 8 -2.327603 -0.102259 -0.637759 8 -1.959555 0.703213 0.301162 8 -1.439806 0.081640 1.308081	**Frequencies (cm^{-1}):** -219.5759, 45.0444, 76.7721, 135.7788, 202.6958, 229.5637, 259.3776, 272.841, 296.8255, 372.1941, 437.0431, 515.2529, 559.4586, 727.5397, 742.7696, 784.913, 912.6843, 936.8623, 955.1531, 967.8978, 1003.1363, 1037.0108, 1075.7696, 1104.1093, 1114.7786, 1149.2049, 1205.6943, 1295.5947, 1329.6573, 1375.6841, 1402.188, 1415.6317, 1449.9339, 1489.8547, 1494.6528, 1506.3371, 1513.2298, 1573.8658, 3022.2136, 3024.3902, 3030.3188, 3083.7976, 3089.4315, 3090.3065, 3099.3316, 3161.8556, 3168.8215, 3257.3082
IRC:  	

Compound: $iPrCHCH_2 + O_3$ POZ 2.1	**Energy (Hartree)** -421.578381691063
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.360596 0.261009 0.342888 6 0.010564 -0.349909 0.663693 6 0.710421 -1.107264 -0.496292 1 0.226755 -0.913108 -1.454083 1 0.784937 -2.178369 -0.321442 8 2.039404 -0.602487 -0.493929 8 1.821406 0.768272 -0.130017 8 0.987678 0.634403 1.045021 1 -0.082212 -0.998618 1.536805 6 -2.380278 -0.849138 0.063939 1 -3.377944 -0.427563 -0.060136 1 -2.142265 -1.393767 -0.852535 1 -2.424817 -1.571070 0.881713 1 -1.667748 0.769399 1.261409 6 -1.330837 1.307867 -0.772571 1 -1.107126 0.867631 -1.745573 1 -2.305652 1.790921 -0.851910 1 -0.587478 2.077648 -0.572792	82.821, 91.1279, 208.8996, 220.8818, 245.3416, 270.0356, 335.8478, 381.5129, 476.0959, 546.1964, 663.2283, 719.5096, 758.6486, 796.0831, 890.6758, 919.0307, 936.1909, 964.8696, 982.6438, 991.8508, 1019.8782, 1034.204, 1140.9352, 1161.544, 1210.05, 1236.8865, 1303.7757, 1333.3372, 1355.0743, 1365.2876, 1399.0781, 1406.6604, 1428.9707, 1489.3204, 1493.3134, 1504.7897, 1511.1692, 1512.835, 3012.7296, 3020.4437, 3032.4462, 3047.309, 3051.6637, 3075.9805, 3085.0632, 3090.7566, 3111.8654, 3118.3225

Compound: $iPrCHCH_2 + O_3$ PRC 2.2	**Energy (Hartree)** -421.487885829932
Reaction Coordinates: 6 1.737850 -0.025217 -0.359528 6 0.705920 0.716044 0.441616 6 -0.075361 1.694433 -0.015482 1 -0.019375 2.029415 -1.044477 1 -0.781369 2.202017 0.625389 1 0.627398 0.428836 1.487324 6 1.454081 -1.534852 -0.371863 1 2.213134 -2.063428 -0.950724 1 0.480285 -1.754737 -0.808877 1 1.463617 -1.940787 0.641881 1 1.694109 0.341721 -1.389128 6 3.145309 0.256504 0.191133 1 3.231696 -0.078656 1.227154 1 3.375256 1.321630 0.163088 1 3.899847 -0.272008 -0.393876 8 -2.776477 0.561860 -0.553041 8 -2.462420 -0.615581 -0.233418 8 -2.010027 -0.803212 0.927333	**Frequencies (cm^{-1}):** 22.2532, 28.7929, 35.8731, 61.6081, 76.1121, 136.9736, 205.2682, 220.7184, 238.6001, 319.3567, 332.0031, 349.0046, 504.0223, 701.1698, 743.0489, 801.63, 928.7501, 933.479, 960.1529, 964.4562, 1008.4367, 1026.7976, 1110.7958, 1175.5333, 1183.8735, 1208.4116, 1219.354, 1321.5608, 1336.3527, 1341.4563, 1397.6683, 1416.7472, 1462.6721, 1487.8229, 1489.8931, 1502.1771, 1510.1935, 1673.181, 3011.9313, 3019.4781, 3024.2273, 3077.2472, 3084.0094, 3093.1686, 3095.4646, 3115.4852, 3132.5411, 3223.2408

Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (Hartree)** -421.478621062929
Reaction Coordinates: 6 1.306992 0.076256 -0.277846 6 0.293489 -0.466937 0.693251 6 -0.515916 -1.530106 0.418630 1 -1.111591 -1.989621 1.191008 1 -0.446717 -2.056977 -0.523082 1 0.339702 -0.102422 1.712352 6 1.749261 1.497439 0.076023 1 2.221931 1.520542 1.060943 1 0.902292 2.180784 0.091864	**Frequencies (cm^{-1}):** -178.2678, 42.4411, 74.4126, 133.5783, 186.9028, 224.4401, 246.0529, 263.4133, 338.0879, 370.4337, 416.7443, 487.0257, 496.7457, 720.7394, 742.5421, 802.6306, 923.0864, 938.2613, 955.6553, 967.9145, 996.1365, 1015.8222, 1083.35, 1107.6349, 1115.7812, 1186.0039, 1208.6418, 1296.3545, 1319.6997, 1337.0796,

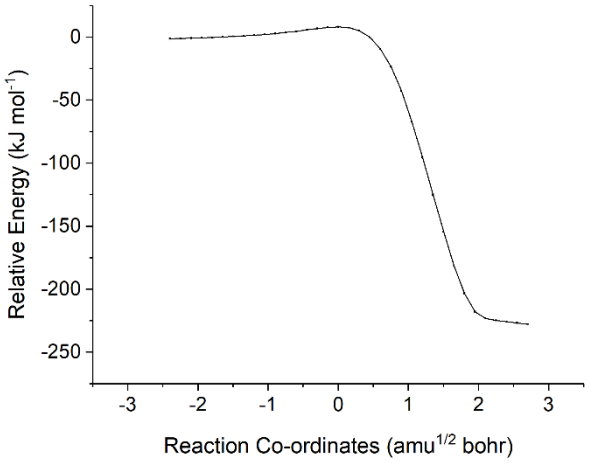
1 2.477303 1.864835 -0.647910 1 0.840665 0.089478 -1.269090 6 2.524389 -0.868605 -0.354958 1 2.233574 -1.873870 -0.658180 1 3.021658 -0.939834 0.614230 1 3.248687 -0.489166 -1.077224 8 -2.390258 -0.569682 -0.369642 8 -1.928934 0.614274 -0.581490 8 -1.415408 1.148905 0.472943	1398.5342, 1419.2666, 1454.8105, 1490.1718, 1490.3326, 1502.3198, 1513.86, 1583.0894, 2995.9028, 3022.4382, 3026.8751, 3080.5498, 3087.175, 3098.1911, 3113.4499, 3153.2697, 3157.4253, 3248.2157
IRC:  	

Compound: $iPrCHCH_2 + O_3$ POZ 2.2	**Energy (Hartree)** -421.579950919226
Reaction Coordinates: 6 1.255989 0.003868 -0.324021 6 -0.020796 0.038356 0.518784 6 -1.016141 1.165007 0.124608 1 -0.718706 1.635515 -0.814736 1 -1.152237 1.916081 0.899837 8 -2.262739 0.500970 -0.024434 8 -1.842211 -0.764521 -0.559207 8 -0.818599 -1.150723 0.382948 1 0.229306 0.084872 1.581503 6 2.092863 -1.236301 -0.003788 1 2.979371 -1.273888 -0.638062 1 2.429966 -1.222178 1.035794 1 1.522645 -2.150207 -0.161178 1 0.946466 -0.045892 -1.372619 6 2.069334 1.285243 -0.109591 1 2.379250 1.379325 0.934115 1 2.972842 1.268972 -0.719369 1 1.511989 2.184549 -0.375698	**Frequencies (cm^{-1}):** 75.4874, 99.7448, 196.6689, 218.3046, 237.882, 313.3533, 350.0876, 380.7715, 445.2364, 489.7946, 686.5078, 717.3874, 764.0131, 819.2826, 894.6433, 919.4475, 937.0786, 961.2906, 983.1729, 992.7684, 1023.6189, 1033.5331, 1134.686, 1184.5308, 1194.982, 1246.2535, 1295.0786, 1317.6712, 1348.6174, 1357.4479, 1396.0621, 1404.672, 1426.4327, 1489.9379, 1494.0473, 1502.9313, 1507.0626, 1514.5139, 3010.1784, 3019.5683, 3023.9182, 3035.4585, 3042.9211, 3077.049, 3082.0234, 3091.726, 3109.6292, 3116.1887

Compound: $iPrCHCH_2 + O_3$ PRC 2.3	**Energy (Hartree)** -421.487653574376
Reaction Coordinates:	**Frequencies (cm^{-1}):**

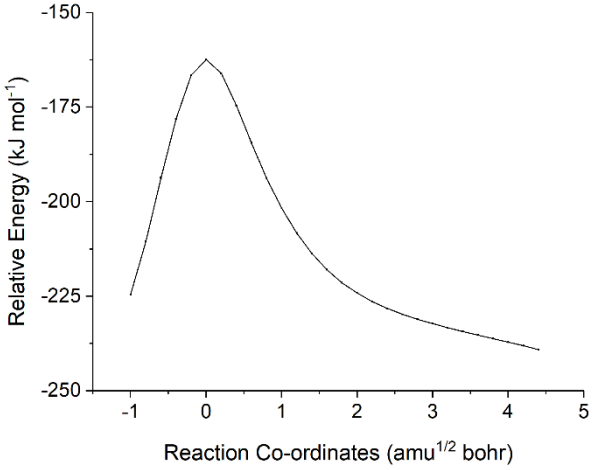
6 -1.890354 0.094090 0.253611 6 -0.724686 -0.482650 1.011480 6 -0.016909 -1.570875 0.704537 1 -0.227708 -2.173005 -0.168889 1 0.791975 -1.904079 1.337973 1 -0.462573 0.057365 1.916800 6 -2.243363 -0.658213 -1.028542 1 -3.116383 -0.208618 -1.502675 1 -2.474055 -1.705685 -0.832580 1 -1.421743 -0.623144 -1.746854 1 -2.752363 0.024611 0.930325 6 -1.668645 1.591802 -0.018571 1 -0.835947 1.743072 -0.707256 1 -1.441341 2.133122 0.900525 1 -2.559975 2.037881 -0.461664 8 2.533801 -0.723897 -0.547862 8 2.233525 0.499002 -0.594617 8 1.953156 1.071590 0.492379	21.5074, 27.5017, 44.4695, 61.0739, 85.3627, 152.4376, 207.7332, 232.1118, 256.8658, 287.3985, 358.6663, 389.0178, 535.2522, 678.3333, 742.6699, 780.5801, 923.369, 932.7311, 958.85, 970.5403, 1027.4387, 1038.7355, 1113.8301, 1156.2272, 1174.783, 1205.9861, 1208.1864, 1315.3885, 1335.3112, 1366.9361, 1402.0741, 1418.148, 1458.394, 1489.9575, 1493.1345, 1504.2896, 1513.6497, 1669.2411, 2967.0229, 3023.7992, 3027.5309, 3083.1816, 3089.6231, 3089.9387, 3092.1859, 3123.3605, 3148.8981, 3230.0246

Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 2.3	**Energy (Hartree)** -421.480159923043
Reaction Coordinates: 6 1.539942 0.347304 -0.183543 6 0.263875 0.480294 -0.976333 6 -0.725909 1.398955 -0.754514 1 -1.467718 1.590406 -1.512651 1 -0.678749 2.099073 0.065786 1 0.249297 -0.047855 -1.921629 6 1.426222 0.785552 1.279843 1 0.724676 0.155468 1.827011 1 1.100823 1.821053 1.377938 1 2.397574 0.702601 1.767781 1 2.241144 1.035346 -0.678240 6 2.146646 -1.055183 -0.306437 1 2.244349 -1.353743 -1.351434 1 1.518136 -1.791284 0.193832 1 3.139445 -1.082368 0.143717 8 -2.321400 0.244128 0.267457 8 -1.613864 -0.744142 0.698365 8 -0.986440 -1.358765 -0.249098	**Frequencies (cm^{-1}):** -213.9187, 51.3942, 77.6188, 140.3079, 189.2169, 218.3342, 243.4297, 286.0037, 349.0132, 366.6713, 422.2983, 487.6518, 538.0044, 722.9933, 739.5276, 776.2754, 926.825, 932.0731, 955.9065, 972.2425, 999.4838, 1045.1925, 1078.4575, 1096.5003, 1113.934, 1166.4033, 1210.0641, 1301.1189, 1318.1692, 1347.9535, 1404.8921, 1417.6824, 1450.2877, 1492.0982, 1493.867, 1506.7324, 1514.7236, 1574.3482, 2947.3346, 3029.5286, 3036.4307, 3088.01, 3094.3135, 3100.3378, 3105.6766, 3159.1343, 3167.4466, 3256.0347
IRC:	



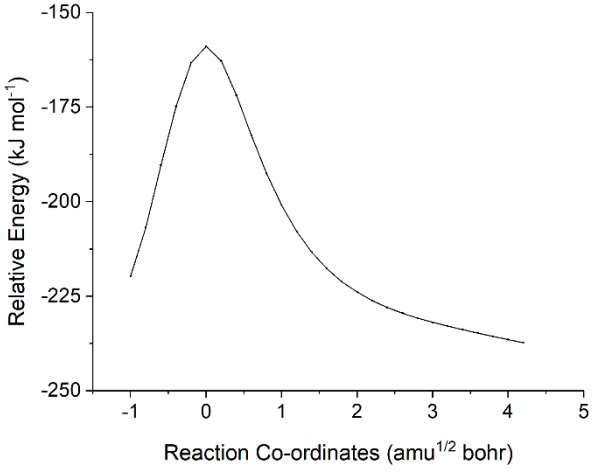
Compound: $iPrCHCH_2 + O_3$ POZ 2.3	**Energy (Hartree)** -421.578474925015
Reaction Coordinates: 6 1.324954 0.108329 0.470433 6 -0.012596 -0.637985 0.374389 6 -1.186545 0.011220 1.153167 1 -0.927810 1.012166 1.501905 1 -1.532133 -0.600130 1.984402 8 -2.252694 0.060050 0.214384 8 -1.543249 0.292716 -1.013072 8 -0.525914 -0.734274 -0.965732 1 0.125054 -1.674107 0.688618 6 1.298037 1.497663 -0.173521 1 2.264203 1.985839 -0.042165 1 1.100807 1.423026 -1.242656 1 0.538307 2.147947 0.258872 1 1.516343 0.227167 1.544279 6 2.453434 -0.744405 -0.118474 1 2.292097 -0.914755 -1.184063 1 3.416429 -0.246531 -0.001539 1 2.517865 -1.717495 0.371745	**Frequencies (cm^{-1}):** 76.1168, 94.3256, 204.5056, 217.4719, 257.6352, 274.1457, 343.5553, 394.9057, 433.8583, 589.0905, 671.5651, 718.1744, 754.702, 795.7339, 894.2209, 917.3276, 933.15, 965.0168, 969.6548, 1001.5387, 1030.8053, 1046.4645, 1124.3664, 1158.6629, 1205.0961, 1233.8928, 1297.9056, 1322.3441, 1350.2114, 1363.4691, 1389.5238, 1406.4913, 1429.4218, 1488.172, 1493.628, 1503.8142, 1511.9128, 1514.6951, 2981.1382, 3024.885, 3036.9716, 3044.9516, 3050.257, 3085.173, 3091.4369, 3095.6789, 3104.9246, 3113.762

Compound: $iPrCHCH_2 + O_3$ TS_{ANTI} 1	**Energy (Hartree)** -421.547189931544
Reaction Coordinates: 6 1.434798 -0.293902 -0.346699 6 -0.047938 -0.098096 -0.561609 6 -0.874712 1.218496 0.531676 1 -0.354995 1.056524 1.486237 1 -0.505563 2.073018 -0.054236 1 -0.363701 0.332016 -1.507713 6 2.187181 1.028569 -0.535717 1 1.973334 1.727897 0.273115 1 3.261236 0.845955 -0.539452 1 1.928692 1.509878 -1.479979 1 1.749762 -0.961580 -1.158741	**Frequencies (cm^{-1}):** -435.9236, 67.8681, 127.5494, 180.5956, 215.2753, 218.2486, 247.7444, 328.531, 342.0147, 423.5645, 452.3003, 516.4436, 561.3426, 630.504, 831.8429, 869.3616, 937.5885, 966.0389, 979.1071, 1015.5748, 1075.5023, 1097.6756, 1155.3994, 1180.6131, 1211.5498, 1225.078, 1263.7704, 1328.11, 1356.9643, 1387.1325, 1391.2113, 1409.8749,

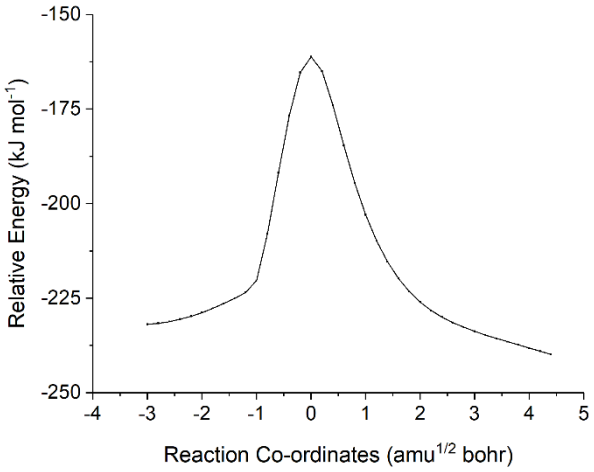
6 1.781644 -0.973228 0.980588 1 1.278519 -1.932357 1.087110 1 2.856451 -1.146267 1.034293 1 1.502037 -0.350155 1.830794 8 -0.821213 -1.110342 -0.166074 8 -2.091895 -0.888630 -0.467569 8 -2.113342 0.943227 0.461035	1434.9429, 1490.4757, 1494.6364, 1508.3109, 1513.4167, 1544.2581, 2922.8952, 2977.8745, 2986.0991, 3032.6127, 3039.9123, 3093.4661, 3096.7007, 3102.6798, 3115.4865, 3120.0678
IRC:  	

Compound: $iPrCHCH_2 + O_3$ C_{ANTI} 1	**Energy (Hartree)** -421.586931902890
Reaction Coordinates: 6 -1.618349 0.117599 -0.367647 6 -0.181988 0.331910 -0.681051 1 0.309646 -0.175311 -1.502394 8 0.484958 1.184415 -0.044691 8 1.836735 1.267128 -0.365357 6 -2.088207 0.845945 0.890533 1 -3.156379 0.683314 1.029387 1 -1.568455 0.468073 1.770830 1 -1.910504 1.918338 0.828866 1 -2.152999 0.525930 -1.238110 6 -1.912942 -1.394207 -0.328296 1 -2.984981 -1.549866 -0.213421 1 -1.592176 -1.889141 -1.244694 1 -1.392665 -1.862425 0.504852 6 2.377690 -0.790924 0.419923 1 2.696854 -0.305152 1.351508 1 3.124554 -0.822688 -0.384930 8 1.324543 -1.408169 0.347215	**Frequencies (cm^{-1}):** 38.391, 81.2123, 91.8229, 125.4783, 191.5909, 211.029, 219.668, 266.0438, 303.1194, 323.4634, 365.3149, 453.553, 465.6094, 557.0607, 601.3829, 832.2031, 921.8562, 931.758, 942.7771, 976.4191, 979.7163, 1108.8914, 1145.4921, 1153.7702, 1208.1421, 1252.2418, 1293.483, 1348.1802, 1375.0067, 1410.3279, 1429.6557, 1488.6357, 1491.4389, 1503.177, 1510.3392, 1512.401, 1562.0059, 1699.3343, 2952.3503, 2957.8868, 3015.1473, 3041.7013, 3044.1515, 3105.4434, 3107.8928, 3113.0262, 3124.5827, 3178.8921

Compound: $iPrCHCH_2 + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -421.548092509859
Reaction Coordinates: 6 -1.379505 0.040935 -0.321837 6 0.005536 -0.140589 0.243875	**Frequencies (cm^{-1}):** -424.7614, 61.1361, 139.3668, 166.4674, 222.0182, 228.4909, 258.0556, 284.9804,

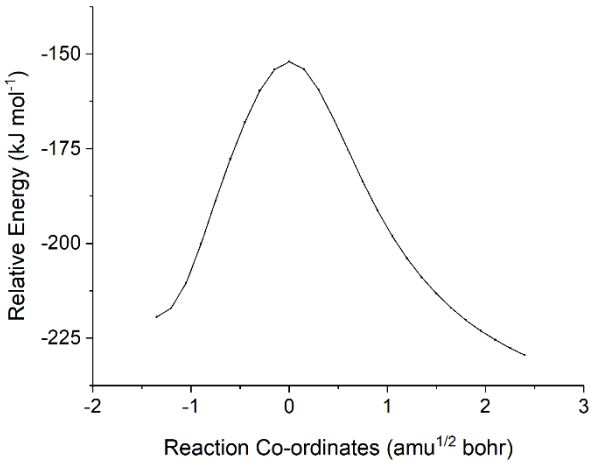
6 1.216241 1.274782 -0.143081 1 0.911384 1.518562 -1.172155 1 0.812877 1.948216 0.628010 1 0.132603 -0.121598 1.323193 6 -2.265986 -1.149587 0.084347 1 -3.261497 -1.036428 -0.345838 1 -1.847446 -2.092558 -0.264635 1 -2.374233 -1.205176 1.169240 1 -1.289108 0.047914 -1.410743 6 -1.996762 1.366717 0.134648 1 -3.013625 1.451808 -0.247360 1 -2.048023 1.422712 1.223902 1 -1.434460 2.227466 -0.224709 8 0.723932 -1.090232 -0.356296 8 1.905411 -1.243297 0.219268 8 2.362456 0.769220 0.053701	352.1543, 448.1485, 466.8311, 517.2809, 530.0917, 598.285, 846.5374, 873.0835, 938.6112, 945.848, 972.7136, 1006.8368, 1083.6508, 1123.1305, 1161.4369, 1187.3312, 1190.0226, 1225.2325, 1256.3155, 1321.4042, 1340.878, 1392.4036, 1403.2855, 1413.1291, 1434.2443, 1489.6905, 1493.2323, 1506.8123, 1513.7905, 1543.4192, 2911.7332, 2974.2782, 3027.8386, 3029.6273, 3036.7375, 3088.7906, 3095.1576, 3106.3509, 3107.9816, 3115.245
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ C$_{ANTI}$ 2	**Energy (Hartree)** -421.586344391043
Reaction Coordinates: 6 -1.540785 0.023982 -0.339574 6 -0.232307 -0.408863 0.212080 1 0.068217 -0.210567 1.234490 8 0.528677 -1.116905 -0.493112 8 1.756654 -1.449180 0.067840 6 -2.667427 -0.765579 0.357071 1 -3.630376 -0.449503 -0.043972 1 -2.564912 -1.838156 0.195862 1 -2.673918 -0.577417 1.431786 1 -1.542869 -0.216384 -1.403835 6 -1.716330 1.540060 -0.153870 1 -2.673769 1.846037 -0.575410 1 -1.710736 1.807132 0.903754 1 -0.917363 2.091820 -0.643233 6 2.581687 0.669642 0.095904 1 3.082249 0.441237 -0.854452 1 3.119014 0.368948 1.005662 8 1.576599 1.363761 0.140232	**Frequencies (cm^{-1}):** 38.6458, 78.3218, 92.3284, 115.713, 184.2876, 210.0883, 213.0463, 265.8411, 297.9685, 316.0486, 358.569, 459.6574, 480.0233, 533.9852, 554.659, 855.2013, 923.6637, 942.1476, 951.8172, 953.7826, 971.8611, 1099.4272, 1151.8702, 1183.9198, 1205.8007, 1252.6154, 1327.8699, 1331.7046, 1370.9554, 1402.8871, 1424.9574, 1487.7594, 1489.8949, 1500.9809, 1510.5609, 1512.6128, 1568.6591, 1701.937, 2951.6084, 3014.3968, 3031.4826, 3037.5118, 3055.7466, 3095.0921, 3101.35, 3106.1457, 3129.2749, 3173.6931

Compound: $iPrCHCH_2 + O_3$ TS_{ANTI} 3	**Energy (Hartree)** -421.547656378960
Reaction Coordinates: 6 1.384417 0.357138 -0.280146 6 -0.018480 -0.181869 -0.417208 6 -1.354485 1.144492 -0.493721 1 -0.971360 1.871503 0.236334 1 -1.162555 1.408849 -1.545088 1 -0.282585 -0.668597 -1.351450 6 1.712600 0.848950 1.132395 1 0.993119 1.586984 1.485020 1 1.720411 0.024311 1.844539 1 2.699680 1.310547 1.140884 1 1.438023 1.208058 -0.966260 6 2.399587 -0.693093 -0.764086 1 2.388024 -1.570766 -0.116593 1 2.186605 -1.019502 -1.782539 1 3.406497 -0.275346 -0.749082 8 -0.501730 -0.817264 0.652772 8 -1.711739 -1.298124 0.414555 8 -2.431243 0.524169 -0.224724	**Frequencies (cm^{-1}):** -429.4656, 63.8621, 124.4903, 180.1246, 213.8114, 225.6088, 251.5155, 265.3578, 370.3811, 411.7229, 501.9678, 535.676, 556.2467, 628.9939, 831.3387, 875.4722, 933.5634, 965.2874, 968.2175, 1027.999, 1064.0366, 1118.9303, 1139.8519, 1181.2976, 1205.0042, 1219.7457, 1263.0199, 1329.9255, 1363.0165, 1385.4375, 1397.503, 1407.6313, 1435.0188, 1489.1033, 1494.051, 1505.1349, 1512.7008, 1543.2454, 2915.0002, 2978.5, 3013.8477, 3029.6345, 3041.6779, 3094.9243, 3096.8056, 3104.7435, 3107.9205, 3121.1286
IRC:  	

Compound: $iPrCHCH_2 + O_3$ C_{ANTI} 3	**Energy (Hartree)** -421.586605259940
Reaction Coordinates: 6 -1.472596 -0.431394 0.018575 6 -0.185451 0.129104 -0.464481 1 0.241295 -0.156184 -1.418003 8 0.405578 1.021690 0.192298 8 1.654236 1.403122 -0.290557 6 -1.879454 0.061114 1.405754 1 -2.792873 -0.443001 1.719430 1 -1.104490 -0.143951 2.142228 1 -2.068375 1.134761 1.404220 1 -1.286320 -1.511431 0.060987 6 -2.564636 -0.194368 -1.044275	**Frequencies (cm^{-1}):** 40.5508, 68.2226, 90.6279, 121.8514, 183.5761, 207.153, 220.4663, 259.7288, 310.3963, 331.5203, 367.7272, 459.9734, 472.8484, 558.9194, 611.0441, 825.8833, 922.661, 931.9843, 944.2274, 975.4644, 976.3257, 1108.8443, 1141.0819, 1151.2537, 1207.7155, 1251.9502, 1296.534, 1354.8658, 1378.1782, 1408.1939, 1428.6715, 1489.3811, 1493.543, 1505.4138, 1509.8474,

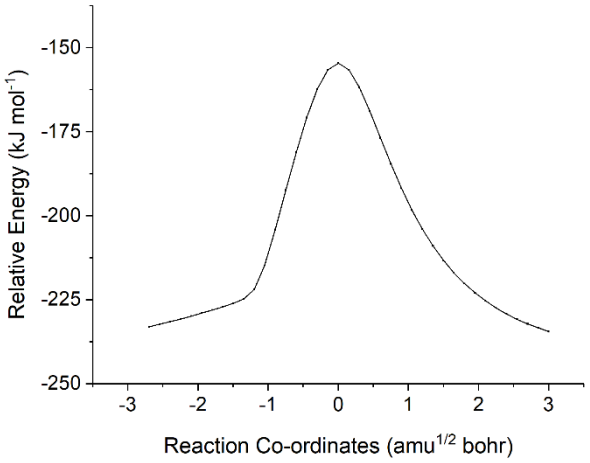
1 -3.474775 -0.717842 -0.753953 1 -2.796797 0.867278 -1.133989 1 -2.262080 -0.563580 -2.024435 6 2.640339 -0.602604 0.082878 1 3.036856 -0.189623 1.019667 1 3.235566 -0.404664 -0.818793 8 1.695535 -1.380171 0.074752	1511.835, 1563.329, 1695.9717, 2953.4456, 3000.0683, 3016.6486, 3033.8952, 3042.5708, 3098.966, 3103.2322, 3107.0985, 3115.8251, 3182.5965

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 1.1	**Energy (Hartree)** -421.545748006541
Reaction Coordinates: 6 -1.404819 -0.300214 0.302582 6 -0.086226 0.179504 0.939912 6 0.886367 1.254290 -0.250220 1 0.230695 1.858478 -0.863866 1 1.528067 1.748146 0.468511 1 -0.234104 1.023766 1.641360 6 -1.204429 -1.323812 -0.813465 1 -2.154273 -1.793850 -1.071201 1 -0.809327 -0.857611 -1.717363 1 -0.508445 -2.101719 -0.504439 1 -1.894090 -0.816416 1.137295 6 -2.316738 0.855811 -0.109300 1 -3.325507 0.493901 -0.308997 1 -2.390788 1.613143 0.674662 1 -1.967732 1.345077 -1.021163 8 1.469021 0.286967 -0.953801 8 2.269559 -0.426686 -0.184098 8 0.796490 -0.673580 1.281417	**Frequencies (cm^{-1}):** -429.0408, 50.0879, 112.5355, 197.6485, 230.3899, 238.4293, 260.4259, 295.1199, 352.0777, 446.7248, 494.3333, 520.1074, 600.0698, 668.6648, 771.6225, 893.1327, 903.5004, 936.0764, 973.6742, 994.4658, 1050.1105, 1079.646, 1140.6606, 1175.5804, 1206.7204, 1221.7753, 1269.2457, 1313.609, 1336.7479, 1351.0271, 1403.1212, 1418.8442, 1454.9626, 1480.6044, 1488.8813, 1496.0494, 1509.581, 1511.2623, 2862.6227, 2987.1409, 3017.7151, 3032.9216, 3071.7465, 3085.7072, 3089.2958, 3112.9217, 3113.7352, 3229.5423
IRC:  	

Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (Hartree)** -421.584591848636
Reaction Coordinates:	**Frequencies (cm^{-1}):**

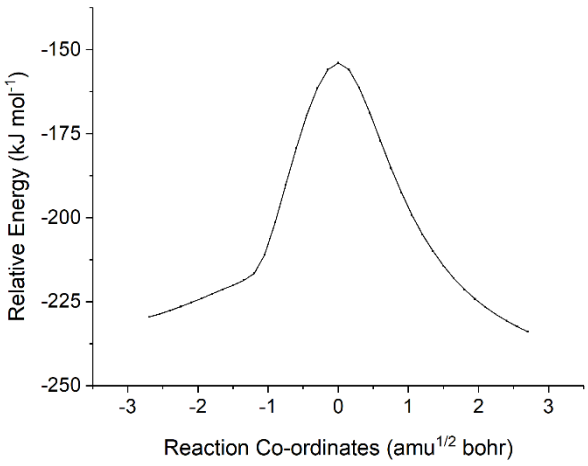
6 -1.737228 0.145395 -0.240931 6 -0.447784 0.471603 -0.960289 1 -0.219359 -0.184589 -1.820225 8 0.265936 1.422289 -0.715075 1 -2.501414 0.565614 -0.913727 6 -1.975289 -1.366611 -0.171787 1 -1.869503 -1.831965 -1.152975 1 -2.982140 -1.575678 0.190253 1 -1.259263 -1.838348 0.499553 6 -1.851468 0.836264 1.114627 1 -1.664828 1.905694 1.031614 1 -2.847274 0.690009 1.533694 1 -1.126804 0.418605 1.814888 6 2.489259 0.535606 0.447457 1 3.361250 1.071747 0.098566 1 1.790455 0.911185 1.180878 8 2.327672 -0.599553 -0.049718 8 1.213134 -1.305963 0.315170	32.5363, 45.8444, 76.1397, 100.4113, 133.9843, 196.1479, 208.482, 219.3935, 240.548, 272.141, 350.5085, 419.7441, 524.0043, 607.0652, 677.2844, 795.4341, 885.5102, 913.994, 925.8915, 948.6476, 974.9734, 993.4003, 1134.6038, 1153.764, 1207.5932, 1240.8374, 1307.6504, 1341.6215, 1401.6542, 1413.0093, 1416.061, 1432.2307, 1487.075, 1494.2573, 1502.2446, 1512.3964, 1566.7968, 1747.5955, 2915.7895, 2946.8097, 3032.2684, 3035.7606, 3089.579, 3093.1937, 3109.0526, 3110.5548, 3132.7528, 3277.7519

Compound: iPrCHCH$_2$ + O$_3$ TS$_{FO}$ 1.2	**Energy (Hartree)** -421.546199608323
Reaction Coordinates: 6 -1.233947 0.052880 -0.323585 6 -0.089776 -0.214373 0.667901 6 1.254540 1.083928 0.427709 1 0.829481 2.060966 0.238667 1 1.808382 0.919981 1.343454 1 -0.293850 0.131163 1.700491 6 -1.975443 1.354792 -0.018451 1 -2.825227 1.476926 -0.690303 1 -2.365825 1.352317 1.002537 1 -1.346056 2.238438 -0.132772 1 -0.793209 0.107146 -1.321983 6 -2.193843 -1.144669 -0.295262 1 -2.665606 -1.245062 0.685279 1 -1.662315 -2.069451 -0.511244 1 -2.985702 -1.016249 -1.034374 8 1.799135 0.561676 -0.666320 8 2.325625 -0.621077 -0.402591 8 0.591583 -1.284539 0.565208	**Frequencies (cm^{-1}):** -426.7675, 45.2426, 106.5045, 189.9068, 207.0405, 244.7019, 292.6715, 309.9316, 346.8872, 410.0374, 491.7873, 533.7123, 593.8846, 635.7118, 802.661, 891.6734, 900.1371, 935.4753, 960.5648, 970.7853, 1048.7729, 1109.1655, 1141.1874, 1169.1915, 1188.6523, 1223.3313, 1266.9753, 1303.1086, 1338.1968, 1344.5213, 1399.6804, 1419.889, 1458.3583, 1478.9255, 1488.4485, 1492.7372, 1506.8467, 1511.6104, 2864.0565, 3019.2365, 3021.9619, 3033.2449, 3075.7067, 3081.8889, 3090.3795, 3113.8663, 3114.0978, 3232.4232
IRC:	



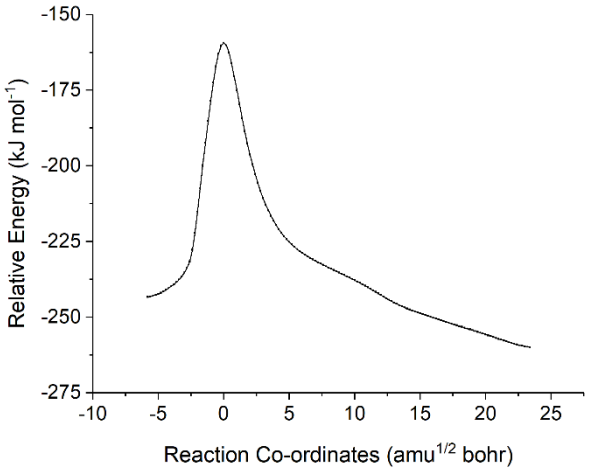
Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (Hartree)** -421.582016760602
Reaction Coordinates: 6 1.270095 -0.243268 -0.032876 6 1.061279 1.239056 0.107996 6 -2.452486 0.672674 -0.178545 1 -2.839793 1.475961 0.431775 1 -2.129072 0.785172 -1.203876 1 1.989445 1.823073 0.286617 6 1.834188 -0.792924 1.287518 1 2.015317 -1.863297 1.190748 1 2.781276 -0.314988 1.548848 1 1.135991 -0.645025 2.111281 1 0.303717 -0.709677 -0.235291 6 2.230125 -0.507376 -1.203035 1 3.195598 -0.020401 -1.047099 1 1.817413 -0.152443 -2.147723 1 2.408694 -1.578471 -1.297354 8 -2.405981 -0.449511 0.367064 8 -1.888672 -1.499073 -0.354797 8 0.002429 1.822475 0.047199	**Frequencies (cm^{-1}):** 31.3179, 37.8505, 63.4785, 85.6428, 96.4421, 108.3427, 194.87, 201.0697, 223.6026, 332.4769, 338.221, 357.4928, 519.6694, 549.5742, 678.1157, 852.3677, 864.9531, 912.0022, 939.3054, 960.9398, 983.6271, 991.164, 1132.2432, 1180.0211, 1193.0407, 1235.2515, 1350.9305, 1365.3009, 1398.0626, 1412.1988, 1413.47, 1428.2433, 1486.3739, 1492.1875, 1503.184, 1510.8698, 1566.5035, 1771.8818, 2863.346, 3021.7069, 3022.7783, 3044.1451, 3083.1966, 3088.2553, 3098.3332, 3101.2328, 3133.3937, 3277.3572

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 1.3	**Energy (Hartree)** -421.545697186692
Reaction Coordinates: 6 -1.319832 0.155799 0.422566 6 -0.162534 -0.805291 0.096118 6 1.326218 -0.363364 1.132707 1 1.021134 0.003395 2.105408 1 1.858731 -1.304385 1.073110 1 -0.273236 -1.788609 0.593306 6 -1.159348 1.529288 -0.226237 1 -2.030664 2.149786 -0.013407 1 -0.276279 2.053102 0.137629 1 -1.063247 1.431808 -1.307024 1 -1.359835 0.270232 1.510884	**Frequencies (cm^{-1}):** -418.9059, 52.0246, 109.3219, 193.5729, 206.0677, 243.9031, 265.0664, 305.9954, 329.9836, 394.3882, 493.3689, 578.8569, 632.1809, 667.3136, 762.6743, 897.5366, 905.8476, 935.8951, 969.0417, 997.115, 1049.2376, 1097.0817, 1113.2446, 1175.3603, 1197.1513, 1221.9977, 1272.3986, 1311.7039, 1339.216, 1353.034, 1400.9797, 1416.1922,

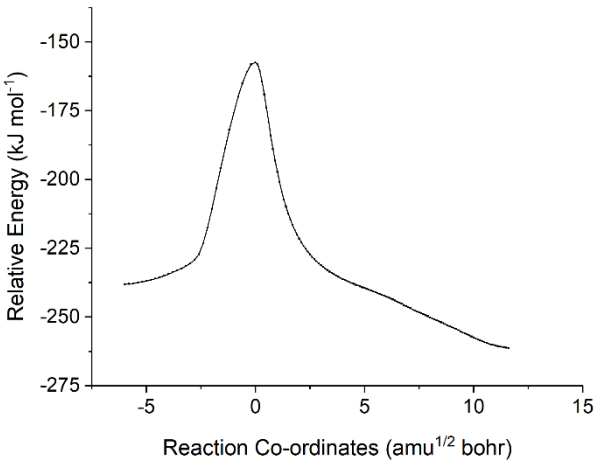
6 -2.626523 -0.520793 -0.021001 1 -3.486199 0.089422 0.258623 1 -2.638985 -0.652732 -1.103860 1 -2.749714 -1.502701 0.439778 8 1.818953 0.609811 0.370650 8 2.175460 0.135698 -0.808961 8 0.336888 -0.835903 -1.076610	1463.159, 1480.0523, 1489.14, 1492.7161, 1502.64, 1513.2438, 2863.1442, 2998.1789, 3022.6606, 3038.3629, 3082.9674, 3092.5045, 3097.7443, 3105.8822, 3110.3199, 3222.2288
IRC:  	

Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 1.3	**Energy (Hartree)** -421.581572894556
Reaction Coordinates: 6 -1.722636 -0.305606 -0.339316 6 -1.132967 1.081061 -0.380817 1 -1.637211 1.770975 -1.089374 8 -0.201225 1.480593 0.277090 1 -1.608884 -0.680429 -1.365898 6 -3.233419 -0.193682 -0.064800 1 -3.723034 0.493448 -0.756897 1 -3.417609 0.158993 0.951326 1 -3.705916 -1.169300 -0.172574 6 -1.004987 -1.243055 0.624118 1 -1.068048 -0.867991 1.646898 1 -1.467798 -2.230058 0.599509 1 0.047442 -1.356024 0.364323 6 2.481840 0.735245 0.541850 1 2.710156 1.783998 0.417945 1 2.065207 0.298812 1.439385 8 2.715881 0.010927 -0.448580 8 2.420182 -1.322294 -0.368617	**Frequencies (cm^{-1}):** 22.7539, 37.1159, 49.3316, 70.0925, 83.7541, 117.5065, 139.6232, 218.2234, 242.228, 279.7377, 348.7099, 401.8489, 521.6848, 640.8711, 671.4196, 793.0007, 877.1105, 915.2473, 929.4863, 950.8389, 977.2944, 986.0585, 1131.597, 1154.9966, 1203.2643, 1239.1947, 1298.623, 1357.7339, 1404.7236, 1413.9475, 1416.2259, 1436.6102, 1491.1116, 1494.9449, 1507.3512, 1518.2229, 1564.0054, 1780.1142, 2869.8082, 2975.9613, 3025.8981, 3028.6648, 3086.142, 3090.1801, 3100.4348, 3100.9371, 3131.5684

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 2.1	**Energy (Hartree)** -421.544395875342
Reaction Coordinates: 6 1.502390 -0.231591 0.309800 6 0.052185 -0.056060 0.831507	**Frequencies (cm^{-1}):** -439.8666, 78.1629, 82.1265, 199.5032, 210.1044, 244.3427, 267.333, 293.6905,

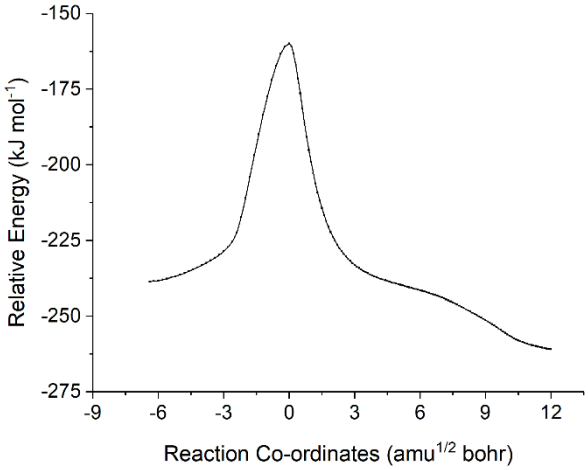
6 -0.801908 1.037413 -0.453065 1 -0.577765 2.081352 -0.275821 1 -0.409801 0.558938 -1.341170 1 -0.009059 0.651744 1.678353 6 2.222963 1.100910 0.103796 1 3.294606 0.939901 -0.016312 1 1.876480 1.620911 -0.791882 1 2.086814 1.767515 0.958094 1 1.987207 -0.733894 1.154726 6 1.606012 -1.163801 -0.893694 1 2.646428 -1.441827 -1.065966 1 1.026311 -2.070410 -0.732064 1 1.246176 -0.692282 -1.811198 8 -2.062660 0.751171 -0.163721 8 -2.306529 -0.530280 -0.364131 8 -0.712967 -1.071288 0.884500	362.9446, 461.5462, 485.116, 509.9775, 593.3666, 605.2207, 783.6659, 892.0257, 914.4268, 936.922, 970.0781, 985.5263, 1063.5387, 1065.4273, 1140.0712, 1175.9006, 1201.8547, 1234.7876, 1265.9508, 1323.3098, 1338.2654, 1362.9375, 1403.1488, 1419.8783, 1459.5708, 1481.1859, 1490.2068, 1498.5271, 1508.9077, 1509.9834, 2885.7259, 2992.5428, 3019.3287, 3026.4885, 3074.4581, 3078.6545, 3087.432, 3113.1138, 3117.5042, 3232.3755
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ CPr$_{FO}$ 2.1	**Energy (Hartree)** -421.580054966628
Reaction Coordinates: 6 -2.381222 -0.219392 -0.353093 6 -1.813590 1.156944 -0.112782 1 -2.573632 1.941267 0.081837 8 -0.641389 1.447646 -0.112654 1 -3.030986 -0.098736 -1.231012 6 -3.288703 -0.601388 0.829947 1 -4.036837 0.166852 1.030926 1 -3.814077 -1.530990 0.614395 1 -2.700763 -0.749307 1.736966 6 -1.313200 -1.265773 -0.648207 1 -1.776329 -2.225636 -0.876271 1 -0.694598 -0.975376 -1.496235 1 -0.654173 -1.404707 0.209150 6 2.571165 0.824812 0.001522 1 3.353665 1.574761 -0.021868 1 1.508202 1.019122 -0.066625 8 2.898563 -0.379528 0.117504 8 4.214428 -0.704176 0.209452	**Frequencies (cm^{-1}):** 10.2663, 13.699, 30.8959, 46.7721, 68.2393, 99.6978, 112.5829, 206.316, 230.6987, 271.3233, 344.3995, 399.7786, 533.256, 641.3325, 712.3574, 792.5133, 900.2259, 914.3051, 929.1468, 947.2759, 974.8744, 999.1053, 1128.3924, 1155.4511, 1201.9968, 1249.955, 1300.4892, 1358.273, 1405.4629, 1412.8991, 1414.5469, 1434.2356, 1487.4563, 1492.9102, 1505.5189, 1510.3041, 1553.5416, 1786.5053, 2879.0591, 2973.9358, 3029.4267, 3039.9024, 3090.2591, 3099.2232, 3099.8437, 3103.3811, 3108.0653, 3251.5759

Compound: iPrCHCH$_2$ + O$_3$ TS$_{FO}$ 2.2	**Energy (Hartree)** -421.545516836548
Reaction Coordinates: 6 1.372831 0.030970 -0.334805 6 0.091169 -0.278473 0.468021 6 -1.115802 1.098860 -0.060019 1 -0.955977 1.997570 0.521446 1 -0.862965 1.098060 -1.113290 1 0.162307 -0.005869 1.537733 6 1.954879 1.408111 -0.013839 1 2.120230 1.521123 1.060409 1 2.919410 1.537176 -0.505383 1 1.314560 2.227479 -0.343419 1 1.109516 -0.025607 -1.394085 6 2.391678 -1.077537 -0.037176 1 3.304941 -0.919903 -0.612909 1 2.662394 -1.085867 1.021304 1 1.983292 -2.054404 -0.290056 8 -2.256009 0.507254 0.255131 8 -2.418937 -0.598369 -0.447382 8 -0.565833 -1.331554 0.190396	**Frequencies (cm^{-1}):** -431.9894, 70.1263, 85.5435, 183.1117, 218.2563, 245.8348, 291.6001, 314.5512, 357.1555, 410.4524, 473.9286, 521.7679, 573.598, 599.763, 823.4206, 886.9454, 906.8937, 935.4618, 969.3827, 973.972, 1061.1257, 1090.7668, 1135.2166, 1170.2598, 1188.0958, 1236.8674, 1267.2271, 1311.4285, 1345.4199, 1355.2409, 1400.2544, 1420.4841, 1454.9737, 1483.5552, 1489.2393, 1491.5733, 1507.4891, 1511.4468, 2880.9168, 3020.4031, 3022.1115, 3028.4609, 3076.9525, 3082.1693, 3089.5753, 3106.5812, 3111.4255, 3229.7746
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ CPr$_{FO}$ 2.2	**Energy (Hartree)** -421.580059414362
Reaction Coordinates: 6 -1.554286 -0.364474 0.000006 6 -1.543689 1.141772 -0.000016 1 -2.549843 1.612705 -0.000036 8 -0.557834 1.840481 -0.000013 6 -2.259649 -0.865076 -1.269671 1 -2.293874 -1.954545 -1.270341 1 -3.287480 -0.499551 -1.321467 1 -1.737665 -0.543515 -2.170986 6 -2.259683 -0.865039 1.269679 1 -3.287515 -0.499513 1.321436 1 -2.293908 -1.954508 1.270380	**Frequencies (cm^{-1}):** 15.319, 17.9783, 36.2105, 52.9113, 70.3453, 101.4084, 120.1214, 204.291, 226.2996, 332.0817, 333.2352, 354.6993, 531.7041, 545.7917, 715.0699, 847.4752, 900.5975, 912.8478, 934.7637, 961.7208, 981.7952, 1000.3116, 1132.8093, 1182.3677, 1187.4294, 1256.2312, 1329.3982, 1345.5344, 1400.0033, 1409.2685, 1413.547, 1429.1656, 1487.5636, 1492.1449, 1504.1205,

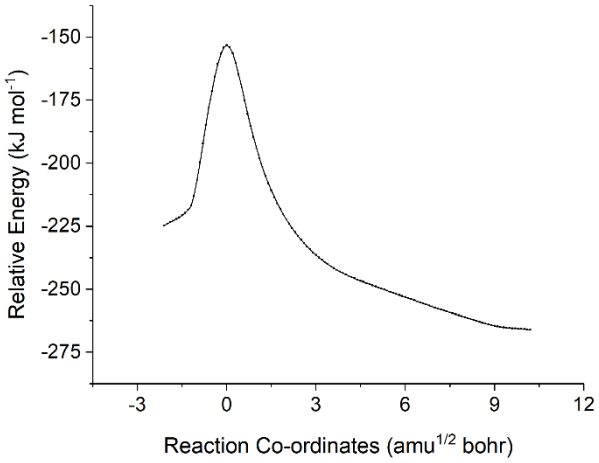
1 -1.737723 -0.543450 2.170999 1 -0.516861 -0.701445 0.000024 6 2.554197 0.892629 0.000010 1 3.558975 1.299323 0.000027 1 1.631242 1.459840 0.000002 8 2.410418 -0.352642 -0.000003 8 3.509081 -1.152116 0.000005	1511.5049, 1546.0075, 1785.1476, 2866.0719, 3024.8071, 3027.1485, 3057.9279, 3086.013, 3092.9092, 3094.8721, 3099.7301, 3100.4623, 3247.4671

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 2.3	**Energy (Hartree)** -421.544980801193
Reaction Coordinates: 6 1.402278 -0.058026 0.418528 6 0.109907 -0.601790 -0.241893 6 -1.186692 -0.315182 1.081621 1 -1.151968 -1.109649 1.817085 1 -0.885364 0.682454 1.375346 1 0.066744 -1.705708 -0.254434 6 2.596299 -0.772165 -0.230881 1 3.526712 -0.475344 0.255248 1 2.508693 -1.856684 -0.149806 1 2.667275 -0.516896 -1.289034 1 1.387816 -0.337832 1.477580 6 1.525161 1.457912 0.296003 1 2.437382 1.801385 0.784972 1 1.558322 1.755677 -0.750866 1 0.686179 1.984867 0.752395 8 -2.278564 -0.382925 0.333498 8 -2.278847 0.577960 -0.572706 8 -0.378028 -0.005880 -1.255636	**Frequencies (cm^{-1}):** -425.0795, 73.4791, 82.5356, 189.9308, 200.5459, 243.528, 278.3522, 305.3909, 334.2694, 411.8505, 470.5816, 572.4617, 596.7529, 632.5925, 784.8118, 895.4903, 910.2779, 940.1711, 966.4427, 999.401, 1059.0369, 1091.4508, 1110.5105, 1178.8193, 1195.1416, 1230.5333, 1265.3799, 1325.1646, 1336.0476, 1364.0623, 1402.6247, 1419.5203, 1461.0714, 1478.8689, 1486.9106, 1491.87, 1501.4695, 1508.556, 2890.9125, 2992.4776, 3024.5372, 3035.325, 3085.9546, 3088.2018, 3093.3389, 3106.5334, 3110.5634, 3224.0383
IRC:  	

Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (Hartree)** -421.580054966628
Reaction Coordinates: 6 -2.663058 -0.000063 0.262332 6 -1.185849 -0.000084 -0.030573	**Frequencies (cm^{-1}):** 8.5524, 9.0358, 27.351, 56.1687, 64.5374, 90.8277, 93.9906, 205.5799, 226.6681,

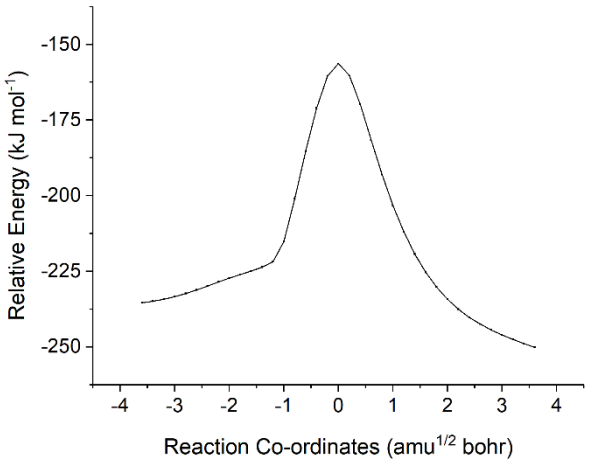
1 -0.926143 0.000323 -1.110573 8 -0.309246 -0.000497 0.800799 6 -3.296368 -1.269699 -0.326607 1 -4.370600 -1.270696 -0.141020 1 -3.146234 -1.321408 -1.406978 1 -2.875115 -2.170964 0.118918 6 -3.296139 1.270145 -0.325617 1 -3.146002 1.322666 -1.405948 1 -4.370370 1.271194 -0.140023 1 -2.874719 2.170987 0.120606 1 -2.776528 -0.000477 1.347363 6 2.969497 -0.000497 0.723987 1 3.639149 -0.001082 1.576662 1 1.886648 -0.000518 0.769399 8 3.465956 0.000280 -0.426985 8 4.817217 0.000362 -0.567506	331.437, 333.0352, 355.1537, 534.2178, 549.0834, 716.6831, 846.0596, 900.732, 913.7206, 934.0091, 962.4529, 981.823, 1000.9913, 1133.0875, 1181.9587, 1187.25, 1252.1426, 1324.0491, 1343.4769, 1400.4597, 1411.6399, 1417.1095, 1429.3722, 1488.3531, 1492.1805, 1504.3814, 1511.9163, 1554.4803, 1786.3737, 2867.9827, 3025.438, 3027.7871, 3054.3511, 3086.3454, 3089.3871, 3092.9249, 3099.0212, 3099.653, 3241.2498

Compound: $iPrCHCH_2 + O_3$ TS_{SYN} 1	**Energy (Hartree)** -421.543111711376
Reaction Coordinates: 6 1.191518 0.216488 -0.350071 6 0.011713 0.769454 0.446775 6 -0.958854 -0.620538 1.243752 1 -0.067181 -1.202491 1.527608 1 -1.433388 -0.086571 2.078896 1 0.284189 1.452789 1.247566 6 2.455757 0.315183 0.512516 1 2.398654 -0.354309 1.373692 1 3.328813 0.022174 -0.069622 1 2.623540 1.328193 0.880728 1 1.280100 0.931702 -1.178084 6 1.062261 -1.177155 -0.971576 1 1.943081 -1.368262 -1.585971 1 1.023840 -1.953858 -0.206804 1 0.174593 -1.262066 -1.587868 8 -1.049021 1.291965 -0.183650 8 -1.522686 0.470900 -1.102107 8 -1.694619 -1.078851 0.314693	**Frequencies (cm^{-1}):** -425.6826, 42.4759, 163.0627, 201.9057, 235.2443, 247.3714, 271.8856, 287.6304, 375.5968, 378.3112, 474.657, 523.043, 576.7051, 701.7327, 842.6803, 880.0824, 925.4797, 932.8609, 965.3255, 975.1141, 1077.7901, 1087.0651, 1149.7792, 1180.8192, 1203.4167, 1224.7214, 1228.8614, 1309.2695, 1338.9401, 1382.9508, 1407.2224, 1418.8307, 1437.2069, 1488.3174, 1491.6007, 1504.8096, 1509.8563, 1543.1175, 2911.6633, 2975.575, 2982.2825, 3024.1978, 3038.792, 3081.4737, 3088.1309, 3100.2355, 3117.5079, 3161.3862
IRC	



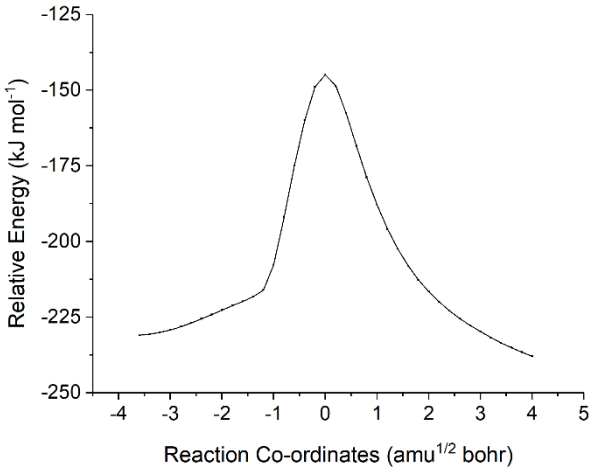
Compound: $iPrCHCH_2 + O_3$ CPr_{SYN} 1	**Energy (Hartree)** -421.581568558205
Reaction Coordinates: 6 -1.637752 -0.075464 0.236235 6 -0.757728 0.606676 -0.734714 1 -0.888131 0.535149 -1.810645 8 0.223614 1.328898 -0.421023 8 0.521543 1.489429 0.915408 6 -3.008563 -0.368417 -0.378281 1 -2.925435 -1.045594 -1.230775 1 -3.651824 -0.845804 0.360304 1 -3.505086 0.542804 -0.713657 1 -1.725314 0.609842 1.084101 6 -0.943363 -1.356204 0.756142 1 -1.567609 -1.806581 1.527917 1 -0.810033 -2.082191 -0.045897 1 0.028387 -1.122486 1.182233 6 3.205163 -0.276724 0.070742 1 2.669689 0.522564 0.608865 1 4.307907 -0.303427 0.166219 8 2.619956 -1.091262 -0.598061	**Frequencies (cm^{-1}):** 16.4307, 31.6879, 50.5018, 56.3772, 94.834, 124.7594, 147.6384, 194.5855, 208.0262, 224.1906, 270.9433, 335.2989, 413.2968, 543.5479, 669.4131, 843.9531, 856.9582, 878.8069, 939.6224, 949.2709, 976.1609, 1109.1502, 1175.761, 1191.5474, 1224.4204, 1282.0887, 1310.7447, 1321.8813, 1376.8559, 1396.9894, 1423.729, 1485.777, 1492.5953, 1502.5179, 1510.4661, 1535.8649, 1569.5776, 1788.7012, 2875.5333, 2979.4695, 3026.0924, 3030.7939, 3040.3919, 3087.5305, 3100.1869, 3102.4617, 3137.7985, 3147.7344

Compound: $iPrCHCH_2 + O_3$ TS_{SYN} 2	**Energy (Hartree)** -421.547239590041
Reaction Coordinates: 6 -1.083471 0.104408 -0.288535 6 0.022308 0.055170 0.750483 6 1.359156 1.254732 0.191279 1 0.651000 2.052943 -0.073064 1 1.908997 1.426899 1.127071 1 -0.254905 0.312017 1.770928 6 -2.003180 1.300613 -0.034042 1 -1.473658 2.252668 -0.076493 1 -2.487741 1.226578 0.942270 1 -2.787911 1.331446 -0.789431 1 -0.621366 0.198762 -1.269787 6 -1.875804 -1.213888 -0.251879	**Frequencies (cm^{-1}):** -438.0669, 75.1877, 137.3063, 197.3475, 210.5116, 235.2839, 270.9712, 312.34, 365.4871, 379.2968, 440.4712, 534.6052, 588.6387, 692.7415, 847.9495, 878.2453, 913.3437, 942.0642, 951.6442, 970.1266, 1068.8619, 1109.3333, 1149.4259, 1186.37, 1190.8205, 1214.1843, 1223.1497, 1326.2098, 1349.3214, 1383.8076, 1401.2727, 1416.3731, 1436.087, 1487.5095, 1494.9006, 1505.4112,

1 -1.236831 -2.069708 -0.457578 1 -2.355034 -1.360025 0.718161 1 -2.658244 -1.186507 -1.010612 8 0.855294 -0.995501 0.790980 8 1.943347 0.649210 -0.762050 8 1.301563 -1.302620 -0.414592	1514.0674, 1539.6042, 2930.5106, 2991.1026, 3024.5625, 3030.6495, 3072.5147, 3085.1524, 3095.4342, 3100.0758, 3114.1698, 3121.7063
IRC  	

Compound: $iPrCHCH_2 + O_3$ CPr_{SYN} 2	**Energy (Hartree)** -421.586425541548
Reaction Coordinates: 6 -1.147352 0.247239 -0.218730 6 -0.405696 -0.306595 0.933722 6 2.499406 0.492058 -0.507544 1 3.217947 -0.140991 0.035070 1 2.438255 0.324402 -1.594330 1 -0.655972 -0.060126 1.962126 6 -1.754342 1.607748 0.126956 1 -0.978857 2.326604 0.388050 1 -2.456744 1.533007 0.960191 1 -2.301287 1.997110 -0.731331 1 -0.429856 0.343163 -1.032068 6 -2.213025 -0.787740 -0.653013 1 -1.749045 -1.739706 -0.902974 1 -2.955076 -0.945773 0.130858 1 -2.729599 -0.411450 -1.535876 8 0.519305 -1.156032 0.866802 8 1.859045 1.356566 0.046379 8 0.962436 -1.543347 -0.384188	**Frequencies (cm^{-1}):** 42.9884, 70.9648, 76.9079, 98.1581, 131.5534, 202.8051, 214.9906, 226.7022, 246.7321, 275.3181, 333.9789, 367.5326, 415.5029, 537.0638, 667.3596, 846.9731, 868.391, 884.7019, 939.9079, 947.5612, 976.0918, 1109.3031, 1168.8733, 1181.766, 1191.8521, 1258.692, 1310.7745, 1323.0421, 1379.8692, 1394.8593, 1421.7396, 1487.6545, 1496.1031, 1501.451, 1513.9828, 1526.6834, 1574.6767, 1763.4748, 2930.2457, 2991.6529, 3027.0187, 3033.3404, 3079.2176, 3090.9542, 3102.4676, 3110.5939, 3120.8249, 3143.9122

Compound: $iPrCHCH_2 + O_3$ TS_{SYN} 3	**Energy (Hartree)** -421.542915962916
Reaction Coordinates: 6 -1.171447 0.404197 0.420856 6 -0.002221 -0.504293 0.778348 6 1.574450 0.539575 0.918625 1 1.058977 1.412862 1.349133	**Frequencies (cm^{-1}):** -424.0332, 54.1921, 164.6446, 197.4006, 217.3173, 248.4357, 257.2572, 282.7579, 367.2125, 413.2314, 423.4476, 535.5042,

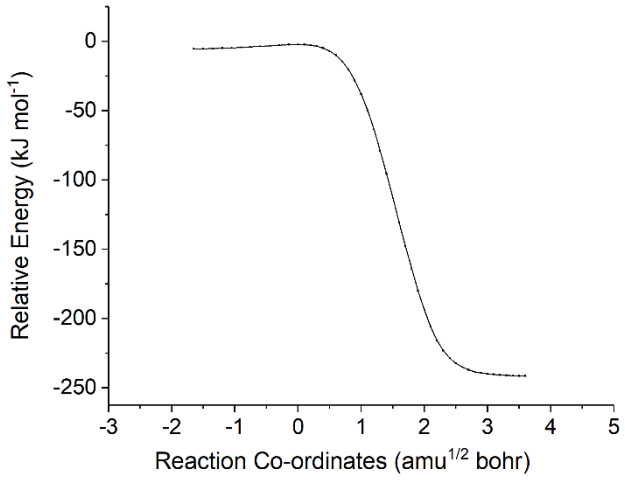
1 2.139969 -0.060094 1.645705 1 -0.122695 -1.014712 1.731411 6 -2.386336 -0.497045 0.122405 1 -2.582748 -1.200546 0.932424 1 -3.274283 0.121300 -0.009762 1 -2.230248 -1.064309 -0.794935 1 -1.375222 0.933553 1.356951 6 -0.979400 1.450389 -0.679341 1 -0.872300 0.982462 -1.654106 1 -1.855118 2.101168 -0.698730 1 -0.099177 2.067053 -0.514161 8 0.520333 -1.382599 -0.082677 8 0.842559 -0.827281 -1.237525 8 2.012430 0.630421 -0.268458	586.4836, 726.4006, 810.2204, 873.0259, 916.2233, 943.0544, 960.0004, 974.2364, 1062.304, 1112.1514, 1126.3256, 1173.6415, 1206.3856, 1224.8545, 1243.9622, 1328.8789, 1372.3091, 1387.4639, 1404.9105, 1423.9809, 1446.1428, 1484.739, 1491.4015, 1501.9742, 1510.407, 1547.5422, 2912.0253, 2975.7323, 3008.9695, 3031.6489, 3043.12, 3094.3905, 3104.4193, 3111.7935, 3114.4054, 3138.1181
IRC  	

Compound: $iPrCHCH_2 + O_3$ CPr_{SYN} 3	**Energy (Hartree)** -421.580710676361
Reaction Coordinates: 6 1.520893 -0.494771 0.434653 6 0.632919 0.533198 1.038950 6 -2.677840 -0.094173 -0.447107 1 -3.054048 0.939278 -0.384252 1 -2.510007 -0.481893 -1.465478 1 0.652659 0.746200 2.103686 6 2.568970 0.176148 -0.481282 1 3.163645 0.912462 0.059771 1 3.244516 -0.591736 -0.858341 1 2.081957 0.664538 -1.321305 1 2.047527 -0.940660 1.281674 6 0.758547 -1.617616 -0.295244 1 0.309503 -1.241983 -1.209453 1 1.467993 -2.408103 -0.542104 1 -0.030059 -2.039044 0.325524 8 -0.174913 1.290629 0.444551 8 -0.357978 1.157600 -0.915332 8 -2.491435 -0.770200 0.534588	**Frequencies (cm^{-1}):** 38.1986, 61.1304, 72.3379, 83.2116, 123.8316, 181.9359, 201.4732, 218.3971, 234.9382, 239.8214, 301.3795, 341.5884, 420.4379, 531.4752, 742.5517, 796.7005, 864.0164, 876.8295, 945.3088, 962.7793, 974.8579, 1100.9033, 1127.4171, 1177.2125, 1197.9032, 1259.3898, 1332.5329, 1374.3637, 1391.6872, 1399.2576, 1422.9729, 1482.0066, 1494.9367, 1501.3647, 1521.5603, 1528.6612, 1573.8011, 1782.731, 2920.2097, 2980.2964, 3031.5362, 3038.4957, 3044.4801, 3097.1427, 3110.1583, 3134.2327, 3146.1413, 3148.9663

S10.6 Ozonolysis of 3,3-dimethyl-1-butene (Alkene 4)

Compound: $tBuCHCH_2 + O_3$ PRC1	**Energy (Hartree)** -460.747918632232
Reaction Coordinates: 6 -1.556018 0.113564 0.050119 6 -0.501900 -0.475325 -0.858447 6 0.229484 -1.571762 -0.658509 1 0.933169 -1.914470 -1.404965 1 0.140387 -2.177469 0.232239 1 -0.367284 0.065792 -1.791902 6 -1.666092 -0.630005 1.385704 1 -2.431535 -0.166096 2.009419 1 -0.724579 -0.601572 1.935257 1 -1.945848 -1.674711 1.242427 6 -1.208285 1.593016 0.311663 1 -1.126842 2.148823 -0.624120 1 -0.259717 1.684714 0.839394 1 -1.986945 2.063635 0.914729 6 -2.908423 0.043277 -0.691849 1 -3.197299 -0.990701 -0.884005 1 -2.860724 0.563782 -1.649922 1 -3.692660 0.512151 -0.094436 8 2.629291 -0.656208 0.703386 8 2.969371 0.173683 -0.179812 8 2.299749 1.238717 -0.268100	**Frequencies (cm^{-1}):** 20.9752, 27.8085, 39.6346, 50.3155, 73.444, 141.2924, 198.0121, 226.7068, 266.0898, 285.0322, 294.4728, 322.6663, 351.7982, 389.5477, 403.2121, 526.4817, 703.8628, 714.621, 743.0282, 881.4047, 928.2036, 939.5606, 956.6683, 965.7845, 1017.0365, 1029.8113, 1047.9629, 1092.1299, 1174.8823, 1207.951, 1219.7564, 1230.4804, 1291.0803, 1339.909, 1396.373, 1400.8877, 1423.0517, 1457.7487, 1481.7299, 1488.8813, 1492.7353, 1504.6754, 1505.6074, 1523.5818, 1668.6011, 3018.4823, 3022.2676, 3028.9033, 3078.6139, 3082, 3086.1262, 3089.7601, 3092.1707, 3103.6297, 3110.9391, 3144.7203, 3222.9043

Compound: $tBuCHCH_2 + O_3$ TS_{OZO} 1	**Energy (Hartree)** -460.740227572465
Reaction Coordinates: 6 -1.320621 -0.060305 0.038067 6 -0.128798 0.417549 -0.764193 6 0.650210 1.498675 -0.468364 1 0.487708 2.089416 0.420142 1 1.321619 1.912694 -1.204706 1 -0.037132 -0.013605 -1.754615 6 -1.563594 -1.556746 -0.223158 1 -2.481449 -1.879181 0.270574 1 -0.742824 -2.163747 0.153255 1 -1.671411 -1.756263 -1.291010 6 -1.147131 0.182542 1.543873 1 -1.067774 1.244163 1.780290 1 -0.256939 -0.318691 1.920326 1 -2.013882 -0.204432 2.081610 6 -2.548449 0.731656 -0.474503 1 -2.697168 0.585824 -1.545667 1 -2.433335 1.800209 -0.291243 1 -3.449215 0.390465 0.039254 8 2.429120 0.574547 0.539637 8 2.517897 -0.469015 -0.208189 8 1.476996 -1.226415 -0.142517	**Frequencies (cm^{-1}):** -173.2116, 53.4758, 74.0635, 130.8142, 188.982, 217.698, 244.989, 267.9473, 277.7023, 294.9671, 356.5905, 366.1715, 405.9267, 417.1546, 485.37, 523.1124, 714.8721, 726.8844, 750.2925, 874.9262, 928.6709, 939.9683, 957.8883, 967.1893, 1003.7728, 1021.1489, 1044.0821, 1086.1013, 1089.1421, 1114.0191, 1213.0876, 1234.2879, 1280.6594, 1315.8212, 1396.066, 1402.4889, 1420.6554, 1454.6801, 1482.1928, 1488.2208, 1491.684, 1503.5983, 1508.1665, 1522.5692, 1579.1913, 3019.6457, 3027.5951, 3034.0885, 3080.5521, 3083.6631, 3087.5153, 3092.8533, 3111.5893, 3117.4544, 3147.2671, 3163.2733, 3248.8463
IRC:	



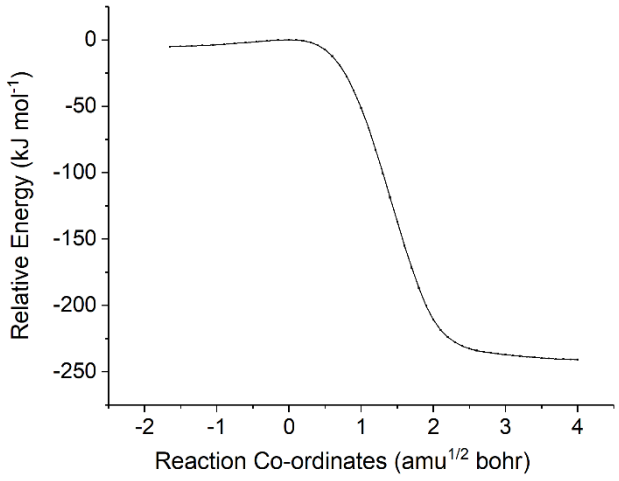
Compound: $tBuCHCH_2 + O_3$ POZ1	**Energy (Hartree)** -460.838705022718
Reaction Coordinates: 6 1.213628 0.005510 0.026760 6 -0.200625 -0.036284 -0.585733 6 -1.153672 1.159420 -0.294663 1 -1.489873 1.622156 -1.224120 1 -0.727867 1.910043 0.366647 8 -2.247924 0.581625 0.407574 8 -2.291035 -0.747106 -0.152567 8 -0.918934 -1.153258 -0.044096 1 -0.116040 -0.163878 -1.669072 6 1.169812 0.174585 1.552218 1 2.185017 0.173935 1.951597 1 0.704530 1.115009 1.850108 1 0.618116 -0.636795 2.023564 6 1.930948 -1.310124 -0.322648 1 2.956443 -1.290487 0.049118 1 1.426098 -2.167057 0.121942 1 1.969221 -1.463830 -1.402892 6 1.973919 1.177962 -0.614300 1 1.520158 2.141126 -0.374652 1 3.000992 1.200547 -0.248043 1 2.012287 1.082740 -1.701285	**Frequencies (cm^{-1}):** 63.0022, 90.2637, 195.919, 204.6776, 248.0985, 257.9683, 283.7115, 316.6226, 344.562, 373.7176, 402.9304, 450.8961, 515.0404, 679.2781, 727.8234, 739.4805, 779.3151, 855.7517, 928.387, 936.6766, 940.5285, 967.5225, 979.334, 1002.6263, 1013.9617, 1027.9546, 1077.1193, 1085.0174, 1219.6125, 1236.7113, 1244.0733, 1282.9195, 1332.0103, 1353.4994, 1382.2459, 1403.8872, 1405.4683, 1438.0277, 1482.1043, 1489.3438, 1491.1048, 1500.5784, 1509.3446, 1515.9998, 1521.8631, 3008.5396, 3020.7625, 3025.7262, 3035.0635, 3042.741, 3079.9965, 3083.095, 3085.4142, 3090.1413, 3102.3099, 3112.5156, 3119.0168

Compound: $tBuCHCH_2 + O_3$ PRC 2	**Energy (Hartree)** -460.748808987932
Reaction Coordinates: 6 -1.580837 -0.099835 0.061272 6 -0.476522 0.428974 -0.825274 6 0.259609 1.526268 -0.650386 1 0.133012 2.182676 0.199753 1 1.010695 1.810622 -1.372802 1 -0.298790 -0.166473 -1.717040 6 -1.229392 -1.544327 0.473327 1 -2.043880 -1.982889 1.052822 1 -0.326401 -1.571760 1.083953 1 -1.061075 -2.174181 -0.401481	**Frequencies (cm^{-1}):** 19.8797, 24.4339, 34.6225, 58.879, 73.3649, 137.9603, 198.6455, 225.6877, 263.6759, 284.5335, 293.2917, 324.5644, 350.3662, 389.846, 402.5291, 526.8701, 703.1615, 714.3252, 743.0764, 881.3986, 927.134, 938.6203, 959.5706, 964.1097, 1016.9046, 1031.535, 1047.9162, 1091.9431, 1176.316, 1209.7032,

6 -1.791684 0.753105 1.316965 1 -2.070846 1.776777 1.063953 1 -0.891519 0.789722 1.932142 1 -2.593076 0.331903 1.925651 6 -2.882288 -0.123204 -0.768454 1 -2.763693 -0.725425 -1.670778 1 -3.171576 0.883750 -1.071339 1 -3.698432 -0.551926 -0.183771 8 2.946779 0.739053 0.424096 8 2.696567 -0.495441 0.427848 8 2.354437 -1.024697 -0.662666	1219.159, 1230.5441, 1290.3448, 1340.0585, 1396.4477, 1400.4938, 1423.2024, 1459.005, 1481.9508, 1487.1665, 1491.2365, 1504.6562, 1505.5852, 1521.7693, 1669.9023, 3018.7848, 3021.3882, 3028.3661, 3080.0748, 3083.0896, 3087.0553, 3088.2139, 3090.9622, 3092.1076, 3116.0388, 3148.8821, 3229.0675

Compound: $tBuCHCH_2 + O_3$ TS_{OZO} 2	**Energy (Hartree)** -460.737652627627
Reaction Coordinates: 6 1.285637 0.055460 0.046996 6 0.136293 -0.502482 -0.768149 6 -0.678974 -1.538343 -0.400520 1 -0.589166 -2.019802 0.561671 1 -1.283996 -2.040466 -1.137707 1 0.129005 -0.210278 -1.811216 6 1.577454 1.505102 -0.374332 1 2.467835 1.874755 0.136348 1 0.741379 2.158749 -0.132820 1 1.757306 1.572258 -1.449075 6 1.023021 -0.002139 1.559048 1 0.880007 -1.023685 1.912298 1 0.145163 0.580959 1.835256 1 1.878827 0.409117 2.096030 6 2.524048 -0.812412 -0.288970 1 2.735945 -0.804062 -1.359270 1 2.375904 -1.847675 0.018735 1 3.401289 -0.421873 0.230371 8 -2.572348 -0.563436 0.221600 8 -2.125891 0.627827 0.433775 8 -1.532308 1.128220 -0.598508	**Frequencies (cm^{-1}):** -202.764, 49.6219, 77.2099, 137.875, 188.8331, 218.2524, 252.4732, 270.1137, 274.6331, 295.8577, 358.3615, 373.0666, 406.5721, 428.1607, 502.4985, 530.3318, 712.853, 736.7001, 747.7878, 873.5424, 928.3474, 939.8311, 956.0588, 967.2812, 1004.035, 1021.6765, 1044.2414, 1078.371, 1091.9471, 1107.0619, 1212.1957, 1233.4846, 1278.6349, 1311.0007, 1396.1306, 1404.006, 1419.7254, 1452.1761, 1481.6375, 1488.4197, 1492.4708, 1503.3567, 1507.462, 1522.3168, 1572.2168, 3019.9344, 3026.7451, 3034.5833, 3080.6697, 3084.7692, 3089.3558, 3094.1474, 3104.545, 3113.6269, 3155.5359, 3166.1779, 3254.8358

IRC:



Compound: $tBuCHCH_2 + O_3$ POZ 2	**Energy (Hartree)** -460.838967030957
Reaction Coordinates: 6 -1.189225 0.018606 0.042206 6 0.186079 0.093560 -0.657133 6 1.166633 1.181269 -0.143814 1 0.850758 1.591874 0.815105 1 1.325979 1.981874 -0.862865 8 2.407416 0.501189 -0.011428 8 1.972152 -0.788134 0.441419 8 0.954839 -1.117064 -0.534157 1 0.026415 0.209977 -1.731335 6 -2.003818 -1.095306 -0.636219 1 -2.995770 -1.168089 -0.187948 1 -2.133020 -0.898031 -1.702513 1 -1.511675 -2.061603 -0.528672 6 -1.058802 -0.295533 1.539374 1 -2.051394 -0.400153 1.980144 1 -0.518605 -1.227675 1.698907 1 -0.540691 0.491376 2.087763 6 -1.905818 1.363702 -0.161391 1 -2.000979 1.608595 -1.221581 1 -2.912021 1.319581 0.257409 1 -1.384539 2.186561 0.330775	**Frequencies (cm^{-1}):** 80.9414, 96.4614, 200.2032, 212.8671, 256.9378, 259.0956, 285.0313, 313.8699, 338.6867, 383.4462, 398.0554, 467.1194, 525.9153, 662.9698, 719.4099, 753.0161, 767.4469, 857.8242, 921.1223, 935.8654, 939.3792, 965.7049, 982.5149, 990.666, 1019.1262, 1022.2703, 1057.7392, 1096.5216, 1224.2869, 1237.3991, 1243.1293, 1277.1558, 1315.738, 1346.8597, 1380.6907, 1402.4183, 1404.8018, 1436.5986, 1482.7128, 1488.6269, 1491.328, 1500.52, 1509.9568, 1514.1966, 1521.3757, 3018.5691, 3023.4876, 3033.3006, 3040.9736, 3055.3828, 3077.4865, 3081.8167, 3084.7365, 3089.6497, 3100.2864, 3108.6759, 3119.808

Compound: $tBuCHCH_2 + O_3$ TS_{ANTI}	**Energy (Hartree)** -460.807913787771
Reaction Coordinates: 6 1.253997 0.031559 -0.008810 6 -0.204651 -0.140817 -0.395275 6 -1.384421 1.279574 0.056988 1 -0.996555 1.569809 1.043229 1 -1.070531 1.931455 -0.771088 1 -0.436465 -0.138641 -1.457013 6 1.757867 1.377363 -0.555548 1 2.832148 1.459731 -0.389759 1 1.580681 1.465801 -1.628852 1 1.279969 2.221311 -0.058837 6 2.039212 -1.113083 -0.688769 1 1.918274 -1.090629 -1.772842 1 1.705670 -2.086091 -0.328699 1 3.102587 -1.012645 -0.467501 6 1.457541 -0.036583 1.511750 1 0.911823 0.753204 2.027524 1 1.130055 -0.992196 1.917949 1 2.516366 0.083873 1.742786 8 -0.864880 -1.084895 0.277728 8 -2.093877 -1.239154 -0.190941 8 -2.540154 0.754917 -0.009152	**Frequencies (cm^{-1}):** -427.9662, 66.9154, 124.4447, 175.8749, 213.3112, 221.0846, 253.6687, 264.0743, 281.5983, 333.5843, 348.8622, 385.5841, 431.0333, 500.0593, 523.79, 556.6287, 595.2725, 786.8686, 861.2057, 920.7543, 939.9291, 951.295, 971.0386, 1016.8353, 1036.0295, 1056.1023, 1112.769, 1161.4557, 1218.2013, 1225.7495, 1232.7398, 1264.3559, 1286.1197, 1382.8615, 1385.9267, 1402.8658, 1408.6055, 1442.1557, 1482.9166, 1489.3431, 1490.6338, 1504.9593, 1508.8828, 1522.8035, 1543.6492, 2924.5942, 2988.4185, 3026.3829, 3030.4646, 3039.8335, 3088.6793, 3092.8236, 3097.3189, 3100.8688, 3103.2336, 3112.1022, 3113.5968
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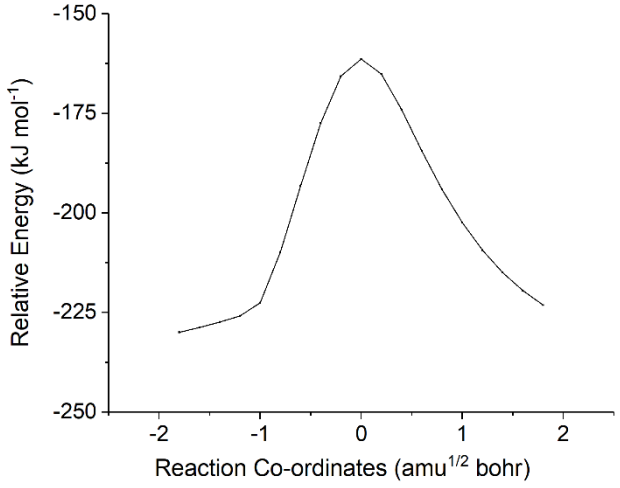
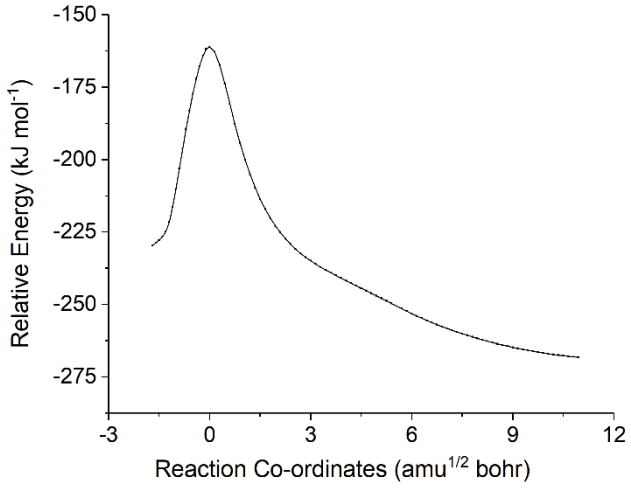
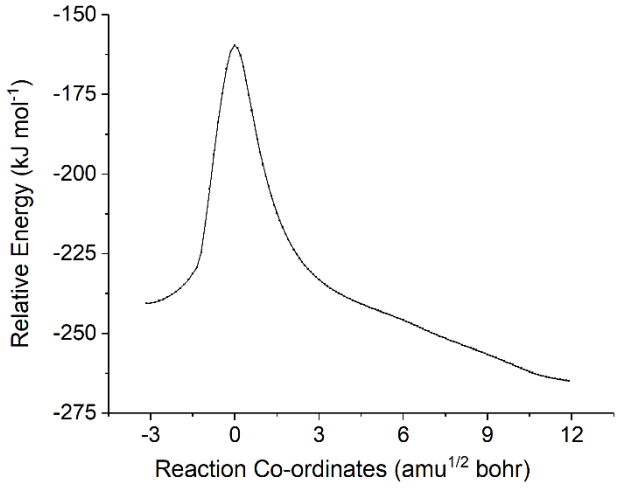


Compound: $tBuCHCH_2 + O_3$ C_{ANTI}	**Energy (Hartree)** -460.847128143048
Reaction Coordinates: 6 1.376085 -0.088090 -0.003468 6 0.016669 0.337877 0.441104 1 -0.386018 0.045284 1.403969 8 -0.660550 1.137025 -0.249674 8 -1.931465 1.442326 0.232323 6 1.468528 -1.617188 0.184869 1 2.475304 -1.946699 -0.073527 1 1.271647 -1.903719 1.218333 1 0.750235 -2.132789 -0.448688 6 2.384829 0.608838 0.943385 1 2.351173 1.692408 0.830799 1 3.392145 0.269670 0.699853 1 2.191382 0.363675 1.988313 6 1.651196 0.298184 -1.460381 1 0.933745 -0.171362 -2.132207 1 1.598094 1.376004 -1.608455 1 2.650541 -0.035315 -1.740026 6 -2.794631 -0.636466 -0.060129 1 -3.406317 -0.427315 0.828095 1 -3.203408 -0.285290 -1.016964 8 -1.812307 -1.362286 -0.010371	**Frequencies (cm^{-1}):** 33.0919, 80.1483, 91.6569, 115.8148, 180.2764, 198.1683, 211.5521, 264.1308, 264.4729, 299.1032, 313.7726, 339.0733, 349.2545, 382.1285, 470.2727, 486.7746, 552.5522, 563.5184, 777.4799, 915.9002, 923.4633, 929.0515, 959.6401, 961.2806, 976.0332, 1045.146, 1068.0272, 1151.7019, 1211.557, 1229.7521, 1252.526, 1299.9684, 1366.0551, 1400.1321, 1409.1103, 1434.8701, 1478.9601, 1488.4947, 1490.0079, 1501.6571, 1503.35, 1511.7506, 1519.6371, 1560.7447, 1701.5902, 2951.1797, 3013.4332, 3029.0496, 3035.5221, 3041.5008, 3094.5849, 3098.5467, 3101.2529, 3105.8247, 3111.5433, 3125.6409, 3172.6784

Compound: $tBuCHCH_2 + O_3$ TS_{FO} 1	**Energy (Hartree)** -460.806199784381
Reaction Coordinates: 6 1.201369 0.045991 0.079732 6 -0.046206 -0.295242 -0.776657 6 -1.380335 1.016967 -0.643277 1 -1.930250 0.771341 -1.543015 1 -0.955838 2.007542 -0.547608 1 0.112311 -0.076139 -1.851531 6 0.899908 -0.037922 1.579254 1 1.825305 0.043928 2.151725	**Frequencies (cm^{-1}):** -415.1607, 47.0558, 111.4634, 192.4328, 221.2597, 246.8507, 256.4116, 279.7969, 290.5369, 320.2342, 361.6341, 382.5604, 427.3794, 500.7077, 550.8053, 602.5383, 658.581, 735.4148, 846.7866, 896.359, 932.0378, 944.9353, 966.8849, 988.5781, 1037.7826, 1051.0339, 1054.0568,

1 0.235332 0.762135 1.905411 1 0.427642 -0.987992 1.824760 6 1.764730 1.422710 -0.292090 1 1.140028 2.238900 0.073735 1 2.753659 1.556650 0.147982 1 1.873136 1.533382 -1.374122 6 2.239030 -1.034392 -0.293794 1 3.168691 -0.867621 0.252639 1 1.864364 -2.027242 -0.047508 1 2.469632 -1.014184 -1.361152 8 -1.946422 0.610029 0.489598 8 -2.468335 -0.593155 0.339173 8 -0.717117 -1.348045 -0.522561	1156.0679, 1219.5508, 1223.3527, 1240.9579, 1259.8389, 1273.9136, 1328.3108, 1396.8159, 1402.3367, 1419.9622, 1452.7957, 1479.8323, 1483.743, 1487.2575, 1492.1477, 1504.6588, 1512.2248, 1520.732, 2853.5784, 3015.7191, 3021.6464, 3033.7038, 3073.935, 3079.3968, 3084.1055, 3090.4353, 3103.575, 3111.3411, 3114.6542, 3232.1718
IRC:  	

Compound: $tBuCHCH_2 + O_3$ CPr_{FO} 1	**Energy (Hartree)** -460.844648712719
Reaction Coordinates: 6 1.466008 -0.073528 -0.048353 6 0.276263 0.495922 0.705736 1 0.081865 0.015772 1.683446 8 -0.379433 1.454849 0.358900 6 1.446832 0.355815 -1.515891 1 0.581423 -0.063741 -2.029259 1 2.345717 0.001273 -2.022455 1 1.403805 1.440137 -1.609536 6 1.467590 -1.603525 0.084340 1 0.602536 -2.041086 -0.410645 1 1.445042 -1.910357 1.131655 1 2.373523 -2.014528 -0.364013 6 2.708227 0.506518 0.668196 1 2.712389 0.256167 1.730826 1 3.612878 0.087693 0.224892 1 2.748832 1.591870 0.572042 6 -2.844089 0.670853 -0.349858 1 -3.591717 1.369487 -0.000054 1 -2.215221 0.825930 -1.214791 8 -2.742582 -0.380363 0.318179 8 -1.781243 -1.283355 -0.046720	**Frequencies (cm^{-1}):** 23.6945, 42.1485, 64.5446, 85.2077, 123.4399, 175.5768, 202.7348, 210.7067, 246.5091, 252.9231, 277.4417, 329.0533, 352.9024, 387.4666, 408.2708, 523.3427, 592.3784, 676.3936, 762.754, 878.7673, 885.5079, 926.9349, 950.8518, 962.2543, 969.7092, 991.9368, 1057.1577, 1066.5102, 1221.2595, 1240.1147, 1240.6531, 1290.0316, 1394.4655, 1401.0826, 1412.4319, 1415.6833, 1436.1343, 1478.7043, 1488.8281, 1490.3426, 1499.859, 1505.1063, 1521.6685, 1566.3558, 1752.8124, 2908.2859, 3021.1246, 3027.0042, 3033.9386, 3081.0367, 3084.9192, 3092.1511, 3094.6096, 3105.9819, 3113.9051, 3132.0401, 3276.994

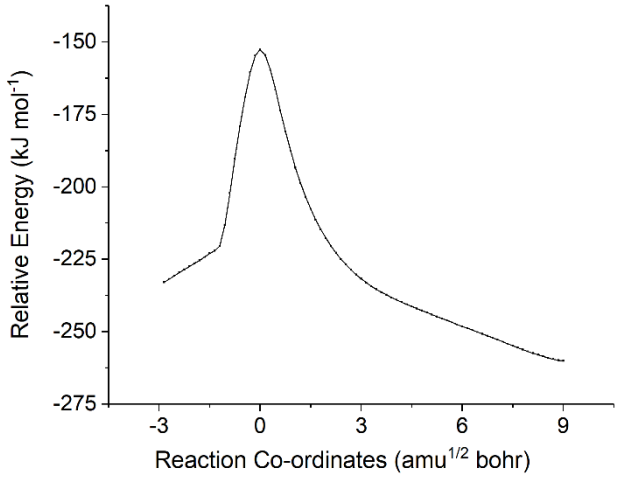
Compound: $tBuCHCH_2 + O_3$ TS_{FO} 2	**Energy (Hartree)** -460.804325711020
Reaction Coordinates: 6 -1.281058 0.040659 0.046612 6 0.096344 -0.236835 -0.634762 6 1.274441 1.103341 -0.003805 1 0.976684 1.085070 1.036260 1 1.151053 2.016732 -0.570950 1 0.102393 0.070453 -1.697524 6 -2.260595 -0.909933 -0.673528 1 -3.272978 -0.764894 -0.292593 1 -2.277468 -0.722742 -1.748965 1 -1.974269 -1.949105 -0.515507 6 -1.731664 1.487092 -0.188276 1 -1.664243 1.758208 -1.244585 1 -2.772893 1.610805 0.112451 1 -1.145971 2.205736 0.387262 6 -1.252942 -0.300436 1.538141 1 -2.264721 -0.272710 1.945449 1 -0.842027 -1.295580 1.698167 1 -0.656529 0.406713 2.117513 8 2.428087 0.511911 -0.274101 8 2.547471 -0.610513 0.409942 8 0.721169 -1.307900 -0.352499	**Frequencies (cm^{-1}):** -428.0647, 75.3955, 79.608, 193.1875, 205.3238, 251.616, 257.8282, 287.8297, 291.2593, 316.8282, 364.852, 380.5214, 448.9984, 474.8079, 548.2433, 589.1872, 599.8295, 747.6811, 848.583, 897.2119, 932.4715, 944.4808, 967.5839, 983.9385, 1033.7093, 1045.8249, 1064.5262, 1153.4286, 1219.2475, 1234.0057, 1240.9096, 1252.7717, 1269.8245, 1356.1125, 1398.0518, 1402.781, 1421.6824, 1453.4631, 1478.1369, 1484.706, 1489.3613, 1491.3458, 1505.7067, 1512.2151, 1518.9386, 2875.7615, 3017.7196, 3022.5193, 3030.7187, 3075.9134, 3078.3586, 3080.7929, 3085.3566, 3103.6193, 3114.6758, 3115.3432, 3276.994
IRC  	

Compound: $tBuCHCH_2 + O_3$ CPr_{FO} 2	**Energy (Hartree)** -460.840586382727
Reaction Coordinates: 6 2.005352 0.212990 0.012082 6 1.430106 -1.176427 -0.177979 1 2.185193 -1.948984 -0.434167 8 0.268313 -1.487847 -0.076311 6 2.701963 0.593459 -1.310145 1 3.205542 1.554099 -1.196390 1 3.453408 -0.144941 -1.595734 1 1.983597 0.682912 -2.125793	**Frequencies (cm^{-1}):** 11.396, 15.5758, 30.163, 48.5833, 67.9821, 98.3662, 102.6532, 200.7514, 245.4581, 249.6845, 275.5111, 322.7194, 347.8046, 387.2013, 400.3139, 533.3561, 595.4158, 713.2967, 763.0783, 880.0023, 901.0339, 925.1852, 949.9415, 963.6473, 967.9614, 999.6208, 1056.6407,

6 3.056302 0.112757 1.136165 1 3.815000 -0.639198 0.911696 1 3.562457 1.071708 1.252621 1 2.593602 -0.143204 2.090031 6 0.915532 1.223205 0.368666 1 1.351854 2.213479 0.503560 1 0.162642 1.288925 -0.416086 1 0.407981 0.947513 1.292635 6 -2.935821 -0.836935 0.076434 1 -3.733822 -1.563266 0.180982 1 -1.876275 -1.059617 0.060770 8 -3.238879 0.373842 -0.038906 8 -4.548406 0.734790 -0.029216	1072.8871, 1225.0375, 1234.1683, 1250.6413, 1294.5485, 1396.9002, 1402.8015, 1411.0335, 1414.6575, 1437.8096, 1480.4426, 1487.8731, 1488.9687, 1500.7793, 1506.9716, 1520.3942, 1553.0467, 1785.6276, 2871.0095, 3023.2964, 3026.3714, 3038.2247, 3086.1542, 3089.2872, 3094.0904, 3094.9936, 3099.1029, 3101.0861, 3106.6603, 3251.5731

Compound: $tBuCHCH_2 + O_3$ TS_{SYN}	**Energy (Hartree)** -460.803227474852
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.077889 -0.070118 0.057406 6 0.145941 0.080572 -0.859902 6 1.463167 -1.214706 -0.439821 1 0.735763 -2.010831 -0.219555 1 1.958812 -1.309768 -1.416219 1 -0.085491 -0.047677 -1.915238 6 -1.970511 -1.157147 -0.566009 1 -1.484363 -2.133849 -0.562467 1 -2.890984 -1.248827 0.010172 1 -2.244491 -0.916546 -1.594863 6 -1.816074 1.287791 -0.003445 1 -2.747169 1.214236 0.559323 1 -2.063448 1.565984 -1.029040 1 -1.215236 2.082065 0.435859 6 -0.792636 -0.424778 1.524041 1 -0.278966 -1.379696 1.620562 1 -0.182397 0.331306 2.006747 1 -1.743965 -0.503917 2.052954 8 2.113478 -0.719334 0.530386 8 1.459820 1.275960 0.458328 8 0.992945 1.111853 -0.766446	-425.4144, 64.6248, 159.5897, 196.802, 217.8585, 246.8033, 262.3699, 263.6354, 290.013, 327.4105, 362.1603, 401.2858, 412.0539, 448.2173, 530.1381, 575.555, 666.662, 802.7782, 858.9804, 885.9071, 935.2734, 936.3068, 964.9808, 973.0021, 1038.6298, 1063.5455, 1080.85, 1155.7967, 1215.7806, 1224.1488, 1225.3731, 1241.812, 1266.0181, 1385.7089, 1399.9014, 1408.858, 1418.4304, 1446.0029, 1480.6968, 1487.578, 1489.5069, 1502.4986, 1507.8014, 1519.9426, 1545.8924, 2920.2693, 2979.9551, 3024.785, 3030.8529, 3041.511, 3084.3356, 3090.8071, 3096.538, 3102.3258, 3111.1659, 3114.6553, 3150.7715

IRC

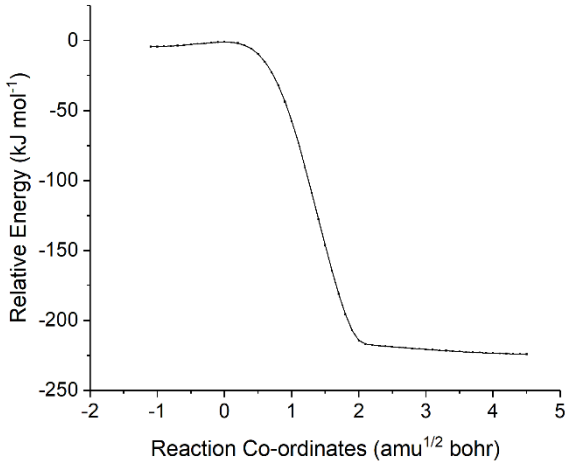


Compound: $tBuCHCH_2 + O_3$ CPr_{SYN}	**Energy (Hartree)** -460.840483767952
Reaction Coordinates: 6 1.351542 0.204034 0.043843 6 0.418919 -0.304587 -1.007634 1 0.569428 -0.056402 -2.054980 8 -0.568410 -1.070800 -0.872154 8 -0.954270 -1.494987 0.381025 6 2.373664 1.117694 -0.653897 1 1.888934 1.984614 -1.105621 1 3.097778 1.481800 0.073989 1 2.922859 0.586008 -1.433190 6 2.074160 -1.007135 0.682417 1 2.752675 -0.638246 1.452626 1 2.665748 -1.549810 -0.055994 1 1.359968 -1.689332 1.135669 6 0.593026 1.003221 1.126650 1 0.013982 1.815533 0.689540 1 -0.082302 0.360413 1.681476 1 1.327794 1.429691 1.811217 6 -3.009798 0.237824 0.281116 1 -3.482952 -0.590481 -0.269965 1 -2.972504 0.124529 1.377271 8 -2.586131 1.220210 -0.275996	**Frequencies (cm^{-1}):** 32.7984, 61.5297, 69.6683, 82.648, 128.3829, 179.6098, 197.3123, 215.4722, 236.5807, 245.008, 268.44, 294.5096, 313.784, 371.082, 393.3987, 397.7969, 539.7448, 662.4144, 787.8568, 862.2408, 874.5096, 922.6193, 939.7233, 949.0031, 975.612, 1048.0368, 1063.4722, 1177.9835, 1213.0975, 1232.5551, 1259.4505, 1272.4446, 1390.3855, 1396.4722, 1402.308, 1430.8369, 1474.9881, 1491.7168, 1493.6594, 1498.4805, 1508.2745, 1525.5754, 1528.888, 1564.637, 1783.9352, 2919.4713, 2979.5986, 3025.4131, 3032.5372, 3039.0573, 3085.6635, 3091.283, 3101.7293, 3105.8382, 3133.8889, 3139.0096, 3151.1234

S10.7 Ozonolysis of Methyl Vinyl Ketone (Alkene 5)

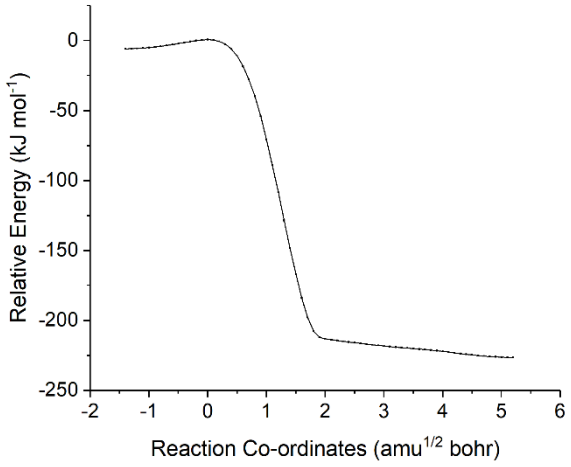
Compound: MVK + O_3 PRC1.1	**Energy (Hartree)** -456.186204464071
Reaction Coordinates: 6 -2.273787 -1.242740 0.247655 6 -1.606138 0.056432 -0.132229 6 -0.652748 0.626881 0.870014 6 0.041622 1.738571 0.622672 1 0.718606 2.162211 1.351241 1 -0.076771 2.253296 -0.321510 1 -0.553592 0.108487 1.816209 8 -1.827993 0.612675 -1.187072 1 -2.827528 -1.121718 1.181878 1 -1.518433 -2.011960 0.423356 1 -2.948578 -1.562280 -0.541270 8 2.319742 0.458297 -0.638151 8 2.367762 -0.558589 0.100102 8 1.409563 -1.375245 0.030299	**Frequencies (cm^{-1}):** 25.1652, 36.7223, 47.9539, 64.4328, 85.0549, 121.6927, 147.0794, 215.8379, 268.6036, 415.6833, 469.5476, 601.0617, 688.15, 743.2286, 775.8423, 959.8374, 1017.9065, 1021.0631, 1046.9848, 1084.0799, 1173.4141, 1194.4722, 1218.4815, 1325.2825, 1385.51, 1438.9693, 1464.814, 1474.0953, 1650.2706, 1764.2321, 3026.8467, 3078.3873, 3142.2081, 3143.8808, 3158.8657, 3236.7308

Compound: MVK + O_3 TS_{OZO} 1.1	**Energy (Hartree)** -456.176463083769
Reaction Coordinates: 6 -2.387645 -0.934084 0.233370 6 -1.455063 0.208841 -0.074384 6 -0.297634 0.391824 0.856578 6 0.598738 1.403158 0.664869 1 1.324943 1.660246 1.420186 1 0.445514 2.092756 -0.152282 1 -0.266929 -0.211445 1.753227 8 -1.615027 0.946886 -1.022435 1 -2.792920 -0.829673 1.242583 1 -1.837258 -1.876817 0.205661 1 -3.198787 -0.958906 -0.488492 8 2.143118 0.389185 -0.503316 8 2.037601 -0.799215 -0.018277 8 0.881191 -1.323681 -0.213908	**Frequencies (cm^{-1}):** -213.8916, 61.1693, 79.3428, 109.1123, 120.8863, 217.2586, 275.777, 336.6449, 426.9135, 445.1228, 559.8212, 602.238, 728.0088, 751.1871, 779.7145, 960.3026, 989.447, 1012.0367, 1047.4411, 1078.1309, 1083.7317, 1125.7044, 1196.8924, 1294.8229, 1387.4039, 1434.7779, 1465.6856, 1474.2813, 1565.1569, 1760.2754, 3029.5558, 3082.5417, 3144.1747, 3161.2936, 3183.7802, 3259.794
IRC:	



Compound: MVK + O_3 POZ1.1	**Energy (Hartree)** -456.263917668777
Reaction Coordinates: 6 -0.035951 0.105209 0.554340 6 -1.390499 -0.239308 -0.078842 8 -1.527315 -1.161856 -0.838353 6 -2.523306 0.677331 0.320785 1 -2.216017 1.725159 0.311114 1 -3.369917 0.529193 -0.343738 1 -2.826409 0.444475 1.344747 6 0.752804 1.185595 -0.263745 1 1.028745 2.025201 0.375819 1 0.229191 1.532983 -1.152714 8 1.896499 0.482653 -0.716978 8 2.127428 -0.434473 0.363108 8 0.817870 -1.022275 0.528469 1 -0.179736 0.457638 1.579588	**Frequencies (cm^{-1}):** 39.8319, 64.6811, 121.8034, 189.8977, 270.7646, 351.0622, 392.0579, 565.2609, 590.1198, 691.094, 726.7123, 743.5035, 802.4903, 921.9484, 944.6164, 965.3995, 989.9505, 1011.3885, 1077.248, 1090.1017, 1181.7339, 1233.4949, 1297.5734, 1351.4365, 1371.1221, 1389.3099, 1463.1151, 1475.8535, 1504.5401, 1807.0867, 3019.1587, 3028.4968, 3044.3941, 3079.2975, 3111.176, 3142.0824

Compound: MVK + O_3 PRC1.2	**Energy (Hartree)** -456.185692055393
Reaction Coordinates: 6 -1.768361 0.036796 -1.411546 6 -1.681642 -0.171711 0.083263 6 -0.804362 0.714471 0.894428 6 -0.114090 1.755807 0.427646 1 0.483356 2.373488 1.084577 1 -0.129655 2.036837 -0.616063 1 -0.784401 0.460127 1.947507 8 -2.315808 -1.046687 0.639997 1 -0.783363 -0.060808 -1.870142 1 -2.140734 1.036440 -1.642461 1 -2.441777 -0.703923 -1.833106 8 2.416744 0.469248 -0.606318 8 2.421691 -0.495439 0.202843 8 1.478286 -1.321415 0.134345	**Frequencies (cm^{-1}):** 13.8291, 37.3665, 39.2477, 54.8898, 69.1285, 122.3891, 147.4387, 182.7936, 277.7078, 439.5153, 492.2799, 536.6631, 699.9927, 746.0101, 760.1504, 946.7037, 999.3233, 1036.6146, 1051.9076, 1075.5961, 1180.009, 1229.3615, 1268.5212, 1309.8637, 1390.1629, 1447.6621, 1473.5714, 1479.3107, 1666.3367, 1742.7163, 3037.2747, 3092.84, 3142.0878, 3146.1354, 3164.5181, 3228.9736

Compound: MVK + O_3 TS_{OZO} 1.2	**Energy (Hartree)** -456.175776837179
Reaction Coordinates: 6 -1.683259 0.752385 -1.148698 6 -1.524203 -0.078889 0.100801 6 -0.312699 0.120778 0.948818 6 0.489210 1.230402 0.901369 1 1.193767 1.433839 1.693466 1 0.286139 2.039912 0.217758 1 -0.223990 -0.584943 1.763210 8 -2.348474 -0.901566 0.440423 1 -0.779529 0.713055 -1.757325 1 -1.862604 1.797958 -0.888416 1 -2.532403 0.381308 -1.715324 8 2.090443 0.578254 -0.421748 8 2.075054 -0.681791 -0.136095 8 0.946018 -1.236045 -0.398468	**Frequencies (cm^{-1}):** -239.7593, 68.4941, 75.2044, 116.3488, 130.2459, 224.2828, 274.6178, 340.3414, 443.9796, 499.1452, 535.892, 556.2633, 732.935, 755.1696, 763.2777, 945.8152, 981.5062, 1013.1847, 1047.4781, 1072.5014, 1077.995, 1122.6638, 1260.3178, 1282.465, 1390.5992, 1430.1312, 1470.6713, 1478.9834, 1566.142, 1750.676, 3035.2025, 3093.5565, 3144.24, 3166.099, 3189.4041, 3255.4817
IRC:  	

Compound: MVK + O_3 POZ1.2	**Energy (Hartree)** -456.270363446280
Reaction Coordinates: 6 -0.031285 0.358251 0.629461 6 -1.439074 0.079243 0.091395 8 -2.286821 0.923778 0.261559 6 -1.676303 -1.203757 -0.652864 1 -1.553361 -2.050217 0.025314 1 -2.678520 -1.201431 -1.071960 1 -0.928591 -1.335010 -1.437115 6 0.833086 1.162575 -0.392286 1 1.355483 1.976828 0.109527 1 0.270625 1.534856 -1.245619 8 1.744399 0.192246 -0.879231 8 2.035349 -0.541726 0.310211 8 0.698954 -0.850860 0.807377 1 -0.119236 0.909595 1.566286	**Frequencies (cm^{-1}):** 39.6444, 62.7843, 157.772, 203.0661, 259.2476, 395.745, 434.2236, 503.8204, 576.6346, 691.8455, 721.1429, 752.237, 770.8312, 917.0796, 939.2981, 973.6672, 988.9329, 1019.4325, 1051.0396, 1086.3571, 1221.5249, 1249.9633, 1277.1828, 1335.4559, 1353.1419, 1393.3151, 1457.525, 1465.6717, 1503.6053, 1783.9411, 3037.9601, 3053.8701, 3067.2296, 3090.0128, 3127.7285, 3145.6386

Compound: MVK + O_3 PRC 2.1	**Energy (Hartree)** -456.184296396009
Reaction Coordinates: 6 -2.510543 -0.844354 0.361809 6 -1.444574 0.043806 -0.231075 6 -0.671913 0.886659 0.729186 6 0.144838 1.855228 0.308677 1 0.696623 2.473113 1.002305 1 0.254157 2.055876 -0.748848 1 -0.813838 0.702348 1.786848 8 -1.214411 0.070406 -1.423669 1 -3.224682 -0.248693 0.934962 1 -2.055280 -1.551810 1.058946 1 -3.027598 -1.386605 -0.424643 8 2.442947 0.288365 -0.268933 8 1.838443 -0.812408 -0.346211 8 1.315993 -1.257896 0.711170	**Frequencies (cm^{-1}):** 28.5327, 47.0216, 54.3142, 62.5386, 94.0142, 120.6781, 162.2295, 244.4381, 270.1362, 411.7715, 477.3651, 602.5921, 690.6836, 747.1234, 780.215, 960.6413, 1015.0252, 1022.7784, 1046.3593, 1087.121, 1170.2996, 1197.2171, 1216.979, 1324.0682, 1386.2987, 1440.2796, 1464.4503, 1474.0336, 1646.1735, 1755.8299, 3027.2917, 3078.6339, 3142.2433, 3147.3774, 3164.6844, 3240.3602

Compound: MVK + O_3 TS_{OZO} 2.1	**Energy (Hartree)** -456.179368879638
Reaction Coordinates: 6 2.527927 -0.565261 -0.351627 6 1.339788 0.186823 0.190265 6 0.331211 0.659887 -0.800352 6 -0.639299 1.541955 -0.428553 1 -1.293580 1.989541 -1.159882 1 -0.635116 1.948518 0.572338 1 0.452132 0.381444 -1.837530 8 1.181462 0.396852 1.376498 1 3.064351 0.047907 -1.079365 1 2.189479 -1.462207 -0.874455 1 3.195318 -0.842919 0.459125 8 -2.264033 0.167262 0.195920 8 -1.560736 -0.869788 0.480517 8 -0.897986 -1.319665 -0.520264	**Frequencies (cm^{-1}):** -192.9949, 65.8813, 84.2054, 109.0036, 120.1139, 203.9969, 280.0962, 324.2855, 432.5692, 454.4184, 561.5867, 605.2774, 735.4113, 748.2964, 786.3104, 961.3039, 990.8427, 1011.2114, 1047.5052, 1081.9072, 1088.7532, 1131.49, 1202.0299, 1293.8501, 1387.2427, 1432.7407, 1465.2213, 1475.0606, 1568.3899, 1746.8556, 3030.0093, 3083.0507, 3143.437, 3162.745, 3188.5901, 3261.8399

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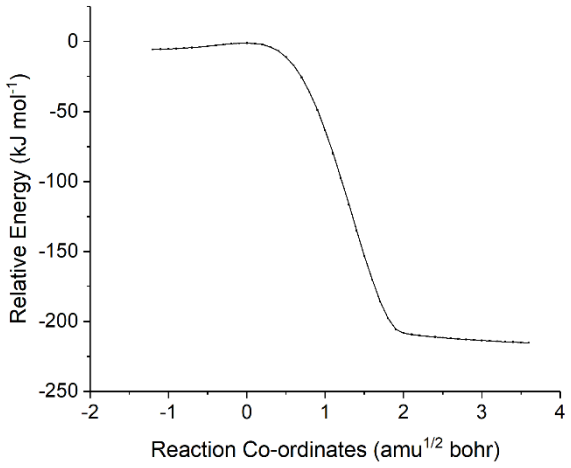


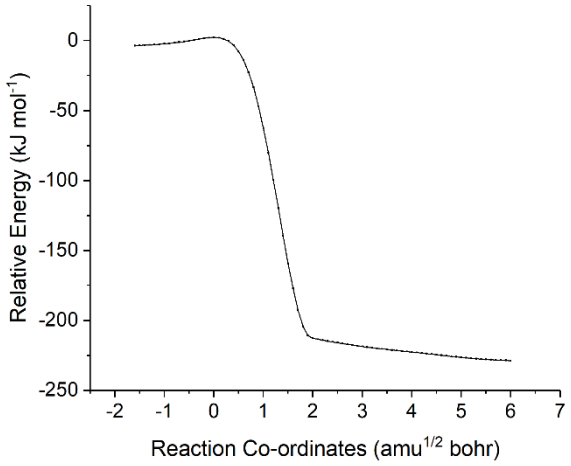
Compound: MVK + O_3 POZ 2.1	**Energy (Hartree)** -456.265703924772
Reaction Coordinates: 6 -0.035242 0.173014 0.623559 6 -1.355177 -0.250626 -0.039235 8 -1.477161 -1.314060 -0.587657 6 -2.473979 0.761864 0.060758 1 -2.132344 1.765046 -0.203161 1 -3.296286 0.468816 -0.585971 1 -2.828279 0.807665 1.093683 6 0.751479 1.197577 -0.257803 1 0.822766 2.186513 0.189161 1 0.330793 1.256701 -1.263909 8 2.060857 0.659753 -0.289564 8 1.786438 -0.748815 -0.319917 8 0.881561 -0.890936 0.800614 1 -0.232699 0.576760 1.618703	**Frequencies (cm^{-1}):** 52.8009, 80.8099, 103.7238, 196.4219, 274.3911, 345.5381, 416.1223, 569.7839, 598.237, 667.9194, 713.6482, 760.1832, 809.3153, 915.5681, 944.5131, 949.5872, 984.8064, 1009.3554, 1064.4978, 1102.975, 1183.7054, 1235.1508, 1264.5745, 1350.1193, 1368.1806, 1387.8929, 1462.8419, 1476.727, 1502.2969, 1810.0178, 3026.8142, 3034.1231, 3053.519, 3078.8035, 3120.8821, 3141.2057

Compound: MVK + O_3 PRC 2.2	**Energy (Hartree)** -456.187382728015
Reaction Coordinates: 6 2.425476 1.005867 0.680379 6 1.932136 -0.295615 0.085829 6 0.840730 -0.272955 -0.921717 6 0.213240 0.819267 -1.355136 1 -0.577141 0.757639 -2.089935 1 0.462587 1.808675 -0.996085 1 0.575191 -1.253132 -1.299348 8 2.414006 -1.362098 0.417422 1 1.615582 1.535755 1.184439 1 2.810794 1.665641 -0.098788 1 3.215332 0.790513 1.394237 8 -2.414953 0.999763 0.495639 8 -2.512945 -0.232768 0.720966 8 -2.557588 -1.010456 -0.262858	**Frequencies (cm^{-1}):** 9.797, 16.8509, 25.4758, 44.4003, 54.9495, 115.0277, 126.6031, 134.7706, 278.9148, 438.2648, 492.3555, 537.7589, 701.4315, 746.4181, 760.2428, 946.3918, 1002.6917, 1041.5976, 1051.5711, 1074.9138, 1186.1202, 1240.3115, 1269.8393, 1310.5861, 1390.6799, 1448.7888, 1473.2662, 1479.277, 1673.9462, 1738.7122, 3036.8061, 3090.947, 3141.8085, 3147.7784, 3165.2429, 3230.0541

Compound: MVK + O_3 TS_{OZO} 2.2	**Energy (Hartree)** -456.175406279816
Reaction Coordinates: 6 1.519955 0.061624 1.424156 6 1.496447 0.001629 -0.086230 6 0.345567 0.604978 -0.816453 6 -0.505193 1.537388 -0.290670 1 -1.151260 2.112205 -0.935650 1 -0.413137 1.877649 0.729823 1 0.349622 0.415394 -1.880480 8 2.397442 -0.504411 -0.722426 1 0.579539 -0.285034 1.854822 1 1.674020 1.089708 1.759013 1 2.338716 -0.552274 1.788273 8 -2.273724 0.310659 0.238019 8 -1.668686 -0.806032 0.458157	**Frequencies (cm^{-1}):** -218.8368, 77.9261, 80.3525, 112.5567, 123.3632, 207.2237, 279.5787, 331.2025, 438.7483, 502.2717, 533.7703, 558.2824, 739.3775, 744.4426, 759.1417, 945.1165, 984.0621, 1013.1188, 1046.2286, 1075.6671, 1084.0607, 1123.9207, 1259.9483, 1284.8398, 1393.1264, 1428.8224, 1469.4788, 1479.8746, 1570.963, 1746.9756, 3034.3912, 3088.9007, 3142.9581, 3165.9298, 3193.8383, 3255.4499

8 -1.019801 -1.236637 -0.561327	

IRC:

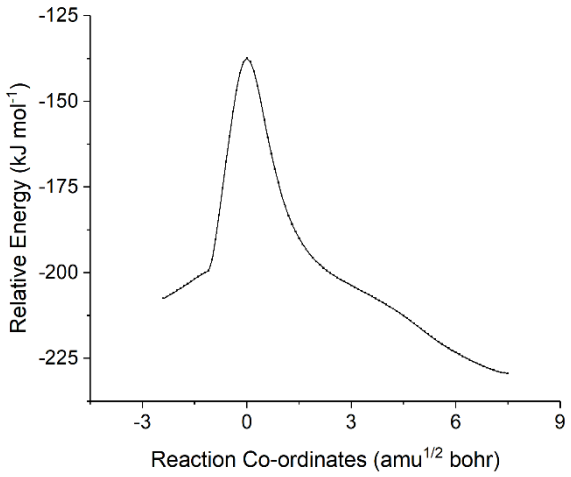


Compound: MVK + O_3 POZ 2.2	**Energy (Hartree)** -456.271438670647
Reaction Coordinates: 6 0.004679 0.255744 0.682591 6 -1.386097 0.202221 0.037909 8 -1.973784 1.247021 -0.122354 6 -1.948706 -1.138616 -0.336073 1 -1.988150 -1.788880 0.539857 1 -2.941407 -1.011921 -0.758501 1 -1.289894 -1.632256 -1.052805 6 0.977789 1.183280 -0.106377 1 1.332609 2.029213 0.476566 1 0.521645 1.524366 -1.035317 8 2.105492 0.349740 -0.348915 8 1.503661 -0.947277 -0.460654 8 0.689115 -0.989517 0.737658 1 -0.116669 0.583968 1.716020	**Frequencies (cm^{-1}):** 34.5265, 79.0622, 153.5949, 209.6666, 275.4099, 375.1588, 452.7262, 517.9064, 587.9968, 676.0139, 717.0244, 761.6569, 787.437, 915.128, 935.5392, 978.1459, 994.8769, 1008.856, 1040.2699, 1103.1051, 1213.7379, 1225.4835, 1262.8074, 1326.3301, 1350.5372, 1390.8592, 1457.7724, 1467.1364, 1513.2989, 1781.1544, 3037.6102, 3062.8456, 3069.4897, 3090.0735, 3132.4128, 3146.0905

Compound: MVK + O_3 TS_{ANTI} 1	**Energy (Hartree)** -456.232838272659
Reaction Coordinates: 6 -2.458428 0.667027 -0.670521 6 -1.455944 -0.164573 0.088034 6 -0.040128 -0.092384 -0.424514 6 0.950213 1.220919 0.520934 1 0.499447 2.082061 0.004250 1 0.592293 1.051275 1.544311 1 0.145060 0.272464 -1.429105 8 -1.732988 -0.836843 1.050963 1 -3.404250 0.676437 -0.136674 1 -2.097605 1.687993 -0.809695 1 -2.607463 0.242763 -1.666559 8 2.153822 0.930557 0.228631	**Frequencies (cm^{-1}):** -449.43, 48.0396, 108.4031, 135.0767, 156.1429, 211.2839, 301.2834, 381.1411, 439.5015, 516.3249, 570.4161, 593.8925, 621.5032, 852.6618, 928.2131, 963.8644, 1015.0169, 1035.4144, 1122.2323, 1144.733, 1193.2912, 1219.5422, 1247.5718, 1373.9191, 1386.2511, 1403.7405, 1463.5923, 1472.9588, 1538.14, 1781.3333, 2925.3479, 3004.7894, 3029.8908, 3082.2954, 3140.8823, 3146.3752

8 1.954555 -0.949425 -0.536329 8 0.736890 -1.119154 -0.067029	

IRC:

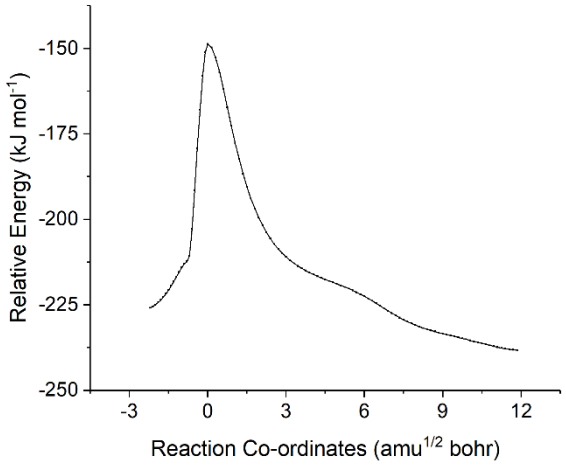


Compound: MVK + O_3 C_{ANTI} 1	**Energy (Hartree)** -456.267801791220
Reaction Coordinates: 6 -2.313645 1.148745 -0.444768 6 -1.629663 -0.092598 0.056606 6 -0.264681 -0.323729 -0.523253 1 0.131893 0.226325 -1.366285 8 0.455298 -1.211056 0.004113 8 1.721768 -1.342938 -0.461588 8 -2.099222 -0.859251 0.862592 1 -3.283615 1.250495 0.032610 1 -1.695079 2.023352 -0.231145 1 -2.437857 1.101040 -1.529471 6 2.453150 0.869761 0.348764 1 2.788378 0.357529 1.262191 1 3.149346 0.852082 -0.502392 8 1.406652 1.485257 0.308683	**Frequencies (cm^{-1}):** 45.7147, 61.8857, 76.731, 117.3614, 125.4511, 195.9322, 238.7194, 257.1303, 289.2984, 375.6091, 410.0717, 466.1412, 566.7143, 617.4489, 894.6049, 905.2813, 936.3848, 1028.7522, 1049.4599, 1170.7255, 1196.8241, 1257.836, 1364.7633, 1393.0743, 1463.0653, 1469.3671, 1509.0535, 1524.0342, 1737.9055, 1772.8094, 2943.3546, 3011.6883, 3028.1983, 3081.0098, 3149.6295, 3193.5725

Compound: MVK + O_3 TS_{ANTI} 2	**Energy (Hartree)** -456.236589638640
Reaction Coordinates: 6 -2.057532 -0.868478 0.786278 6 -1.476243 0.134125 -0.172302 6 -0.021452 0.024332 -0.530276 6 1.010622 1.196305 0.539354 1 0.752409 2.094704 -0.037022 1 0.505212 1.110168 1.511416 1 0.280837 0.409170 -1.497265 8 -2.105202 1.047011 -0.657506 1 -3.092236 -0.609192 0.990469 1 -2.002589 -1.871275 0.358266 1 -1.484191 -0.893049 1.714253	**Frequencies (cm^{-1}):** -454.4496, 66.3455, 113.74, 126.7112, 155.9432, 206.879, 315.6977, 408.9368, 459.1389, 526.205, 545.709, 590.9745, 608.6009, 830.2059, 882.2389, 1011.3585, 1015.3091, 1040.9621, 1119.7995, 1155.8763, 1214.9454, 1232.7255, 1260.9556, 1359.6662, 1369.2914, 1397.2725, 1461.5483, 1470.043, 1542.254, 1769.1678, 2935.0892,

8 2.190147 0.727559 0.425238 8 1.866597 -1.066757 -0.467415 8 0.586982 -1.102592 -0.147623	3003.5502, 3039.3273, 3092.9248, 3148.778, 3157.962

IRC:

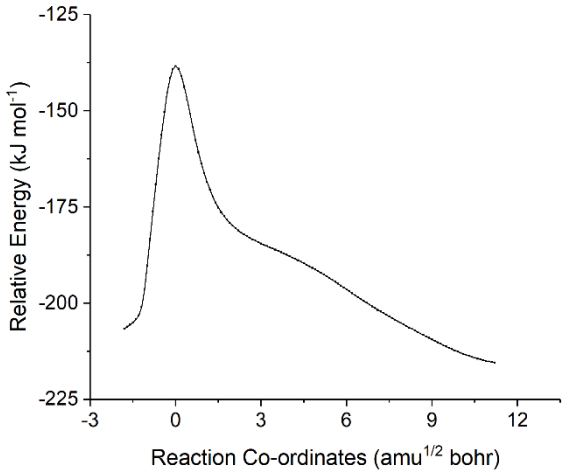


Compound: MVK + O_3 C_{ANTI} 2	**Energy (Hartree)** -456.269159459781
Reaction Coordinates: 6 -0.095987 1.744241 1.034569 6 0.046603 1.027027 -0.277427 6 -0.891099 -0.070254 -0.593223 1 -0.807241 -0.654813 -1.501844 8 -1.829189 -0.321468 0.213992 8 -2.696457 -1.307620 -0.068713 8 0.887748 1.298684 -1.114904 1 0.639166 2.542132 1.085788 1 -1.100829 2.154887 1.142120 1 0.054760 1.043937 1.857150 6 2.688557 -1.094402 -0.023073 1 2.759318 -0.302587 -0.788526 1 3.577636 -1.732129 0.124772 8 1.686490 -1.255983 0.624058	**Frequencies (cm^{-1}):** 31.8563, 54.4678, 65.0592, 92.0449, 99.277, 152.6856, 165.1055, 168.7825, 191.0045, 227.4592, 399.4823, 501.0133, 559.9164, 572.1996, 834.7722, 916.1473, 1008.3183, 1028.9119, 1049.1463, 1212.0972, 1248.4071, 1267.9762, 1344.9359, 1399.4626, 1463.5812, 1472.3116, 1493.5808, 1523.9992, 1729.5467, 1797.6411, 2905.0197, 2977.0259, 3043.8875, 3100.6183, 3147.7651, 3182.2422

Compound: MVK + O_3 TS_{FO} 1.1	**Energy (Hartree)** -456.233801783071
Reaction Coordinates: 6 -2.629214 0.312303 0.428051 6 -1.343745 -0.109337 -0.245885 6 -0.179214 -0.431588 0.718856 6 0.914085 1.169718 0.479058 1 0.326442 2.033673 0.195555 1 1.366901 1.124219 1.460933 1 -0.405375 -0.265321 1.786257 8 -1.217153 -0.214423 -1.436327 1 -3.358436 0.612078 -0.319201 1 -3.026330 -0.521053 1.012488	**Frequencies (cm^{-1}):** -392.7443, 51.2519, 88.9853, 122.2145, 160.5978, 260.383, 294.056, 362.806, 478.4695, 512.9117, 585.4505, 619.9948, 655.6298, 777.028, 888.3772, 944.2673, 968.7236, 1025.7637, 1051.8813, 1127.388, 1169.3956, 1230.2424, 1274.0007, 1353.6089, 1383.0153, 1457.3047, 1462.4967, 1471.3267, 1485.0196, 1801.985, 2907.1447,

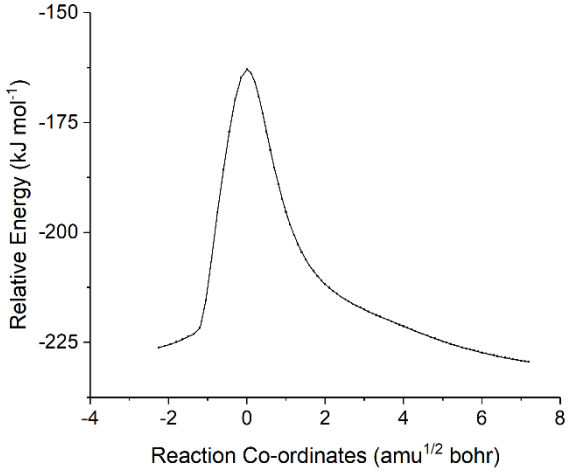
1 -2.452449 1.131210 1.129093 8 0.616726 -1.362508 0.415935 8 2.328084 -0.356360 -0.154706 8 1.644563 0.713119 -0.518102	3027.6863, 3078.4389, 3112.8737, 3142.3558, 3234.7384

IRC:



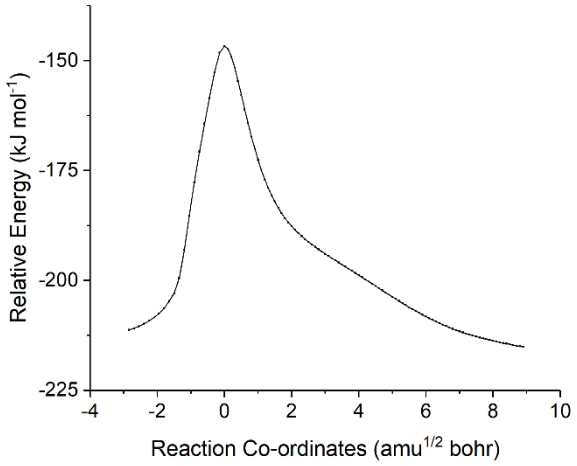
Compound: MVK + O_3 CPr_{FO} 1.1	**Energy (Hartree)** -456.261237431394
Reaction Coordinates: 6 -3.471710 -0.927226 0.000001 6 -2.075395 -0.376525 0.000000 6 -1.952762 1.172903 0.000005 1 -2.903106 1.740678 0.000017 8 -0.889620 1.726544 -0.000003 8 -1.073417 -1.044661 -0.000005 1 -3.451577 -2.012871 -0.000003 1 -4.016866 -0.565446 0.876013 1 -4.016870 -0.565438 -0.876004 6 2.040938 -0.155399 -0.000001 1 1.230484 0.560462 -0.000009 1 1.910578 -1.230673 0.000009 8 3.199967 0.319872 -0.000004 8 4.263186 -0.527908 0.000006	**Frequencies (cm^{-1}):** 12.9334, 24.298, 47.6598, 55.5461, 60.2228, 68.9387, 93.8572, 131.3223, 269.9692, 403.9261, 464.447, 527.9565, 638.8827, 704.2435, 801.0064, 880.213, 894.1198, 974.9287, 1002.235, 1076.7572, 1181.5843, 1231.1907, 1390.1438, 1399.8388, 1406.2772, 1458.9949, 1466.4791, 1549.7646, 1788.28, 1820.4789, 2907.3685, 3023.1795, 3070.8322, 3115.6541, 3148.6348, 3266.5354

Compound: MVK + O_3 TS_{FO} 1.2	**Energy (Hartree)** -456.243731375558
Reaction Coordinates: 6 1.584190 1.248293 -0.664278 6 1.422135 -0.068875 0.036400 6 0.153060 -0.260498 0.881494 6 -0.987986 -1.213735 -0.309987 1 -0.409060 -1.842610 -0.974512 1 -1.606640 -1.669346 0.452403 1 0.254268 -1.100657 1.589124 8 2.230454 -0.967500 0.002510 1 2.487109 1.238048 -1.267901	**Frequencies (cm^{-1}):** -399.1707, 58.541, 96.225, 115.3489, 165.4963, 248.2229, 300.9156, 431.8369, 475.537, 516.3623, 577.3178, 602.245, 638.934, 757.5777, 898.9444, 954.5515, 1007.2087, 1024.4438, 1050.7534, 1149.9669, 1214.1893, 1225.073, 1273.2002, 1301.795, 1390.4748, 1445.8418, 1460.4305, 1463.7953,

1 0.709396 1.463191 -1.279862 1 1.631960 2.046425 0.078654 8 -0.545370 0.745167 1.210764 8 -2.180950 0.593623 -0.070399 8 -1.516062 -0.167061 -0.925336	1486.2758, 1776.3068, 2926.6784, 3041.8535, 3094.4734, 3114.4965, 3148.2134, 3236.7337
IRC:  	

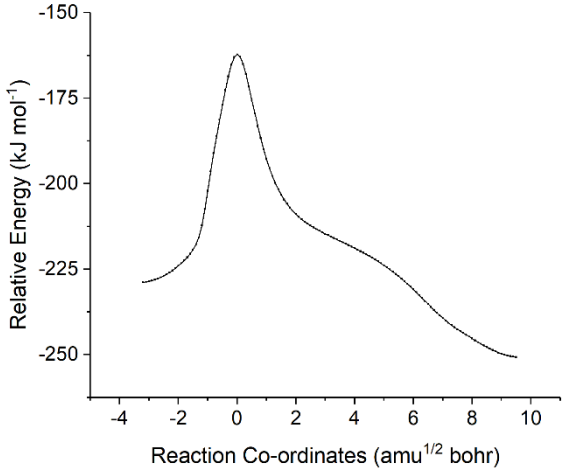
Compound: MVK + O_3 CPr_{FO} 1.2	**Energy (Hartree)** -456.275225635743
Reaction Coordinates: 6 1.190383 1.310987 1.000471 6 0.725366 0.640164 -0.255196 6 1.380465 -0.690316 -0.630040 1 0.908518 -1.182935 -1.498786 8 2.351372 -1.128176 -0.073536 8 -0.069630 1.127068 -1.041284 1 0.600458 2.204108 1.187318 1 1.126959 0.620667 1.839930 1 2.243317 1.580446 0.890716 6 -2.404595 0.015632 -0.516346 1 -3.230413 0.713732 -0.544386 1 -1.955023 -0.438451 -1.387586 8 -1.993079 -0.273829 0.628030 8 -0.919103 -1.119610 0.726724	**Frequencies (cm^{-1}):** 53.9394, 60.686, 76.1751, 104.1622, 126.9361, 177.1163, 195.0446, 226.753, 256.5464, 474.1684, 489.1827, 525.4362, 585.7249, 678.047, 785.7371, 883.2559, 922.3838, 1002.9041, 1014.9957, 1066.272, 1240.8945, 1251.3296, 1367.3749, 1392.1778, 1416.4431, 1455.3903, 1467.1276, 1566.9828, 1727.7281, 1795.1644, 2937.3654, 3041.4918, 3104.7907, 3132.6877, 3147.2852, 3278.1482

Compound: MVK + O_3 TS_{FO} 2.1	**Energy (Hartree)** -456.235933348061
Reaction Coordinates: 6 2.674078 -0.053627 0.678362 6 1.457783 0.056468 -0.207402 6 0.151656 -0.497014 0.446727 6 -0.917679 1.092169 0.238209 1 -0.648792 1.840918 0.973852 1 -0.671998 1.230406 -0.809083	**Frequencies (cm^{-1}):** -373.8862, 47.9332, 104.9092, 128.5647, 192.7982, 262.3019, 292.3149, 329.2256, 469.2277, 508.4486, 578.1971, 590.179, 635.4187, 781.1971, 893.6734, 942.9455, 994.9344, 1033.9196, 1051.5928, 1128.5684, 1164.1758, 1235.6424,

1 0.201937 -0.583732 1.546082 8 1.480277 0.482159 -1.330164 1 2.500351 0.452882 1.630100 1 2.863169 -1.103960 0.910439 1 3.536950 0.375404 0.176888 8 -2.074599 0.524168 0.509964 8 -2.400842 -0.375867 -0.402107 8 -0.501916 -1.355447 -0.198148	1265.8626, 1374.3464, 1381.9386, 1461.7703, 1462.263, 1468.5781, 1484.837, 1799.9629, 2909.0047, 3031.5805, 3084.6314, 3090.8587, 3144.0005, 3223.9552
IRC:  	

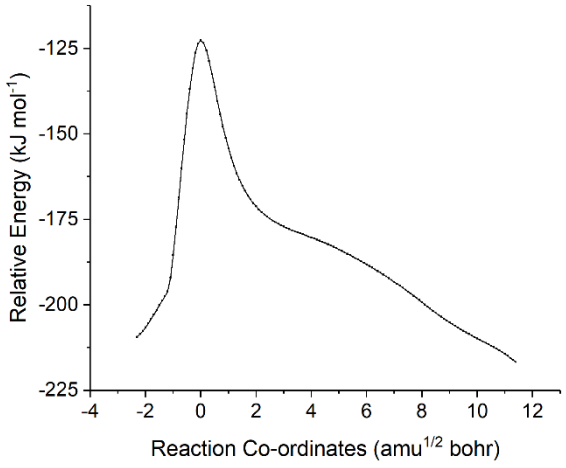
Compound: MVK + O_3 CPr_{FO} 2.1	**Energy (Hartree)** -456.271731817866
Reaction Coordinates: 6 -1.721235 -1.482475 0.092313 6 -0.929117 -0.287327 -0.357640 6 -1.075631 0.996973 0.475093 1 -1.536612 0.867110 1.470286 8 -0.736911 2.076456 0.065379 8 -0.277558 -0.266802 -1.388274 1 -1.704627 -1.587203 1.175181 1 -2.762377 -1.345382 -0.216645 1 -1.336323 -2.383464 -0.377532 6 1.954812 0.275095 -0.574796 1 2.646569 0.050486 -1.376199 1 1.437029 1.218110 -0.468830 8 1.845731 -0.623968 0.289823 8 0.904160 -0.414842 1.281061	**Frequencies (cm^{-1}):** 59.3232, 94.9443, 107.7437, 127.4285, 139.6416, 188.7177, 216.2572, 286.1673, 297.1954, 407.7125, 507.3407, 529.2019, 647.9601, 704.8725, 838.4876, 871.6352, 907.7392, 991.3869, 1041.0014, 1060.635, 1192.0423, 1246.3283, 1391.2578, 1400.2652, 1423.2827, 1459.141, 1476.8179, 1569.3358, 1713.6052, 1789.1469, 2931.6461, 3023.6138, 3100.183, 3127.243, 3146.0529, 3271.4158

Compound: MVK + O_3 TS_{FO} 2.2	**Energy (Hartree)** -456.242451639511
Reaction Coordinates: 6 1.912254 1.044420 0.745859 6 1.498110 -0.141046 -0.078343 6 0.115006 -0.058808 -0.771984 6 -0.870364 -0.972833 0.591237 1 -0.681174 -2.035210 0.506292	**Frequencies (cm^{-1}):** -382.7959, 83.3289, 93.8653, 112.8644, 168.3644, 265.3785, 275.6913, 411.6495, 474.4676, 522.5809, 573.4957, 584.1742, 591.8783, 764.769, 887.8157, 983.7593, 1001.0583, 1019.419, 1057.1311,

1 -0.521360 -0.431210 1.461742 1 0.018954 -0.798494 -1.581889 8 2.186568 -1.109132 -0.282359 1 2.206537 1.845327 0.063664 1 1.081734 1.436881 1.330714 1 2.755955 0.779525 1.377164 8 -2.067067 -0.628918 0.148927 8 -2.255744 0.676508 0.236152 8 -0.462592 1.058140 -0.862508	1138.0785, 1191.0141, 1224.6572, 1270.1325, 1335.5451, 1389.7996, 1456.5515, 1460.1777, 1466.8585, 1479.9492, 1783.6133, 2953.0055, 3042.316, 3100.474, 3109.3534, 3148.5338, 3235.1353
IRC:  	

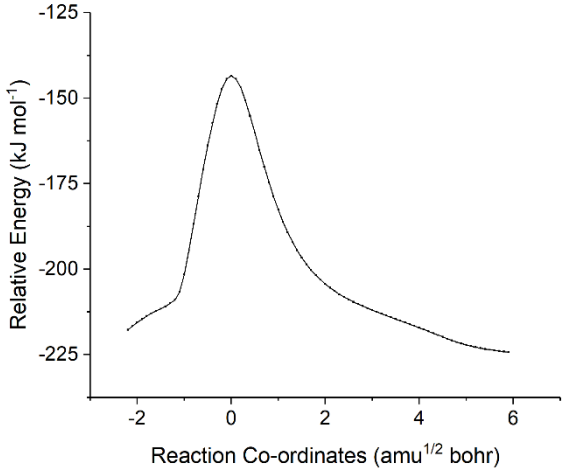
Compound: MVK + O_3 CPr_{FO} 2.2	**Energy (Hartree)** -456.275122940607
Reaction Coordinates: 6 -1.247554 1.382559 0.870913 6 -0.682153 0.606821 -0.279470 6 -1.296199 -0.761873 -0.575032 1 -0.732533 -1.343716 -1.325648 8 -2.330732 -1.136621 -0.090723 8 0.142119 1.045960 -1.068018 1 -2.275115 1.666053 0.630845 1 -1.288999 0.765117 1.766004 1 -0.658282 2.279076 1.045297 6 2.403063 0.315613 -0.142601 1 3.157830 0.343420 -0.916879 1 2.118274 1.163478 0.462928 8 1.889084 -0.806215 0.060931 8 0.876515 -0.869643 0.984635	**Frequencies (cm^{-1}):** 58.8116, 71.3915, 86.0205, 118.2147, 135.5804, 194.4754, 212.675, 255.0958, 269.9623, 472.6693, 487.2115, 527.8133, 591.9795, 685.0056, 785.8178, 889.4603, 931.3019, 1004.9923, 1015.2932, 1062.4168, 1237.3704, 1249.4216, 1367.5519, 1394.5357, 1414.4214, 1456.963, 1465.5547, 1566.407, 1711.392, 1792.1496, 2941.2295, 3040.1755, 3104.7426, 3135.8213, 3144.6956, 3280.2475

Compound: MVK + O_3 TS_{SYN} 1	**Energy (Hartree)** -456.227716334814
Reaction Coordinates: 6 2.426203 0.672562 0.099725 6 1.236581 -0.240875 -0.097325	**Frequencies (cm^{-1}):** -412.3666, 68.8092, 77.0806, 102.8744, 166.2176, 214.635,

6 0.072437 0.049665 0.831626 6 -0.936919 1.440575 -0.120451 1 -0.104140 1.863063 -0.701729 1 -1.213333 2.012960 0.776513 1 0.352374 0.421767 1.813176 8 1.235358 -1.166289 -0.863419 1 3.035772 0.669197 -0.799809 1 2.131689 1.690750 0.352528 1 3.028338 0.286787 0.926186 8 -1.838214 0.802117 -0.737073 8 -1.460716 -1.141768 -0.193520 8 -0.938993 -0.803571 0.962973	303.8893, 348.8722, 443.0383, 517.5128, 534.1209, 607.3324, 691.7491, 826.0602, 905.1487, 946.9895, 987.6442, 1033.3464, 1079.1374, 1132.2614, 1172.1207, 1218.7098, 1232.7591, 1382.7142, 1390.2723, 1432.6396, 1467.5, 1478.2829, 1549.8312, 1795.0323, 2922.0895, 2981.0897, 3034.3827, 3094.5817, 3134.144, 3143.3892
IRC  	

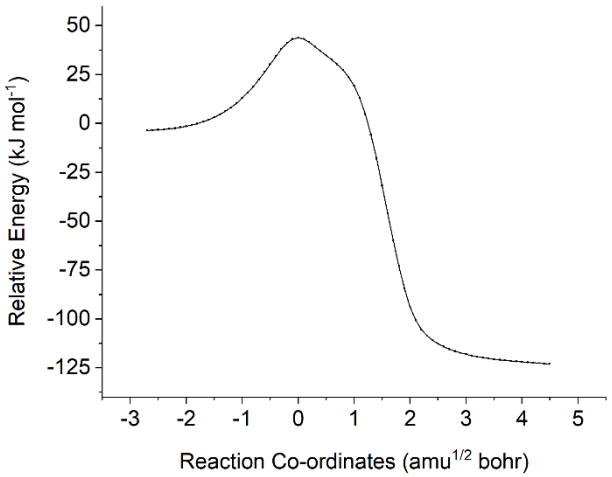
Compound: MVK + O_3 CPr_{SYN} 1	**Energy (Hartree)** -456.254760711605
Reaction Coordinates: 6 -1.425189 1.440524 0.003720 6 -1.411455 -0.061487 -0.045699 6 -0.047306 -0.778545 -0.117003 1 -0.218768 -1.851133 -0.227530 8 0.706005 -0.618752 1.092319 8 1.561684 0.522397 0.791353 8 -2.407208 -0.744557 -0.015773 1 -2.437369 1.788714 0.189564 1 -0.746691 1.803049 0.776453 1 -1.067055 1.838842 -0.947135 6 1.956056 0.184044 -0.515482 1 2.322196 1.089429 -0.996199 1 2.702501 -0.615165 -0.505658 8 0.766087 -0.254207 -1.148238	**Frequencies (cm^{-1}):** 40.8735, 94.5141, 133.6361, 197.8858, 248.6756, 366.4592, 420.9936, 534.36, 595.9659, 728.2163, 770.948, 788.7789, 866.3244, 918.818, 962.3184, 1022.4898, 1042.8244, 1050.1093, 1098.7346, 1154.3248, 1231.5943, 1251.7324, 1294.2001, 1342.3101, 1390.1755, 1390.7328, 1466.3643, 1468.781, 1519.158, 1789.2763, 3020.1158, 3042.417, 3064.6143, 3099.495, 3116.7905, 3144.441

Compound: MVK + O_3 TS_{SYN} 2	**Energy (Hartree)** -456.235446436955
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.405586 1.160045 -0.783167 6 -1.309263 -0.076261 0.057198 6 -0.038809 -0.406207 0.830238 6 1.057850 -1.298079 -0.439971 1 0.233184 -1.795317 -0.969724 1 1.620397 -1.947312 0.244549 1 -0.225806 -1.084522 1.656213 8 -2.211027 -0.873039 0.183576 1 -1.119898 2.043605 -0.212163 1 -0.700275 1.096177 -1.612281 1 -2.425033 1.250852 -1.148361 8 1.675215 -0.360806 -1.039178 8 1.262039 1.250734 0.174166 8 0.872808 0.503052 1.188434	-430.9151, 34.0089, 116.1417, 188.1295, 210.7973, 248.366, 308.054, 355.0012, 467.6908, 520.673, 532.1735, 606.878, 682.2697, 818.9488, 888.0324, 953.8825, 1023.8396, 1044.7669, 1069.8456, 1155.004, 1211.2032, 1217.5216, 1241.0192, 1365.5391, 1397.2773, 1400.6883, 1453.1952, 1463.6239, 1546.387, 1760.1253, 2935.1069, 3001.7206, 3046.3406, 3103.6425, 3145.2972, 3156.4383
IRC  	

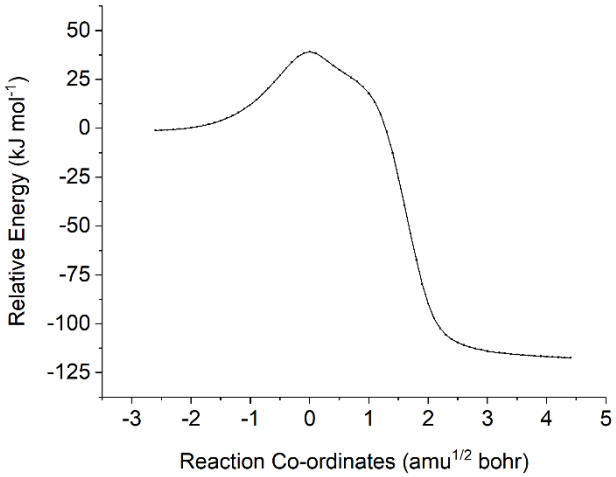
Compound: MVK + O_3 CPr_{SYN} 2	**Energy (Hartree)** -456.266282922429
Reaction Coordinates: 6 1.234499 -0.424668 1.440329 6 1.462391 -0.358324 -0.034013 6 0.700090 0.581001 -0.913190 1 0.903906 0.528467 -1.975872 8 -0.145538 1.469853 -0.616023 8 -0.537283 1.683428 0.660400 8 2.275421 -1.040122 -0.627906 1 1.894262 -1.177924 1.863317 1 1.408909 0.552141 1.892422 1 0.189221 -0.660725 1.637915 6 -2.786998 -0.693538 0.061734 1 -2.754285 0.281330 0.574482 1 -3.781454 -1.150814 -0.091184 8 -1.782657 -1.238071 -0.320251	**Frequencies (cm^{-1}):** 27.5161, 53.8334, 60.2462, 77.6675, 79.4991, 94.2378, 117.2288, 190.828, 241.7392, 324.3854, 348.1024, 498.3069, 586.7428, 667.394, 818.0278, 861.8707, 912.8046, 1041.7754, 1051.2307, 1214.8147, 1258.3245, 1269.8904, 1361.0742, 1398.4759, 1442.5145, 1455.2084, 1503.0485, 1526.4095, 1732.9327, 1793.6549, 2899.5505, 2984.8016, 3046.6356, 3105.4746, 3145.0683, 3186.8609

Compound: MVK + O_3 TS_{EPOX} 1.1	**Energy (Hartree)** -456.157741160206
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.372363 1.219189 0.145472 6 1.970434 -0.228531 -0.034048 6 0.596743 -0.558118 -0.421492 6 -0.420982 0.361131 -0.689668 1 -0.177387 1.413846 -0.727808 1 -1.228915 0.088851 -1.371390 1 0.371587 -1.616720 -0.440846 8 2.771677 -1.137223 0.129112 1 2.253593 1.775819 -0.786236 1 1.752594 1.707392 0.899753 1 3.412976 1.258793 0.453735 8 -1.314430 0.284856 0.756217 8 -2.490470 -0.371010 0.562760 8 -3.153751 0.049626 -0.451689	-363.7337, 70.6413, 76.1798, 84.4809, 124.0222, 207.0942, 284.7645, 300.9347, 423.627, 490.6217, 531.8628, 560.5861, 702.0273, 768.2866, 818.2928, 852.9195, 936.3861, 1037.872, 1048.3906, 1111.3101, 1138.6885, 1200.9445, 1261.2767, 1273.2853, 1393.6342, 1417.5546, 1469.592, 1479.968, 1530.8559, 1684.8269, 3033.0059, 3036.7886, 3086.3731, 3143.8248, 3178.9395, 3195.9407
IRC  	

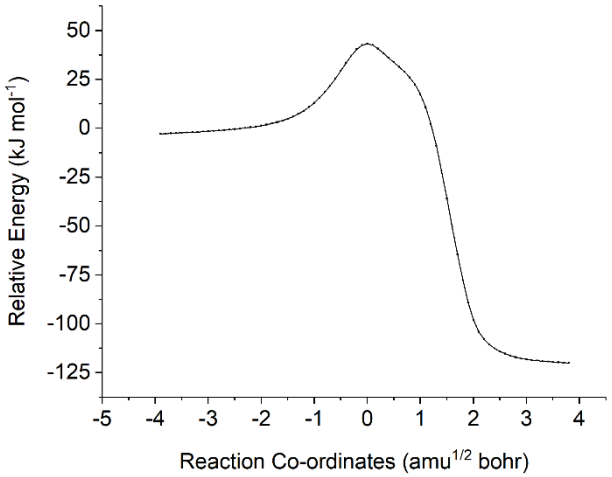
Compound: MVK + O_3 C_{EPOX} 1.1	**Energy (Hartree)** -456.237983457170
Reaction Coordinates: 6 -2.466710 -0.972373 -0.347683 6 -1.800689 0.351252 -0.078622 6 -0.307932 0.371180 0.112919 6 0.347410 -0.456722 1.139433 1 1.267840 -0.088363 1.585213 1 -0.233879 -1.132757 1.756100 1 0.162801 1.308445 -0.160892 8 -2.404177 1.398571 -0.019369 1 -2.165255 -1.729251 0.377202 1 -2.151484 -1.340928 -1.326042 1 -3.545162 -0.843779 -0.331474 8 3.219396 0.408674 0.221193 8 2.754970 0.010874 -0.826116 8 0.433894 -0.809792 -0.232756	**Frequencies (cm^{-1}):** 25.1203, 50.8199, 64.6142, 79.9012, 102.2431, 116.7645, 168.8343, 241.2261, 289.4099, 478.6073, 505.1174, 594.4314, 739.1458, 848.2764, 899.2998, 926.9053, 1010.4641, 1065.0937, 1100.3737, 1155.5005, 1163.8258, 1248.5124, 1270.2424, 1388.2352, 1393.7366, 1457.9456, 1469.3082, 1516.7315, 1554.5188, 1776.2175, 3039.7218, 3074.572, 3092.5363, 3145.6767, 3147.8589, 3168.1347

Compound: MVK + O_3 TS_{EPOX} 1.2	**Energy (Hartree)** -456.157706885861
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 3.014242 -0.928622 0.054496 6 1.918270 0.106674 -0.031066 6 0.607854 -0.349513 -0.516208 6 -0.466132 0.528120 -0.650178 1 -0.263312 1.578892 -0.493819 1 -1.266120 0.319286 -1.359043 1 0.460984 -1.404367 -0.709081 8 2.099927 1.272407 0.285261 1 2.735758 -1.709644 0.765841 1 3.159284 -1.414683 -0.912638 1 3.941363 -0.461088 0.373183 8 -1.343355 0.147453 0.785998 8 -2.471177 -0.539072 0.501250 8 -3.187064 -0.011830 -0.423346	-357.4571, 70.5253, 74.51, 83.0025, 94.6134, 212.0457, 280.3727, 288.4289, 418.7204, 430.0018, 567.1329, 600.699, 703.0029, 778.5998, 806.8366, 865.016, 960.8074, 1036.3252, 1047.0311, 1110.9736, 1137.764, 1191.1131, 1216.2221, 1266.7283, 1388.3592, 1427.8315, 1465.1762, 1474.4465, 1518.0095, 1701.9516, 3028.5546, 3065.2749, 3079.8954, 3143.4076, 3174.3138, 3203.067
IRC  	

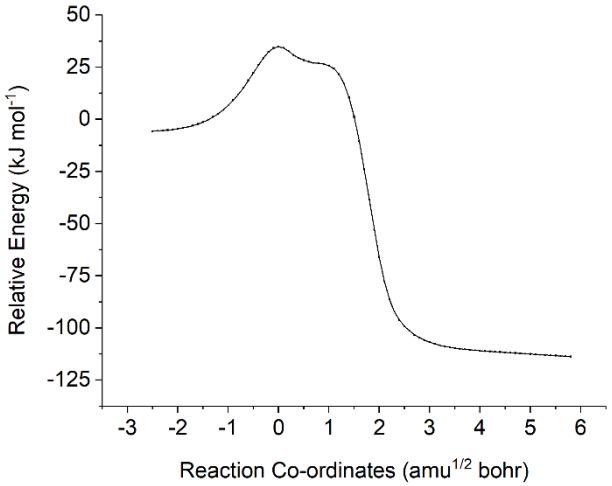
Compound: MVK + O_3 C_{EPOX} 1.2	**Energy (Hartree)** -456.234735203125
Reaction Coordinates: 6 -2.561677 1.317820 0.127750 6 -1.780184 0.042353 -0.058778 6 -0.288075 0.150714 0.162389 6 0.424578 -0.952380 0.830713 1 1.323848 -0.723407 1.399011 1 -0.135004 -1.830635 1.130949 1 0.129506 1.149012 0.236082 8 -2.290305 -1.012335 -0.349626 1 -2.270517 2.041739 -0.637536 1 -2.330747 1.770845 1.094753 1 -3.626788 1.117628 0.055544 8 3.078768 0.510274 0.431040 8 2.699711 0.412998 -0.719481 8 0.529558 -0.770465 -0.568338	**Frequencies (cm^{-1}):** 34.6389, 46.4953, 72.4901, 91.0171, 105.0959, 135.9993, 194.9677, 245.2737, 307.073, 374.7759, 592.0944, 610.8883, 761.7105, 853.6271, 894.101, 955.6863, 994.5565, 1057.3085, 1107.2086, 1160.1364, 1164.5938, 1198.2811, 1276.333, 1385.7006, 1414.6763, 1463.3374, 1473.2375, 1496.8147, 1539.317, 1790.8004, 3026.0246, 3063.0831, 3076.7372, 3133.7968, 3144.0415, 3174.4668

Compound: MVK + O_3 TS_{EPOX} 1.3	**Energy (Hartree)** -456.159268181460
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.100004 -1.472390 0.247930 6 -1.716304 -0.116765 0.008501 6 -0.911324 1.093518 0.203876 6 0.409197 1.134834 0.667464 1 0.828115 2.104743 0.896577 1 0.797971 0.344659 1.310857 1 -1.416309 2.012450 -0.064903 8 -2.883146 0.009446 -0.334982 1 -0.296647 -1.655242 -0.469522 1 -0.658196 -1.543019 1.243338 1 -1.863794 -2.236040 0.133481 8 1.288781 0.744845 -0.739246 8 1.880990 -0.475764 -0.624488 8 2.528309 -0.636368 0.471659	-367.6924, 62.9416, 83.0145, 129.5713, 164.9946, 229.5626, 263.4659, 304.0192, 410.1843, 491.8636, 530.175, 558.7169, 700.8537, 769.7833, 817.9027, 839.9033, 947.1561, 1038.4806, 1052.7228, 1118.1603, 1122.8942, 1194.1948, 1253.3892, 1279.4904, 1396.6796, 1424.4495, 1465.1276, 1477.7338, 1525.679, 1686.1108, 3031.8076, 3050.8528, 3084.8806, 3143.4686, 3177.4848, 3196.6632
IRC  	

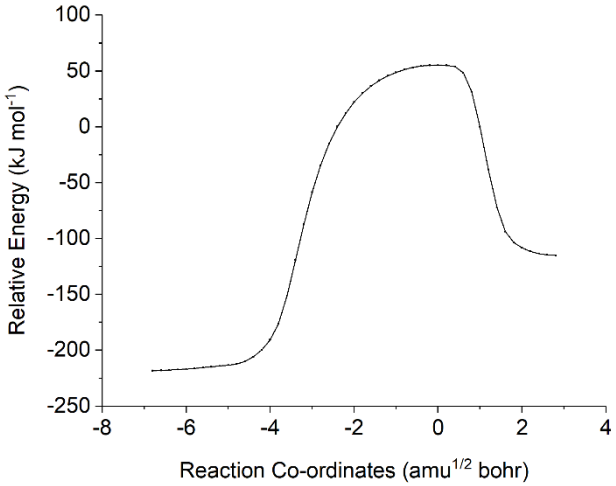
Compound: MVK + O_3 C_{EPOX} 1.3	**Energy (Hartree)** -456.239363946836
Reaction Coordinates: 6 -0.947337 -1.544387 0.430551 6 -1.740907 -0.388633 -0.119293 6 -1.035570 0.922878 -0.336345 6 -0.304729 1.588122 0.756627 1 -0.251005 2.670719 0.760772 1 -0.228975 1.107597 1.725539 1 -1.490304 1.541761 -1.101888 8 -2.914915 -0.467467 -0.405331 1 -0.206120 -1.857279 -0.307391 1 -0.389130 -1.260583 1.323270 1 -1.618949 -2.368636 0.653078 8 0.396868 0.943959 -0.300298 8 2.580900 -0.719127 0.179568 8 3.481615 -0.170047 -0.404267	**Frequencies (cm^{-1}):** 9.1118, 27.9221, 34.1713, 53.0674, 80.1511, 97.5841, 113.6791, 235.0531, 264.1927, 477.9423, 505.4664, 595.5412, 738.6975, 855.4518, 895.1486, 930.5145, 1012.6362, 1065.7933, 1097.5099, 1154.6552, 1166.67, 1249.5061, 1272.2579, 1386.4063, 1394.6362, 1457.7288, 1469.7615, 1523.3998, 1603.3764, 1772.8361, 3040.9856, 3092.9062, 3095.3302, 3140.6298, 3145.2591, 3182.5121

Compound: MVK + O_3 TS_{EPOX} 1.4	**Energy (Hartree)** -456.161450630123
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.866111 -0.343622 0.309847 6 1.435323 -0.201171 -0.152587 6 0.852398 1.131606 -0.192321 6 -0.485444 1.281591 -0.570254 1 -0.903374 2.277224 -0.616460 1 -0.904004 0.580987 -1.291808 1 1.412262 1.973692 0.192915 8 0.748401 -1.174022 -0.451960 1 2.938344 -0.107642 1.374158 1 3.204960 -1.363295 0.149176 1 3.518567 0.352434 -0.220368 8 -2.420032 -0.739798 -0.450706 8 -1.702127 -0.610001 0.589450 8 -1.285877 0.658344 0.818751	-352.1461, 66.5184, 86.5413, 91.8222, 158.4674, 224.8126, 293.1177, 308.8633, 400.0719, 445.4994, 565.2864, 604.9671, 706.1094, 784.3287, 816.3389, 846.3034, 966.4721, 1039.5382, 1049.2005, 1126.7536, 1152.712, 1204.979, 1217.6897, 1251.6471, 1389.2156, 1434.2369, 1467.2904, 1476.7039, 1512.018, 1664.9899, 3029.8556, 3065.2683, 3082.5204, 3140.0903, 3174.7555, 3205.9886
IRC  	

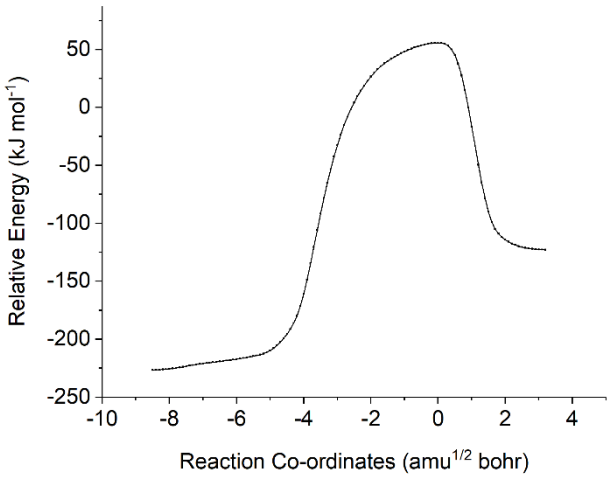
Compound: MVK + O_3 C_{EPOX} 1.4	**Energy (Hartree)** -456.236649707373
Reaction Coordinates: 6 -2.730401 -0.946037 0.057627 6 -1.292892 -0.503632 -0.064152 6 -1.070793 0.987399 -0.109234 6 0.001966 1.580083 0.715178 1 -0.117174 2.595753 1.076412 1 0.622634 0.916370 1.306136 1 -1.939181 1.596700 -0.340448 8 -0.369481 -1.282166 -0.110642 1 -2.778393 -2.020012 0.212785 1 -3.224668 -0.425827 0.881202 1 -3.272671 -0.683641 -0.854261 8 0.147725 1.440681 -0.688563 8 3.007038 -0.265729 -0.336832 8 2.372489 -0.978564 0.401244	**Frequencies (cm^{-1}):** 23.2229, 33.4266, 54.6209, 57.5847, 74.8451, 89.7019, 126.406, 240.0514, 264.8547, 378.2566, 594.8601, 612.5373, 765.0808, 868.8639, 890.9458, 959.1078, 992.8719, 1059.6805, 1101.4825, 1163.7047, 1168.5098, 1198.8924, 1275.2943, 1384.4136, 1413.7046, 1463.3056, 1474.0393, 1510.6709, 1595.8845, 1782.2923, 3026.5258, 3077.7903, 3089.6637, 3117.0276, 3143.4864, 3186.1079

Compound: MVK + O_3 TS_{EPOX} 2.1	**Energy (Hartree)** -456.207090721319
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -2.525269 1.274093 0.090767 6 -1.723976 -0.001329 -0.011252 6 -0.470436 -0.067549 0.732453 6 0.424324 -1.196506 0.581243 1 1.071414 -1.445372 1.415599 1 -0.038486 -2.073687 0.140394 1 -0.133673 0.795312 1.291221 8 -2.096697 -0.953373 -0.687533 1 -3.502370 1.131891 -0.362117 1 -2.639524 1.585563 1.130517 1 -2.000676 2.078243 -0.430637 8 1.270898 -0.610280 -0.515622 8 2.421510 0.050819 0.080373 8 2.531221 1.247308 -0.320248	-86.0721, 61.5282, 80.5549, 92.1182, 131.3281, 210.6785, 267.1186, 374.2067, 415.951, 470.0315, 547.7153, 555.5953, 600.6825, 751.2049, 799.6452, 832.2505, 961.7915, 1036.1848, 1061.7961, 1148.5126, 1191.7029, 1204.667, 1241.011, 1306.8374, 1389.6297, 1433.6452, 1466.357, 1474.9238, 1481.2252, 1669.8823, 3030.55, 3083.3839, 3104.6617, 3141.9797, 3169.7833, 3191.4557
IRC  	

Compound: MVK + O_3 C_{EPOX} 2.1	**Energy (Hartree)** -456.235187855083
Reaction Coordinates: 6 -2.597595 1.338121 0.296928 6 -1.817456 0.129646 -0.157397 6 -0.409673 0.021142 0.382525 6 0.094467 -1.296948 0.811670 1 0.843878 -1.343941 1.593661 1 -0.556118 -2.156043 0.696309 1 0.004901 0.907809 0.850400 8 -2.273317 -0.714642 -0.890198 1 -3.626137 1.269000 -0.045419 1 -2.570660 1.425740 1.385573 1 -2.137148 2.244382 -0.104539 8 0.523792 -0.713926 -0.409588 8 2.778965 0.318236 0.317884 8 3.523414 0.672994 -0.565391	**Frequencies (cm^{-1}):** 12.8046, 35.3243, 38.3182, 63.3625, 75.8602, 130.2572, 149.0878, 241.6124, 280.1794, 374.7716, 593.1864, 610.7994, 762.6553, 860.2161, 889.0018, 957.0572, 996.8388, 1058.9601, 1103.4358, 1160.5276, 1167.6973, 1197.5962, 1275.1535, 1384.7566, 1411.5156, 1463.4876, 1473.5678, 1504.0555, 1579.1126, 1790.0219, 3025.8806, 3076.6983, 3094.1536, 3128.5998, 3143.0947, 3190.5796

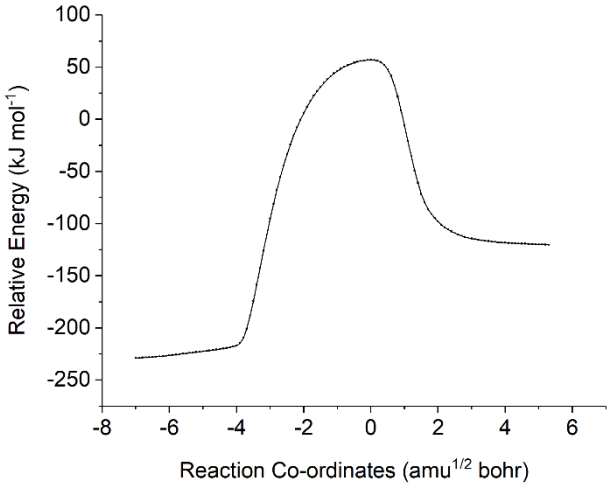
Compound: MVK + O_3 TS_{EPOX} 2.2	**Energy (Hartree)** -456.239749900564
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -2.198022 -0.842130 -0.798111 6 -1.725015 0.316839 0.050115 6 -0.481115 0.208743 0.798232 6 0.353846 -0.977538 0.860630 1 1.021033 -1.052006 1.713918 1 -0.142865 -1.925697 0.678723 1 -0.129795 1.124873 1.253954 8 -2.380652 1.347681 0.152102 1 -3.081076 -0.534799 -1.350828 1 -1.422438 -1.162099 -1.495610 1 -2.454867 -1.700108 -0.172742 8 1.178417 -0.724763 -0.364927 8 2.430063 -0.041563 0.034590 8 2.586152 1.045440 -0.583342	-140.927, 61.3467, 82.0327, 117.8929, 120.8358, 174.3052, 253.4492, 368.6125, 395.881, 489.7979, 514.8858, 521.7892, 565.3176, 762.7579, 811.414, 816.1383, 943.6449, 1035.4237, 1055.4192, 1144.522, 1204.4331, 1231.448, 1269.5706, 1308.9908, 1393.375, 1409.7861, 1467.8536, 1480.6684, 1496.7281, 1660.1279, 3031.7993, 3086.7827, 3097.6008, 3143.0359, 3154.2245, 3195.6897
IRC  	

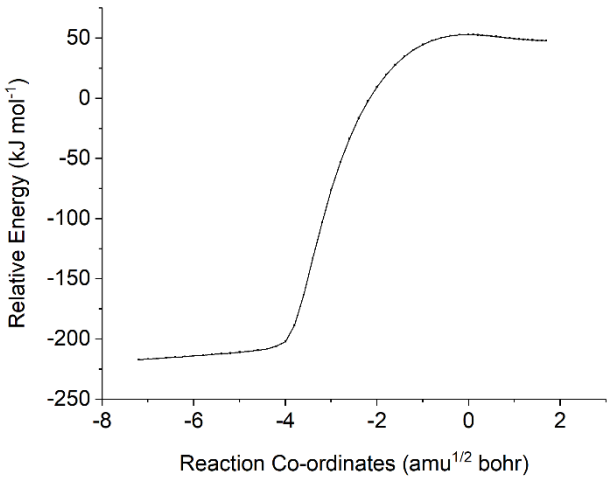
Compound: MVK + O_3 C_{EPOX} 2.2	**Energy (Hartree)** -456.238757609375
Reaction Coordinates: 6 -2.367449 0.991278 0.698101 6 -1.867264 -0.318038 0.146462 6 -0.438703 -0.393401 -0.320776 6 0.080158 0.530613 -1.343786 1 0.871466 0.184492 -1.998096 1 -0.558691 1.311556 -1.740680 1 -0.007462 -1.386366 -0.261381 8 -2.554253 -1.312038 0.073125 1 -3.441600 0.933126 0.849120 1 -1.870480 1.191447 1.649677 1 -2.121045 1.826180 0.041583 8 0.443986 0.681654 0.025067 8 2.756959 -0.561137 0.135563 8 3.689228 0.076129 0.563717	**Frequencies (cm^{-1}):** 13.5566, 27.7392, 38.7466, 66.8704, 89.832, 110.5237, 140.7518, 240.2713, 267.3185, 478.6085, 505.4428, 594.8274, 739.5614, 854.3641, 893.2068, 931.5211, 1011.0585, 1066.0952, 1097.0819, 1154.877, 1166.3532, 1248.4917, 1271.0409, 1386.7338, 1393.335, 1457.8282, 1469.3377, 1519.1993, 1585.0243, 1774.8071, 3039.7628, 3092.6438, 3096.3196, 3143.6444, 3145.5243, 3185.9899

Compound: MVK + O_3 TS_{EPOX} 2.3	**Energy (Hartree)** -456.239534637013
Reaction Coordinates:	**Frequencies (cm^{-1}):**

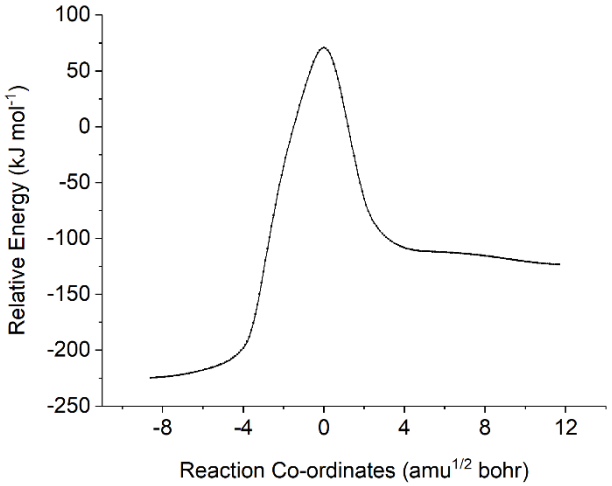
6 1.382671 -1.073501 0.998718 6 1.582362 -0.066321 -0.109978 6 0.674141 1.063942 -0.245949 6 -0.448286 1.380006 0.623101 1 -0.483209 0.866937 1.579755 1 -0.657625 2.438824 0.751545 1 0.834580 1.686808 -1.115275 8 2.541813 -0.129904 -0.871658 1 1.652910 -0.630438 1.960515 1 0.347328 -1.406391 1.066171 1 2.029797 -1.926761 0.816491 8 -1.541068 0.861038 -0.245332 8 -1.946615 -0.495044 0.232647 8 -1.912768 -1.342807 -0.697477	-143.8671, 66.0133, 88.3301, 125.9508, 144.7397, 214.3804, 266.7079, 358.8235, 369.6951, 483.4673, 517.0622, 528.9597, 578.6371, 763.1323, 800.161, 833.3356, 938.1357, 1036.81, 1051.1124, 1163.9752, 1191.7029, 1231.4974, 1272.4487, 1306.667, 1396.7201, 1404.2236, 1466.3143, 1479.996, 1491.6341, 1654.6656, 3032.7011, 3087.6458, 3095.4503, 3143.661, 3145.9739, 3198.7947
IRC	



Compound: MVK + O_3 TS_{EPOX} 2.4	**Energy (Hartree)** -456.170075488032
Reaction Coordinates: 6 -2.527515 -0.516057 -0.494703 6 -1.310040 0.079714 0.168222 6 -0.561201 1.124309 -0.474544 6 0.662505 1.562053 0.173797 1 1.068386 2.504332 -0.182465 1 0.650043 1.505711 1.257245 1 -0.772239 1.426473 -1.490242 8 -0.908239 -0.334102 1.264440 1 -3.387173 -0.398271 0.165851 1 -2.748769 -0.054463 -1.455370 1 -2.370423 -1.584974 -0.637814 8 1.673328 0.571186 -0.343110 8 1.561657 -0.714260 0.340070 8 1.420465 -1.635189 -0.498130	**Frequencies (cm^{-1}):** -114.9096, 35.2276, 62.0296, 98.3181, 190.8973, 303.1027, 330.8209, 380.3819, 438.5761, 466.5193, 537.0944, 572.1773, 602.3298, 763.3434, 787.4825, 839.994, 995.7693, 1044.4555, 1048.6377, 1142.9794, 1187.0258, 1231.0255, 1255.3566, 1315.5502, 1395.6089, 1418.2141, 1466.6435, 1474.373, 1486.9352, 1596.0938, 3041.7783, 3099.4685, 3104.3762, 3120.5399, 3164.0651, 3201.0748
IRC	



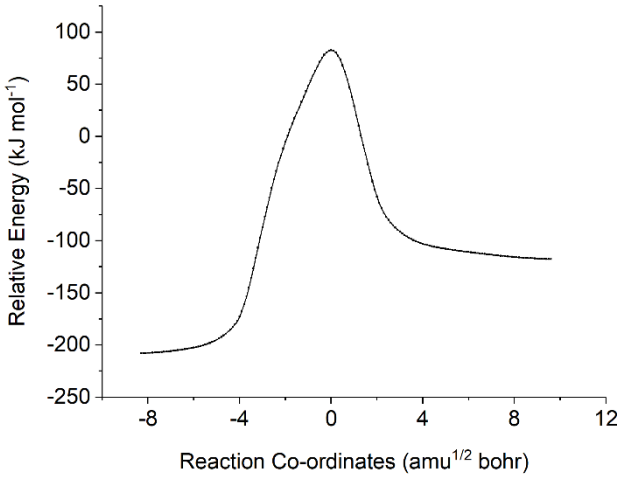
Compound: MVK + O_3 TS_{EPOX} 2.5	**Energy (Hartree)** -456.140995312962
Reaction Coordinates: 6 2.244027 1.241931 0.075347 6 1.664927 -0.132289 -0.098745 6 0.135124 -0.176100 -0.327525 6 -0.593388 -1.339473 0.165593 1 -1.290241 -1.908305 -0.426688 1 -0.445722 -1.619850 1.196857 1 -0.045996 0.033562 -1.389680 8 2.307067 -1.152116 -0.084070 1 1.923658 1.897917 -0.736133 1 3.328151 1.179572 0.109006 1 1.860640 1.682043 0.997080 8 -2.801311 -0.185309 0.127790 8 -2.195945 0.774277 -0.377679 8 -0.564139 0.709478 0.504152	**Frequencies (cm^{-1}):** -582.8387, 36.408, 88.6967, 98.073, 128.0061, 238.3455, 275.1063, 300.5924, 358.7715, 436.4891, 457.6764, 523.0491, 575.4716, 654.2201, 715.7341, 916.568, 955.4286, 965.945, 1021.9861, 1071.9431, 1172.866, 1206.0052, 1250.1492, 1306.4664, 1319.9653, 1388.4954, 1457.6884, 1463.9446, 1489.7269, 1785.0036, 2985.9202, 3039.8861, 3094.6417, 3145.3742, 3182.252, 3298.1299
IRC	



Compound: MVK + O_3 TS_{EPOX} 2.6	**Energy (Hartree)**

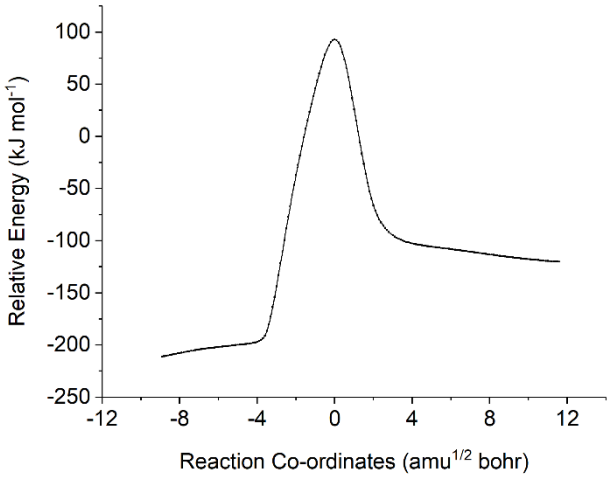
Reaction Coordinates:	**Frequencies (cm^{-1}):**
IP	

IRC



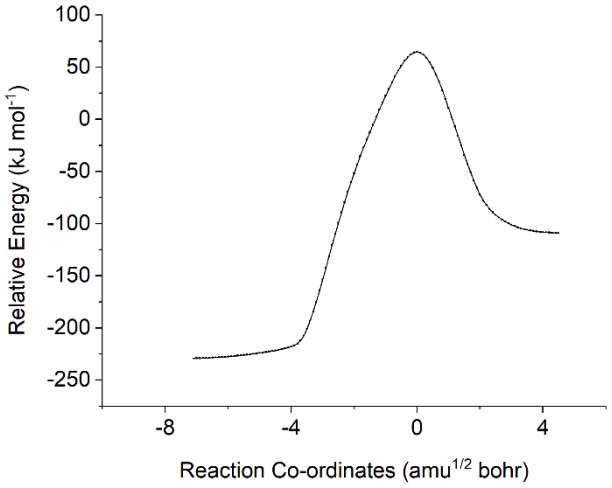
Compound: MVK + O_3 TS_{EPOX} 2.7	**Energy (Hartree)** -456.131026262361
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.559630 1.335613 0.446486 6 1.324371 -0.064243 -0.051866 6 0.165934 -0.885134 0.568704 6 -0.772768 -0.277559 1.505843 1 -1.465600 -0.931894 2.011692 1 -0.871480 0.783319 1.662291 1 0.589083 -1.836485 0.903597 8 2.012122 -0.599072 -0.881974 1 1.681000 1.343000 1.532930 1 0.699576 1.965105 0.211142 1 2.451388 1.740940 -0.023129 8 -2.038945 0.922954 -0.337820 8 -1.171608 0.380109 -1.071316 8 -0.894940 -1.168496 -0.348081	-612.1042, 48.9171, 79.9614, 171.1517, 179.1742, 201.3574, 283.7233, 329.6669, 385.9884, 449.8581, 480.121, 512.5975, 595.6981, 622.9532, 733.6496, 869.1024, 930.1304, 948.0312, 1032.2486, 1071.5627, 1154.2291, 1206.9229, 1216.3691, 1242.1888, 1334.183, 1387.1018, 1464.0067, 1474.0593, 1499.3154, 1797.2576, 3026.0223, 3027.791, 3083.2109, 3143.0931, 3182.6501, 3295.4538

IRC



Compound: MVK + O_3 C_{EPOX} 2.7	**Energy (Hartree)** -456.239011910976
Reaction Coordinates: 6 -0.721038 -1.369346 0.901061 6 -1.542402 -0.593314 -0.094557 6 -1.081022 0.787273 -0.475011 6 -0.847589 1.822895 0.546905 1 -1.013508 2.860364 0.279868 1 -0.967274 1.580926 1.597156 1 -1.407842 1.102608 -1.459761 8 -2.545364 -1.032453 -0.612145 1 -0.500346 -0.776903 1.789599 1 0.242267 -1.620696 0.452434 1 -1.250324 -2.277288 1.175834 8 3.397034 -0.220028 0.241116 8 2.660443 -0.529221 -0.660439 8 0.244054 1.187445 -0.106721	**Frequencies (cm^{-1}):** 14.4582, 18.8435, 34.5707, 40.6433, 43.7643, 93.0459, 124.065, 235.1491, 262.7402, 477.9341, 505.8821, 596.6135, 739.489, 856.8866, 896.4518, 931.2599, 1013.5987, 1066.161, 1097.5602, 1155.0101, 1166.1634, 1249.5477, 1272.3087, 1387.3625, 1394.8734, 1459.2456, 1469.572, 1524.0603, 1615.3489, 1772.8742, 3039.3582, 3091.2514, 3093.62, 3139.6631, 3144.7228, 3179.8683

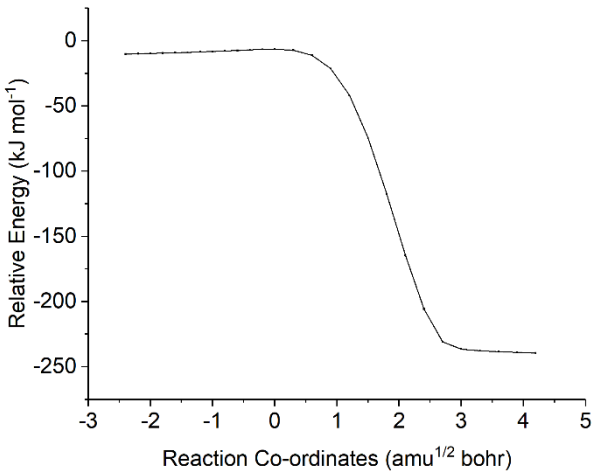
Compound: MVK + O_3 TS_{EPOX} 2.8	**Energy (Hartree)** -456.145645098218
Reaction Coordinates: 6 1.949533 -1.110688 0.213964 6 1.268653 0.172000 -0.156985 6 0.152354 0.676282 0.787241 6 -0.854189 1.503362 0.133579 1 -1.583622 1.997480 0.756505 1 -0.938010 1.577966 -0.938275 1 0.678614 1.180987 1.613499 8 1.577922 0.872556 -1.088212 1 1.222403 -1.921946 0.223970 1 2.351365 -1.032155 1.227014 1 2.750605 -1.323921 -0.488288 8 -2.095908 -0.461871 -0.834762 8 -1.169550 -1.144952 -0.371325 8 -0.759897 -0.256252 1.261646	**Frequencies (cm^{-1}):** -574.156, 58.1182, 92.0327, 110.7515, 180.2315, 225.1498, 275.1356, 297.7817, 354.8015, 426.1749, 430.8497, 522.81, 597.5208, 611.6522, 747.5041, 908.9684, 953.2755, 977.7138, 1062.4634, 1092.9248, 1146.6984, 1198.0341, 1215.1123, 1307.5732, 1333.0691, 1390.9814, 1459.3196, 1469.081, 1479.5574, 1789.5379, 2935.2123, 3037.5242, 3101.2038, 3147.7217, 3178.7451, 3297.6719
IRC	


100
50
0
-50
-100
-150
-200
-250
Relative Energy (kJ mol-1)
-8
-4
0
4
Reaction Co-ordinates (amu1/2 bohr)

S10.8 Ozonolysis of 2-methyl-2-butene (Alkene 6)

Compound: $MeCHCMe_2 + O_3$ PRC1	**Energy (Hartree)** -421.490704382920
Reaction Coordinates: 6 0.617958 -1.738134 -0.847548 6 1.160318 -0.482303 -0.232014 6 0.817788 0.722130 -0.730886 6 1.228567 2.075100 -0.254696 1 0.345186 2.656941 0.020752 1 1.728190 2.627048 -1.055503 1 1.895261 2.049366 0.603867 1 0.161888 0.725122 -1.595772 6 2.072541 -0.693526 0.940121 1 1.566970 -1.279829 1.711620 1 2.416178 0.232472 1.392362 1 2.951302 -1.269950 0.637003 1 1.424669 -2.429968 -1.104406 1 -0.026102 -2.267153 -0.136714 1 0.036317 -1.536620 -1.745393 8 -2.692863 0.200343 -0.511708 8 -2.104248 -0.355829 0.471919 8 -1.188250 0.304608 1.042579	**Frequencies (cm^{-1}):** 27.1784, 50.1606, 53.6577, 75.2081, 102.8604, 118.194, 127.0791, 178.0945, 255.2214, 276.1835, 298.1965, 388.2708, 456.2367, 528.1489, 731.5779, 771.3455, 838.3277, 958.8451, 970.2319, 1002.4463, 1058.0042, 1075.0445, 1096.3981, 1135.3897, 1143.4019, 1166.3998, 1244.4755, 1380.4423, 1410.1982, 1415.0271, 1420.5919, 1469.6599, 1475.4336, 1480.3338, 1489.7206, 1492.6476, 1495.7423, 1679.7275, 3001.8539, 3016.2956, 3018.3243, 3043.7022, 3054.3052, 3054.4137, 3104.8866, 3110.9907, 3128.0823, 3135.6233

Compound: $MeCHCMe_2 + O_3$ TS_{OZO} 1	**Energy (Hartree)** -421.488197362492
Reaction Coordinates: 6 1.141143 -1.399325 -1.095080 6 0.972841 -0.198514 -0.208950 6 0.322740 0.912992 -0.685697 6 0.249553 2.232717 0.008353 1 1.197219 2.774223 -0.079378 1 0.033345 2.116685 1.069826 1 -0.528600 2.856009 -0.427453 1 -0.021866 0.883196 -1.711558 6 1.785812 -0.175686 1.052941 1 1.820552 -1.162035 1.513466 1 1.396451 0.529878 1.782586 1 2.816863 0.114235 0.825336 1 2.149954 -1.412818 -1.520953 1 1.018188 -2.325984 -0.535149 1 0.432562 -1.394583 -1.922359 8 -1.937684 0.406110 -0.269118 8 -1.790979 -0.824332 0.080348 8 -0.914738 -0.983267 1.010801	**Frequencies (cm^{-1}):** -136.2357, 69.9513, 97.1473, 113.1259, 132.8794, 157.0309, 162.2988, 181.2724, 260.3192, 289.9223, 388.6736, 430.8786, 493.8605, 527.7861, 739.5736, 774.8147, 843.5158, 955.376, 975.3407, 1007.9985, 1040.2137, 1074.0844, 1086.2863, 1090.372, 1110.1244, 1137.0213, 1241.886, 1368.0393, 1407.6949, 1410.9587, 1419.3948, 1472.2655, 1473.4018, 1479.7303, 1482.5358, 1492.2253, 1502.9971, 1593.0708, 3007.963, 3009.7503, 3013.8158, 3071.6638, 3077.9598, 3081.9531, 3109.0578, 3114.1663, 3126.0383, 3160.7213
IRC:	



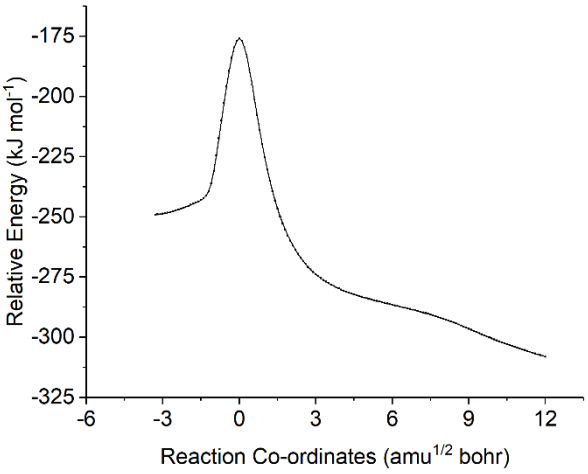
Compound: $MeCHCMe_2 + O_3$ POZ1	**Energy (Hartree)** -421.589334220594
Reaction Coordinates: 6 1.101822 1.196014 -1.047195 6 0.684040 0.173905 0.000722 6 -0.806760 0.278334 0.501228 6 -1.600548 1.517231 0.143171 1 -1.663038 1.656540 -0.934013 1 -2.611955 1.435145 0.539513 1 -1.139167 2.399873 0.586425 1 -0.806591 0.134098 1.585354 8 -1.445405 -0.846198 -0.105810 8 -0.397122 -1.824940 -0.078572 8 0.687478 -1.100568 -0.688230 6 1.646165 0.136944 1.183570 1 1.572065 1.055397 1.769638 1 2.674210 0.034719 0.837387 1 1.411965 -0.704448 1.834562 1 0.410532 1.206593 -1.887081 1 2.092545 0.946409 -1.426485 1 1.151512 2.194759 -0.613386	**Frequencies (cm^{-1}):** 53.6351, 213.4189, 235.2693, 251.6887, 275.9539, 292.1465, 306.9803, 346.0847, 411.0663, 480.6846, 520.2624, 600.6938, 701.9449, 724.326, 767.0573, 861.1894, 892.3931, 933.2719, 939.0378, 954.3417, 1014.6864, 1054.8716, 1098.5972, 1159.5296, 1184.6188, 1216.3731, 1264.8323, 1352.7203, 1389.2551, 1404.2704, 1416.6102, 1424.2986, 1475.6044, 1486.0936, 1489.1246, 1500.635, 1500.9913, 1515.6267, 3014.3141, 3030.0947, 3042.4794, 3046.8643, 3092.5638, 3103.2686, 3106.4043, 3112.3538, 3119.5643, 3126.7663

Compound: $MeCHCMe_2 + O_3$ PRC 2	**Energy (Hartree)** -421.495697865614
Reaction Coordinates: 6 1.338362 -1.481189 -0.970225 6 1.224914 -0.200943 -0.196144 6 0.600374 0.866522 -0.731027 6 0.359114 2.200580 -0.105301 1 -0.714310 2.372083 0.029823 1 0.714633 3.002707 -0.756992 1 0.835919 2.315764 0.865119 1 0.219252 0.757717 -1.740579 6 1.895925 -0.219283 1.147715 1 1.547624 -1.071276 1.735089 1 1.727869 0.682519 1.729755 1 2.975271 -0.346684 1.022583 1 2.385515 -1.776619 -1.083131	**Frequencies (cm^{-1}):** 36.9586, 48.5349, 58.774, 75.81, 87.4943, 122.1003, 148.8737, 177.9751, 267.2774, 290.6169, 299.6627, 388.7022, 463.2547, 526.5619, 738.9726, 770.9035, 833.5889, 959.1562, 970.2212, 1006.5445, 1054.7353, 1073.1955, 1099.0366, 1132.8514, 1154.1765, 1171.5029, 1241.1897, 1377.034, 1410.2, 1415.1913, 1421.1811, 1469.0695, 1476.3614, 1477.595, 1488.3415, 1493.8922, 1496.422, 1675.6447, 3004.0927,

1 0.837262 -2.292110 -0.434698 1 0.890144 -1.401474 -1.958703 8 -2.099525 -0.285338 -0.824124 8 -2.114687 -0.102944 0.430069 8 -1.277202 -0.766311 1.109258	3009.8783, 3018.3636, 3044.5664, 3051.4083, 3060.9297, 3108.5119, 3110.3783, 3128.2449, 3141.4631

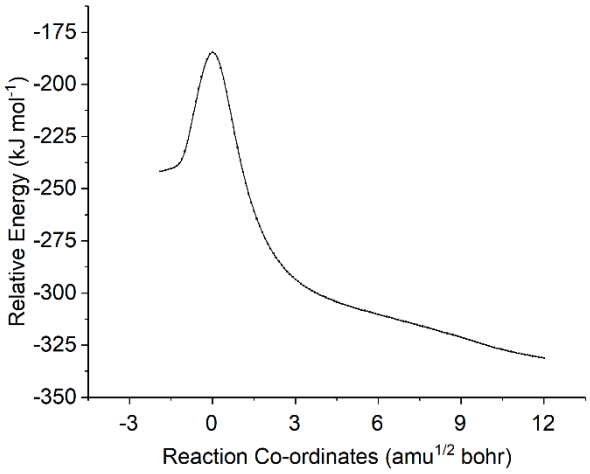
Compound: MeCHCMe$_2$ + O$_3$ TS$_{OZO}$ 2	**Energy (Hartree)** -421.486931933269
Reaction Coordinates: 6 -1.559672 -1.077952 1.054445 6 -1.006578 0.001822 0.176915 6 -0.152071 0.945013 0.701523 6 0.321347 2.155449 -0.037576 1 -0.508244 2.827327 -0.277361 1 0.790687 1.883615 -0.986412 1 1.049135 2.712187 0.547865 1 0.049427 0.899998 1.762214 6 -1.669464 0.181671 -1.161013 1 -1.923591 -0.778804 -1.605857 1 -1.050939 0.732390 -1.865653 1 -2.603568 0.739424 -1.032614 1 -2.611584 -0.876738 1.281865 1 -1.518312 -2.044152 0.550601 1 -1.012411 -1.155926 1.991667 8 1.822796 -0.244108 0.679771 8 1.711213 -0.634259 -0.544601 8 0.683244 -1.393550 -0.731680	**Frequencies (cm^{-1}):** -166.479, 66.823, 128.0688, 140.1025, 151.3913, 167.7468, 175.382, 190.4718, 268.1285, 283.3042, 386.8183, 453.6647, 505.9947, 531.6042, 738.9611, 775.9025, 848.6449, 958.6579, 978.941, 1006.8509, 1037.4865, 1072.6977, 1078.3327, 1089.7411, 1105.7005, 1132.3285, 1242.2939, 1359.4497, 1409.4788, 1413.2695, 1419.6259, 1469.7945, 1474.898, 1480.0535, 1481.6523, 1490.1522, 1502.9366, 1581.474, 3006.1939, 3010.4183, 3012.2715, 3051.4727, 3071.5928, 3083.8299, 3115.8701, 3116.0134, 3124.7305, 3180.0494
IRC: Reassess	

Compound: MeCHCMe$_2$ + O$_3$ POZ 2	**Energy (Hartree)** -421.588054479771
Reaction Coordinates: 6 1.822185 0.322617 -1.041390 6 0.715074 0.085934 -0.023353 6 -0.707787 0.448168 -0.593236 6 -1.445900 1.600267 0.065664 1 -2.414158 1.730562 -0.415927 1 -0.889834 2.532821 -0.043876 1 -1.613113 1.415411 1.124908 1 -0.623761 0.626479 -1.666520 6 1.038334 0.716356 1.327811 1 2.015344 0.366308 1.659275 1 0.301606 0.433953 2.076806 1 1.071231 1.803793 1.265062 1 1.932718 1.390362 -1.233219 1 2.773678 -0.051722 -0.664619 1 1.596356 -0.181472 -1.979955 8 -1.451036 -0.779588 -0.487624 8 -0.744709 -1.511813 0.542224 8 0.610557 -1.346917 0.128536	**Frequencies (cm^{-1}):** 38.6134, 214.0229, 246.9177, 269.816, 279.0017, 279.7958, 308.925, 340.7614, 434.1964, 489.808, 504.9436, 611.6695, 692.605, 740.8897, 772.0819, 862.7097, 888.8831, 932.4031, 937.883, 957.7792, 1019.0646, 1051.0518, 1074.9168, 1124.2582, 1189.5732, 1230.7942, 1246.6571, 1330.3106, 1384.6717, 1404.4642, 1412.6955, 1423.3656, 1477.6914, 1485.0787, 1489.6134, 1500.7606, 1504.0664, 1515.415, 3037.1044, 3038.4508, 3045.239, 3049.5332, 3098.6085, 3101.2893, 3108.4609, 3113.8191, 3119.2866, 3125.9615

Compound: $MeCHCMe_2 + O_3$ TS_{ANTI}	**Energy (Hartree)** -421.558157771816
Reaction Coordinates: 6 -1.782165 0.236012 -1.091068 6 -0.874306 -0.264360 0.043812 6 0.770417 0.551827 -0.431907 6 0.913304 1.994077 -0.058972 1 1.031170 2.113714 1.015917 1 0.039549 2.556114 -0.383758 1 1.784635 2.425011 -0.556244 1 0.730017 0.300814 -1.486883 6 -1.223231 0.268505 1.435859 1 -2.154761 -0.200205 1.757749 1 -0.448886 -0.004383 2.150151 1 -1.370033 1.348374 1.450396 1 -2.801214 -0.093587 -0.882391 1 -1.794218 1.323344 -1.170786 1 -1.474364 -0.199688 -2.039316 8 1.572185 -0.263284 0.268364 8 1.440624 -1.510683 -0.157766 8 -0.558560 -1.511767 -0.015746	**Frequencies (cm^{-1}):** -466.3525, 89.6845, 176.2857, 193.9454, 222.5575, 235.3344, 247.1831, 296.438, 339.7262, 376.8853, 412.9267, 485.6561, 524.767, 559.3632, 627.6716, 770.2026, 905.2958, 910.0071, 981.8117, 1009.4561, 1014.5526, 1064.8005, 1118.5438, 1146.5144, 1161.7471, 1189.4767, 1261.1009, 1373.0331, 1384.6445, 1390.8201, 1403.6407, 1422.5666, 1473.3562, 1479.8921, 1488.9339, 1490.883, 1497.2512, 1505.5882, 3030.8364, 3035.6217, 3038.8522, 3089.1983, 3093.7419, 3099.8496, 3119.6383, 3121.0775, 3124.4951, 3136.2108
IRC:  	

Compound: $MeCHCMe_2 + O_3$ C_{ANTI}	**Energy (Hartree)** -421.605132678016
Reaction Coordinates: 6 3.226302 -0.638153 0.168365 6 1.818787 -0.129682 -0.048385 6 -1.866763 -0.375132 -0.350313 6 -2.204602 -1.731438 0.121341 1 -2.588917 -1.708894 1.138098 1 -1.307388 -2.352057 0.076703 1 -2.947171 -2.182390 -0.542049 1 -1.475935 -0.168670 -1.340142 6 1.621460 1.363727 -0.029196 1 2.119112 1.796186 -0.902129 1 0.564229 1.627452 -0.046492	**Frequencies (cm^{-1}):** 24.6817, 44.6322, 74.7078, 85.5727, 92.8105, 99.4911, 130.2591, 152.2036, 199.0116, 269.2797, 325.2901, 395.5072, 498.9114, 545.1685, 550.271, 791.9803, 863.5713, 875.7613, 891.1069, 904.2128, 960.206, 1074.031, 1093.1404, 1125.8131, 1162.7069, 1247.1089, 1348.7825, 1388.207, 1403.0531, 1408.7298, 1459.3169, 1462.5566, 1467.2691, 1468.5009, 1476.6733, 1494.4853,

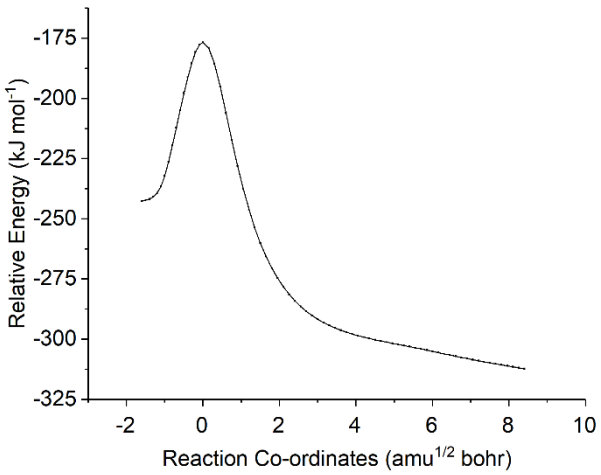
1 2.105787 1.798500 0.847730 1 3.926210 -0.129741 -0.497011 1 3.540601 -0.409141 1.189463 1 3.271565 -1.712188 0.009315 8 -2.044909 0.603692 0.408725 8 -1.700863 1.863783 -0.066705 8 0.898371 -0.904349 -0.230064	1593.4248, 1756.1197, 3009.9083, 3026.5708, 3031.296, 3070.2546, 3077.4937, 3084.7504, 3103.7982, 3135.1382, 3137.0156, 3171.8886

Compound: $MeCHCMe_2 + O_3$ TS_{AO} 1	**Energy (Hartree)** -421.562412908607
Reaction Coordinates: 6 1.076547 1.726726 -0.342731 6 0.730735 0.306270 0.016816 6 -1.011017 0.107900 0.642501 6 -1.948613 1.044531 -0.104046 1 -1.965690 0.804259 -1.166031 1 -2.957663 0.903853 0.285678 1 -1.679995 2.092538 0.028470 1 -0.751714 0.436042 1.662253 6 1.588496 -0.348858 1.072799 1 1.737647 0.341480 1.901364 1 2.564046 -0.580680 0.638311 1 1.143043 -1.268510 1.435639 1 0.515339 2.064281 -1.210802 1 2.142979 1.806347 -0.563201 1 0.862091 2.387546 0.495748 8 -1.211069 -1.158836 0.524305 8 0.177948 -1.669761 -0.814101 8 0.504750 -0.422223 -1.112637	**Frequencies (cm^{-1}):** -464.4145, 125.8449, 178.4565, 182.8643, 209.148, 233.3068, 274.6675, 294.9501, 337.3068, 373.3082, 411.4326, 492.8246, 538.8472, 596.9151, 648.3781, 780.8192, 901.5617, 953.308, 967.1753, 989.2816, 1003.0883, 1041.5102, 1104.9221, 1127.7686, 1164.8217, 1276.1836, 1281.9841, 1299.9895, 1396.1905, 1403.5467, 1417.8383, 1422.9553, 1471.7498, 1477.4423, 1485.3375, 1492.333, 1500.7002, 1505.8269, 2922.4449, 3033.895, 3036.1349, 3039.1887, 3094.9116, 3098.7751, 3103.713, 3116.6291, 3131.9684, 3160.173
IRC:  	

Compound: $MeCHCMe_2 + O_3$ CPr_{AO} 1	**Energy (Hartree)** -421.612023626196
Reaction Coordinates: 6 -2.512406 -0.932241 -0.440998 6 -1.530899 0.069185 0.045685	**Frequencies (cm^{-1}):** 39.7403, 44.8699, 77.4796, 88.4943, 103.3423, 124.2875, 157.4773, 160.3839,

6 -1.299755 0.363030 1.470542 1 -2.021213 -0.149676 2.101141 1 -1.330527 1.444666 1.618757 1 -0.285024 0.054362 1.730761 8 -0.885480 0.683163 -0.849624 8 0.083956 1.589891 -0.436400 1 -2.537007 -0.958109 -1.527163 1 -3.507651 -0.704282 -0.053081 1 -2.234761 -1.918664 -0.061764 6 1.898688 -0.597448 -0.407457 6 2.986679 0.186524 0.258868 1 3.032243 -0.030912 1.323698 1 3.943989 -0.056027 -0.210997 1 2.803941 1.249244 0.094482 1 1.786830 -0.415176 -1.491145 8 1.188441 -1.404269 0.150458	190.9702, 293.528, 309.4418, 367.8338, 480.8197, 512.8259, 594.2307, 782.8576, 812.6365, 891.1953, 913.9003, 930.4715, 988.146, 1073.3978, 1097.6353, 1127.3188, 1135.0153, 1306.0908, 1373.8141, 1387.5912, 1405.7322, 1426.6915, 1443.9167, 1458.5583, 1459.9681, 1470.3089, 1471.2569, 1479.7331, 1570.7409, 1776.5179, 2926.9447, 3024.8398, 3027.0652, 3034.2594, 3075.4222, 3082.484, 3087.2993, 3131.4625, 3137.6628, 3139.0482

Compound: $MeCHCMe_2 + O_3$ TS_{AO} 2	**Energy (Hartree)** -421.559064397801
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.078887 -1.637625 -0.778188 6 -0.638144 -0.432392 0.006330 6 1.080095 0.130026 -0.545203 6 2.068641 -0.796198 0.164622 1 3.052246 -0.626531 -0.274908 1 2.130442 -0.565035 1.225123 1 1.819582 -1.848541 0.026164 1 0.981853 -0.091613 -1.620694 6 -0.584410 -0.562017 1.508062 1 -0.121712 -1.504135 1.790976 1 -1.611634 -0.559964 1.882476 1 -0.052056 0.264168 1.966030 1 -1.235095 -1.382760 -1.824629 1 -2.008582 -2.040172 -0.370960 1 -0.325814 -2.421720 -0.716426 8 1.109775 1.372783 -0.220251 8 -0.824805 1.764468 0.161602 8 -1.249095 0.683442 -0.468462	-480.2753, 104.3204, 172.4186, 197.7865, 216.2532, 239.2856, 264.4242, 318.009, 330.4402, 388.6542, 399.715, 487.3769, 527.8877, 571.8559, 644.806, 783.2927, 896.5886, 955.4545, 983.2999, 997.8347, 1009.8732, 1039.2419, 1084.9956, 1141.5825, 1189.7616, 1279.8408, 1282.5421, 1338.8266, 1389.5462, 1403.5466, 1418.9586, 1427.4506, 1468.2293, 1479.9942, 1486.0295, 1493.8978, 1497.1086, 1508.1341, 2914.3777, 3032.6749, 3036.2167, 3038.3616, 3093.7143, 3098.1012, 3112.5657, 3125.9276, 3131.3313, 3162.4647
IRC	

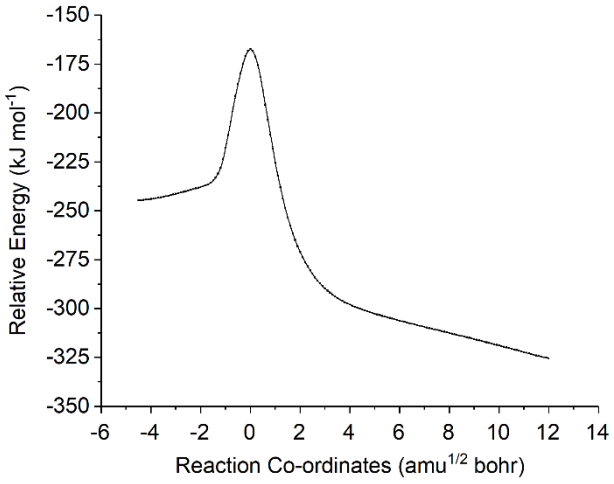


Compound: $MeCHCMe_2 + O_3$ CPr_{AO} 2	**Energy (Hartree)** -421.610541650470
Reaction Coordinates: 6 -1.815272 -1.389891 -0.771255 6 -1.441415 -0.146777 -0.052760 6 -1.555028 0.022707 1.405656 1 -1.987703 -0.856512 1.874963 1 -2.145169 0.918819 1.613003 1 -0.563005 0.226740 1.812625 8 -1.011875 0.799063 -0.770647 8 -0.617315 1.967007 -0.124686 1 -1.692118 -1.270739 -1.844579 1 -2.849644 -1.658993 -0.545935 1 -1.178830 -2.205702 -0.421583 6 2.425014 -0.721681 0.072252 6 2.570316 0.750564 -0.141048 1 3.053892 0.920136 -1.107820 1 1.613643 1.271192 -0.101840 1 3.256042 1.149597 0.612563 1 3.370095 -1.302176 0.041676 8 1.381828 -1.301307 0.269065	**Frequencies (cm^{-1}):** 41.7998, 58.3635, 65.2839, 79.5834, 97.647, 107.534, 156.371, 164.1727, 180.0062, 289.4071, 308.5627, 366.8994, 479.8787, 527.1083, 593.4557, 780.6412, 812.1044, 894.3221, 911.6484, 928.9357, 989.0279, 1072.5462, 1096.7011, 1144.3467, 1147.9438, 1305.9462, 1387.7099, 1389.2479, 1403.6777, 1426.6526, 1441.7838, 1459.7322, 1467.0467, 1471.5204, 1477.1735, 1481.8101, 1570.2575, 1787.3611, 2873.1107, 3004.6472, 3027.9351, 3034.0048, 3060.2229, 3078.5874, 3081.0599, 3105.6982, 3136.5806, 3140.4641

Compound: $MeCHCMe_2 + O_3$ TS_{SYN}	**Energy (Hartree)** -421.556402140495
Reaction Coordinates: 6 -1.640357 -1.059582 -0.747861 6 -0.892864 -0.074825 0.157072 6 0.668581 0.362641 -0.777078 6 1.317464 1.558995 -0.139940 1 0.833672 2.473271 -0.474039 1 2.362047 1.588488 -0.460360 1 1.293506 1.500698 0.943107 1 0.406995 0.449195 -1.828386 6 -1.600396 1.285836 0.299757 1 -2.596214 1.092071 0.700883 1 -1.075455 1.930019 0.998567 1 -1.717911 1.791781 -0.658488	**Frequencies (cm^{-1}):** -467.3132, 103.2029, 195.4634, 200.243, 226.7866, 258.5396, 289.8417, 304.1453, 311.1064, 346.239, 420.7633, 487.8422, 547.1886, 571.5685, 695.4948, 789.0796, 897.3989, 910.6994, 956.8011, 991.5011, 1023.3904, 1061.597, 1077.3589, 1130.9944, 1163.9672, 1182.657, 1206.2704, 1364.2579, 1393.0693, 1395.4713, 1405.1096, 1424.8817, 1470.623, 1481.0968, 1485.2167, 1495.4393,

1 -2.572878 -1.341705 -0.255833 1 -1.052190 -1.962092 -0.895415 1 -1.889327 -0.625679 -1.717491 8 1.257998 -0.837343 -0.586005 8 1.507719 -1.019128 0.699676 8 -0.404068 -0.560334 1.248298	1498.6324, 1506.6639, 3029.7573, 3036.3222, 3038.0324, 3086.3059, 3094.9386, 3112.3149, 3121.9339, 3127.9074, 3143.1043, 3159.3044

IRC



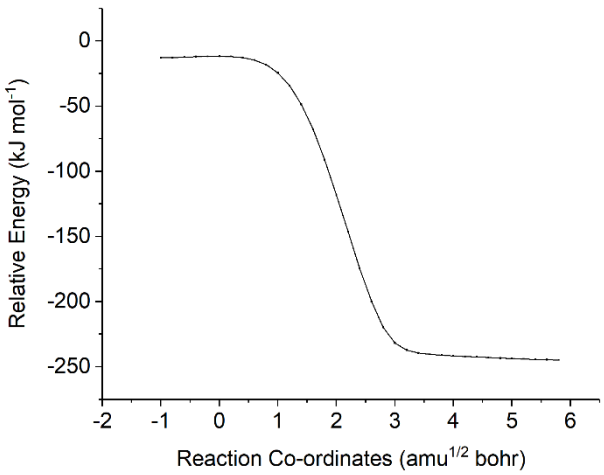
Compound: $MeCHCMe_2 + O_3$ CPr_{SYN}	**Energy (Hartree)** -421.608401293787
Reaction Coordinates: 6 -1.488448 1.338632 -0.286630 6 -1.854330 -0.096253 0.001738 6 1.889394 -0.664075 0.570923 6 2.128980 -1.238853 -0.755259 1 2.150474 -2.323929 -0.714141 1 3.064026 -0.835816 -1.154851 1 1.345868 -0.896240 -1.434895 1 1.729606 -1.246798 1.469673 6 -3.329642 -0.427465 0.047561 1 -3.761668 -0.303519 -0.948398 1 -3.477811 -1.451333 0.380144 1 -3.859087 0.262054 0.707601 1 -2.046749 1.708205 -1.149184 1 -0.418756 1.452958 -0.450077 1 -1.786502 1.958356 0.563704 8 1.865527 0.575688 0.780137 8 2.022237 1.403722 -0.314372 8 -1.014654 -0.953892 0.191788	**Frequencies (cm^{-1}):** 26.1022, 41.0813, 54.7406, 71.8994, 77.7347, 86.7309, 97.3139, 152.8184, 161.0665, 296.7717, 391.7577, 452.845, 497.3666, 540.9522, 669.6858, 764.0928, 788.3718, 876.3052, 888.2451, 900.9167, 986.1014, 1055.4851, 1089.8235, 1112.1629, 1123.7228, 1242.6301, 1354.1102, 1387.8518, 1396.6765, 1399.4392, 1440.0942, 1461.0493, 1462.1664, 1466.7276, 1475.5573, 1494.8781, 1576.2977, 1762.2427, 3019.0949, 3026.9161, 3030.9632, 3072.7577, 3073.0736, 3083.7923, 3122.6784, 3137.047, 3143.3993, 3183.1819

S10.9 Ozonolysis of 2-methyl-2-pentene (Alkene 7)

Compound: $EtCHCMe_2 + O_3$ PRC1.1	**Energy (Hartree)** -460.747340455438
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -2.926431 -1.475814 -0.386089 6 -1.736522 -0.944110 0.425894 6 -0.801170 -0.123331 -0.402321 6 -0.412376 1.154885 -0.223088 6 0.556467 1.792245 -1.175016 6 -0.872458 2.040682 0.897410 1 1.490925 2.043468 -0.661643 1 0.159821 2.732333 -1.567837 1 0.795951 1.140772 -2.013611 1 -0.015520 2.387482 1.480770 1 -1.358724 2.934926 0.497538 1 -1.566088 1.553234 1.576623 1 -0.401677 -0.639481 -1.271131 1 -2.099906 -0.386042 1.287935 1 -1.175474 -1.795430 0.824746 1 -3.541740 -0.658781 -0.764871 1 -3.557798 -2.118530 0.228378 1 -2.587324 -2.061404 -1.242132 8 1.449466 -0.472725 1.081214 8 2.442836 -0.518140 0.299294 8 2.484260 -1.484121 -0.529947	24.3772, 39.0395, 52.1489, 56.6795, 69.4759, 101.5354, 122.3423, 156.3385, 192.7105, 210.6896, 262.5123, 305.4494, 366.032, 418.5862, 482.2918, 512.7082, 731.7565, 752.2646, 826.8154, 869.7889, 920.3645, 962.6203, 1003.8852, 1015.6723, 1079.2643, 1094.4421, 1098.6073, 1143.5357, 1147.1185, 1167.0006, 1239.2296, 1290.7326, 1337.6765, 1393.3027, 1408.3391, 1414.3389, 1419.4656, 1469.915, 1475.9219, 1487.2231, 1491.0555, 1495.4187, 1498.928, 1506.5892, 1675.1502, 3001.9397, 3010.1237, 3017.1463, 3025.9382, 3043.6647, 3053.8741, 3069.224, 3090.55, 3091.6538, 3104.5644, 3119.7839, 3127.8807

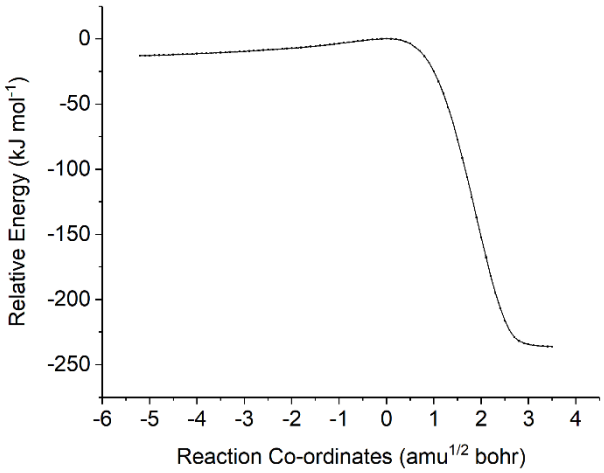
Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 1.1	**Energy (Hartree)** -460.744901381960
Reaction Coordinates: 6 3.070359 -0.360149 0.108386 6 1.660901 -0.888308 -0.207046 6 0.597663 -0.176813 0.568100 6 -0.069520 0.960791 0.177542 6 -0.938176 1.682539 1.168994 6 0.244327 1.701946 -1.090320 1 -1.821607 2.104339 0.691028 1 -0.384251 2.514758 1.616030 1 -1.258309 1.027084 1.978052 1 0.672892 1.059699 -1.855002 1 -0.651203 2.168967 -1.498254 1 0.960536 2.503321 -0.883164 1 0.486292 -0.479461 1.602977 1 1.467298 -0.809970 -1.276691 1 1.615687 -1.950503 0.036204 1 3.175172 0.689398 -0.168216 1 3.821902 -0.929343 -0.439971 1 3.295278 -0.447932 1.172378 8 -1.812563 -0.211244 -0.916951 8 -2.026263 -1.076576 0.014105 8 -1.007801 -1.833479 0.236683	**Frequencies (cm^{-1}):** -148.1205, 54.1249, 65.1226, 107.6598, 126.0068, 153.4591, 169.4816, 179.9395, 182.1914, 215.7886, 313.0412, 357.4286, 399.0068, 444.0117, 511.7577, 547.3871, 740.4461, 749.8615, 824.3318, 883.1431, 912.0016, 957.3278, 1005.8709, 1011.9397, 1065.3115, 1080.7093, 1086.6118, 1094.9507, 1115.5838, 1149.9181, 1237.5583, 1294.3723, 1337.9675, 1376.0062, 1406.7923, 1410.381, 1419.3049, 1472.8497, 1479.6381, 1481.9242, 1492.6201, 1498.4052, 1503.0607, 1511.6697, 1587.1901, 3008.281, 3016.5786, 3026.927, 3046.1347, 3072.6226, 3072.7756, 3081.6067, 3090.5786, 3096.0364, 3109.7847, 3128.8697, 3146.0254
IRC:	



Compound: $EtCHCMe_2 + O_3$ POZ1.1	**Energy (Hartree)** -460.844826485851
Reaction Coordinates: 6 1.726537 -0.747415 0.329396 6 0.356559 -0.595628 -0.315866 6 -0.532778 0.659786 0.031630 6 -0.722567 1.547477 -1.193997 1 -1.372356 2.389784 -0.958182 1 0.235710 1.939768 -1.539840 1 -1.172539 0.977958 -2.006301 6 -0.116607 1.455738 1.261655 1 0.017222 0.806456 2.124222 1 0.805906 2.005831 1.080125 1 -0.894427 2.180129 1.502940 8 -1.795585 0.047508 0.401689 8 -1.762202 -1.243175 -0.236261 8 -0.447294 -1.697684 0.106936 1 0.458280 -0.641425 -1.404884 1 2.016807 -1.793823 0.215279 1 1.659150 -0.561621 1.400877 6 2.797042 0.139066 -0.308735 1 2.569363 1.200482 -0.207539 1 3.764150 -0.033649 0.162782 1 2.904267 -0.077216 -1.372878	**Frequencies (cm^{-1}):** 52.8853, 113.4263, 187.0898, 214.8036, 230.4054, 251.427, 291.0146, 303.4499, 331.9844, 382.0785, 419.3479, 466.621, 515.5523, 608.5525, 699.1929, 711.1992, 771.1634, 824.6508, 860.66, 933.7451, 938.7342, 940.1331, 963.0493, 1003.4908, 1023.3307, 1060.4343, 1110.9264, 1159.7843, 1182.9483, 1216.0754, 1255.0844, 1297.3725, 1334.5637, 1373.7122, 1402.6847, 1404.4904, 1420.5908, 1424.2249, 1478.7767, 1489.1409, 1493.9075, 1499.9695, 1502.3072, 1508.7366, 1515.988, 3003.7631, 3031.3114, 3032.5537, 3041.8825, 3046.379, 3075.619, 3094.2251, 3096.9861, 3098.0272, 3106.8693, 3111.6073, 3123.6411

Compound: $EtCHCMe_2 + O_3$ PRC1.2	**Energy (Hartree)** -460.747724375538
Reaction Coordinates: 6 1.514008 -1.269378 0.756672 6 0.622896 -0.070354 0.906175 6 0.513660 1.110020 0.260584 6 1.349596 1.607772 -0.883666 1 0.703695 1.887865 -1.719910 1 2.078691 0.894468 -1.243701 1 1.879330 2.517823 -0.586549 6 -0.549355 2.081412 0.692933 1 -1.074408 1.750442 1.586899 1 -1.288830 2.218113 -0.103830	**Frequencies (cm^{-1}):** 25.6604, 44.3871, 51.0711, 53.7853, 83.6472, 101.5725, 111.5851, 174.1157, 238.9903, 251.4035, 275.4482, 316.4937, 336.1399, 397.371, 462.9088, 619.2409, 730.9618, 740.3755, 776.6171, 885.0587, 895.453, 961.3383, 1007.8813, 1032.7309, 1079.2222, 1094.997, 1104.0563, 1140.7121, 1147.8444, 1163.6155,

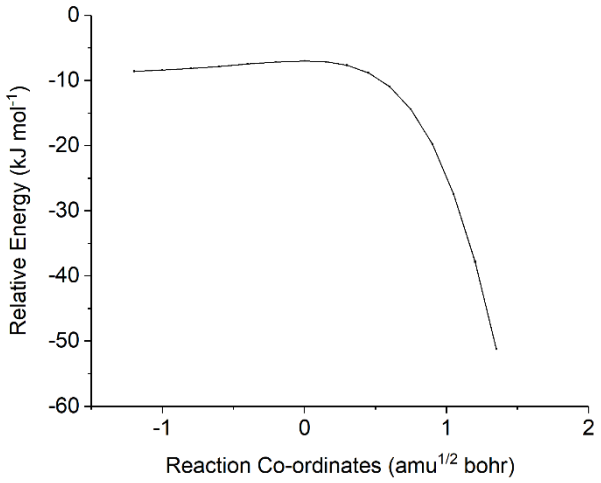
1 -0.121667 3.068858 0.886398 1 -0.075941 -0.205984 1.727055 1 0.843025 -2.130363 0.661652 6 2.568339 -1.351450 -0.344308 1 3.324342 -0.571842 -0.251919 1 2.125811 -1.287109 -1.337879 1 3.082301 -2.311249 -0.278471 1 2.004921 -1.416429 1.726386 8 -1.171745 -0.677283 -1.036562 8 -2.321842 -0.404536 -0.583605 8 -2.705930 -1.051022 0.445608	1224.1557, 1312.257, 1382.8257, 1400.693, 1411.8033, 1420.3499, 1427.533, 1465.1825, 1470.8392, 1479.773, 1491.4561, 1497.5721, 1511.2134, 1515.2005, 1674.1797, 2987.5776, 3000.3032, 3006.8705, 3016.2611, 3033.5309, 3042.6471, 3050.6253, 3087.4138, 3100.844, 3105.5098, 3116.6265, 3184.6047

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 1.2	**Energy (Hartree)** -460.739786646692
Reaction Coordinates: 6 -2.517389 0.046252 -0.472549 6 -1.819378 -0.769219 0.628382 6 -0.377775 -0.441323 0.916786 6 0.702277 -0.883915 0.182516 6 2.082458 -0.753494 0.763092 6 0.556397 -1.802240 -0.996841 1 2.161339 0.114828 1.416673 1 2.839419 -0.674003 -0.015414 1 2.318912 -1.637634 1.364018 1 1.330991 -1.606804 -1.737146 1 -0.410924 -1.711338 -1.482297 1 0.675215 -2.841190 -0.671817 1 -0.164801 -0.022691 1.891504 1 -1.881728 -1.829795 0.365439 1 -2.384237 -0.656002 1.554830 1 -2.605922 1.091877 -0.190624 1 -3.517892 -0.353819 -0.641555 1 -1.968904 0.010457 -1.412243 8 0.877242 0.995325 -1.129709 8 0.866211 1.850904 -0.160878 8 -0.262328 1.871241 0.469377	**Frequencies (cm^{-1}):** -184.7692, 50.4835, 86.4092, 113.7601, 137.8623, 147.3028, 164.4755, 191.3028, 201.9791, 234.44, 285.7862, 343.2962, 394.391, 442.8648, 510.9799, 591.2409, 735.1897, 744.0848, 826.9125, 870.1603, 899.3584, 957.4594, 1007.6298, 1020.4367, 1058.9903, 1073.302, 1088.0406, 1100.7156, 1110.7763, 1134.2899, 1235.3982, 1302.7241, 1357.5725, 1373.2093, 1407.9464, 1413.5969, 1420.4798, 1472.6008, 1480.0011, 1480.8523, 1490.4083, 1492.8335, 1506.1366, 1512.2903, 1574.2953, 3006.6021, 3010.109, 3014.2479, 3042.1801, 3056.0302, 3074.7985, 3084.4545, 3104.1582, 3112.7303, 3129.7948, 3136.1839, 3163.6699
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ1.2	**Energy (Hartree)** -460.841474813509
Reaction Coordinates: 6 1.743490 -0.439424 0.783544 6 0.358621 0.214437 0.766326 6 -0.831376 -0.467249 -0.022909 6 -2.028609 -0.663614 0.905749 1 -2.870966 -1.080670 0.354598 1 -1.776029 -1.347694 1.718098 1 -2.331513 0.287350 1.341226 6 -0.514041 -1.742532 -0.789863 1 -1.398525 -2.068054 -1.336938 1 0.291958 -1.597387 -1.502786 1 -0.238514 -2.540709 -0.100893 8 -1.138444 0.528552 -1.021177 8 -0.850125 1.757360 -0.340904 8 0.476537 1.505535 0.160495 1 0.022033 0.340278 1.799141 1 1.606289 -1.499856 1.007186 1 2.285008 -0.026756 1.637272 6 2.605437 -0.260637 -0.468328 1 2.836668 0.789223 -0.635493 1 3.545488 -0.799746 -0.346243 1 2.123227 -0.633452 -1.369594	**Frequencies (cm^{-1}):** 31.4557, 97.9497, 173.3504, 211.4148, 236.1125, 259.6678, 264.073, 285.9836, 341.214, 357.6992, 406.0484, 501.7996, 564.0141, 627.5542, 699.0777, 717.6724, 761.8879, 808.9397, 860.4008, 917.9469, 930.4121, 934.0109, 954.1294, 975.5551, 1021.6561, 1086.9356, 1098.312, 1141.2577, 1186.327, 1206.6786, 1256.9978, 1305.117, 1346.9067, 1371.5275, 1398.596, 1405.4694, 1423.6047, 1428.4515, 1477.2474, 1488.2502, 1489.5688, 1496.7173, 1501.3657, 1506.1677, 1517.4918, 3008.5522, 3031.9684, 3034.1431, 3045.7197, 3050.0698, 3055.6507, 3094.7489, 3104.6311, 3104.9209, 3115.4515, 3120.6432, 3144.2798

Compound: $EtCHCMe_2 + O_3$ PRC1.3	**Energy (Hartree)** -460.747724375538
Reaction Coordinates: 6 -1.528255 -2.408615 -0.110197 6 -1.976308 -0.944957 -0.030330 6 -0.994301 -0.003626 -0.657275 6 -0.639514 1.231222 -0.250401 6 0.359265 2.031354 -1.032997 6 -1.199335 1.921692 0.958828 1 0.671289 1.520989 -1.942599 1 1.251486 2.230300 -0.429899 1 -0.049450 3.007845 -1.307121 1 -0.391776 2.295008 1.592614 1 -1.837492 1.281787 1.562039 1 -1.787859 2.792826 0.655777 1 -0.536041 -0.369073 -1.572324 1 -2.168225 -0.674373 1.007981 1 -2.936838 -0.844433 -0.550921 1 -0.588078 -2.557650 0.419014 1 -1.378789 -2.716079 -1.146597 1 -2.278585 -3.067411 0.327844 8 1.202822 -0.331289 1.065809 8 2.268628 -0.235307 0.390553 8 2.516181 -1.166173 -0.441559	**Frequencies (cm^{-1}):** 25.3411, 38.1564, 46.1916, 62.1397, 72.7198, 102.7148, 121.6829, 167.3478, 197.6592, 207.2022, 253.2639, 289.9318, 350.3514, 418.1852, 470.7755, 512.796, 730.7464, 746.4923, 824.0487, 865.476, 926.2027, 964.4243, 1001.8646, 1025.4569, 1086.8402, 1093.9333, 1098.4524, 1141.9493, 1146.0957, 1165.8577, 1237.7572, 1289.2825, 1338.3482, 1395.2342, 1409.9316, 1415.715, 1419.883, 1469.1078, 1474.3306, 1481.436, 1490.5559, 1494.4989, 1498.9472, 1507.7617, 1673.6631, 2981.2833, 3003.1462, 3016.5654, 3030.8419, 3043.5369, 3057.4094, 3062.1603, 3089.4291, 3103.5251, 3107.05, 3118.6057, 3125.6229

Compound: $EtCHCMe_2 + O_3$ TS_{ozo} 1.3	**Energy (Hartree)** -460.745048402460
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -3.003459 -0.232966 0.218382 6 -1.693548 -0.748272 -0.373478 6 -0.510738 -0.521799 0.515472 6 0.779968 -0.883888 0.220106 6 1.844579 -0.788076 1.275002 6 1.125176 -1.655769 -1.020962 1 1.554590 -0.117395 2.082811 1 2.788974 -0.442421 0.855539 1 2.029012 -1.775108 1.711936 1 1.021286 -2.729528 -0.833369 1 2.157205 -1.476167 -1.318794 1 0.477770 -1.399694 -1.856163 1 -0.716644 -0.182554 1.523842 1 -1.507235 -0.267510 -1.338019 1 -1.782883 -1.819739 -0.587671 1 -2.951217 0.840414 0.399510 1 -3.227357 -0.723912 1.167379 1 -3.837776 -0.420843 -0.457380 8 1.275637 1.138352 -0.896046 8 0.794931 1.959291 -0.028715 8 -0.477767 1.839743 0.130167	-126.491, 68.9222, 76.5664, 112.5713, 123.5622, 150.6893, 156.4756, 181.0043, 193.376, 209.4068, 288.478, 329.1104, 421.1836, 430.5905, 492.2905, 517.4084, 738.6056, 752.5652, 814.2382, 869.5764, 930.2156, 958.748, 1009.0385, 1036.3133, 1070.9306, 1086.9033, 1089.5301, 1099.3898, 1114.1089, 1139.2754, 1232.4285, 1289.9454, 1340.3804, 1382.917, 1408.0571, 1416.1403, 1418.9474, 1461.1663, 1473.1831, 1480.6995, 1483.5446, 1500.625, 1501.5581, 1506.1808, 1589.6959, 2990.1223, 3008.1951, 3013.7395, 3026.3928, 3031.5984, 3071.7701, 3082.5418, 3087.4777, 3101.8727, 3109.1984, 3124.5935, 3149.3621
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ1.3	**Energy (Hartree)** -460.845901713431
Reaction Coordinates: 6 1.672473 -0.747777 -0.199550 6 0.513832 0.073422 0.339480 6 -0.953385 -0.413689 0.034679 6 -1.670419 -0.796857 1.325247 1 -2.693753 -1.107462 1.116577 1 -1.156306 -1.623029 1.820911 1 -1.695486 0.050545 2.009221 6 -1.087757 -1.488648 -1.035441 1 -0.574404 -1.202557 -1.950762 1 -0.685300 -2.437941 -0.682155 1 -2.141390 -1.639102 -1.270005 8 -1.557208 0.770646 -0.541564 8 -0.764883 1.852708 -0.017294 8 0.565550 1.373544 -0.252371	**Frequencies (cm^{-1}):** 50.885, 98.4154, 179.7514, 214.5487, 229.8212, 257.0531, 283.636, 299.8391, 321.321, 347.0321, 443.3669, 488.5574, 505.5981, 600.0054, 700.7677, 749.1161, 775.0452, 810.0957, 865.2591, 932.9256, 936.3662, 939.0062, 967.3431, 975.3204, 1019.3547, 1062.3722, 1117.8919, 1160.6095, 1184.1923, 1213.5223, 1259.1745, 1302.7511, 1344.2241, 1358.8357, 1403.7369, 1408.8623, 1418.4758, 1424.2717, 1473.9708, 1483.9326, 1490.184, 1498.2063,

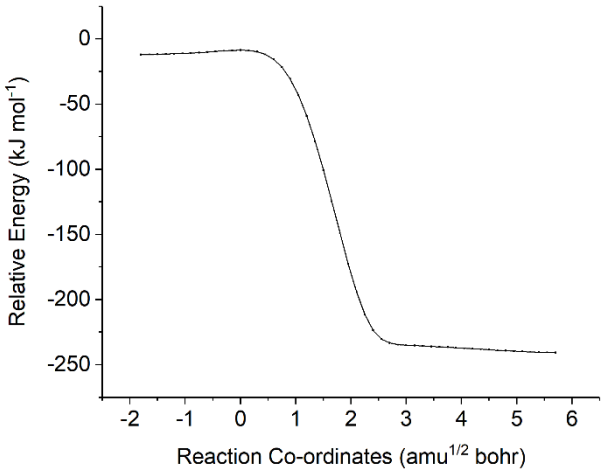
1 0.612346 0.183647 1.424295 1 1.556572 -1.770529 0.167259 1 1.609302 -0.790614 -1.287323 6 3.035988 -0.201019 0.225423 1 3.124432 -0.163640 1.312713 1 3.838966 -0.833866 -0.152727 1 3.192963 0.806770 -0.157191	1500.1633, 1507.6806, 1510.4988, 3002.5993, 3029.7136, 3030.8764, 3031.2636, 3044.2585, 3071.4208, 3092.1848, 3092.6604, 3103.6445, 3105.7702, 3112.4243, 3123.6743

Compound: $EtCHCMe_2 + O_3$ PRC 2.1	**Energy (Hartree)** -460.751783712005
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.001608 1.052763 0.198353 6 -1.637208 0.725716 -0.423354 6 -0.780670 -0.112455 0.471376 6 -0.134832 -1.259034 0.181313 6 0.713261 -1.936271 1.217679 6 -0.218846 -1.987250 -1.130137 1 0.376408 -2.963249 1.386052 1 1.750536 -1.995819 0.877005 1 0.699729 -1.404488 2.167021 1 0.781746 -2.173632 -1.525892 1 -0.786946 -1.454879 -1.887784 1 -0.682631 -2.966847 -0.981932 1 -0.679968 0.265061 1.484517 1 -1.777973 0.252435 -1.394376 1 -1.114039 1.669995 -0.621498 1 -3.583664 0.145733 0.365649 1 -3.578486 1.710073 -0.453067 1 -2.884327 1.554850 1.160039 8 1.925602 0.431374 -0.932292 8 1.700829 1.555159 -0.394783 8 1.603448 1.570962 0.868685	29.2275, 39.6196, 48.3274, 66.479, 73.649, 92.3192, 148.0055, 161.3737, 201.1173, 211.2481, 273.1839, 304.5078, 363.7559, 421.248, 488.8513, 510.2296, 738.8918, 750.5936, 824.8152, 862.694, 922.278, 962.9471, 1006.5153, 1018.8988, 1081.1436, 1093.9354, 1099.5826, 1143.6492, 1154.4732, 1171.8565, 1236.5816, 1292.091, 1338.4629, 1391.6324, 1408.2846, 1413.6368, 1419.4938, 1469.3301, 1474.9754, 1484.1329, 1489.0941, 1495.9253, 1499.2529, 1505.2213, 1671.4855, 2977.5611, 3009.919, 3018.4747, 3026.53, 3051.2988, 3059.8369, 3068.5702, 3091.0571, 3091.4878, 3108.8168, 3125.3984, 3128.0445

Compound: $EtCHCMe_2 + O_3$ TS_{ozo} 2.1	**Energy (Hartree)** -460.742913889416
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 3.013184 -0.288539 0.004775 6 1.611362 -0.913995 -0.095548 6 0.574447 -0.126895 0.648329 6 -0.101753 0.972647 0.160745 6 -0.922865 1.809094 1.094706 6 0.190095 1.581615 -1.183780 1 -1.862578 2.105240 0.628123 1 -1.149367 1.277675 2.016799 1 -0.383173 2.727539 1.348147 1 -0.697255 2.058358 -1.596503 1 0.555686 0.856456 -1.906837 1 0.954092 2.358318 -1.075121 1 0.514424 -0.304809 1.714142 1 1.332293 -1.011486 -1.146224 1 1.643633 -1.924580 0.311238 1 3.040152 0.708789 -0.434403 1 3.743955 -0.906652 -0.518182	-181.1186, 54.02, 72.8453, 119.6983, 145.1096, 165.0871, 183.5146, 186.8669, 195.1584, 218.0639, 309.8123, 354.167, 401.5708, 454.3051, 522.7918, 562.4166, 740.3799, 749.1805, 825.8896, 884.8969, 910.7131, 958.3067, 1006.5499, 1012.1368, 1065.0227, 1075.7464, 1078.9228, 1094.3438, 1114.621, 1145.6073, 1237.9765, 1298.5338, 1339.7951, 1368.9063, 1407.6763, 1410.7949, 1419.6865, 1470.7354, 1478.4169, 1479.7185, 1492.5676, 1498.5335, 1502.571, 1511.2965, 1575.1834, 3008.7156, 3013.3935, 3028.8012, 3039.2506, 3071.7678,

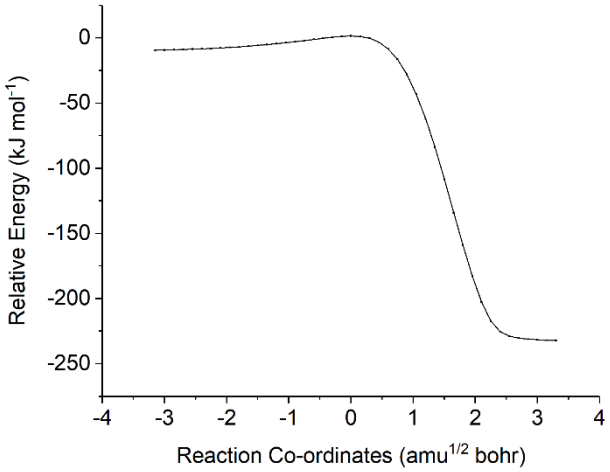
1 3.330296 -0.203388 1.045018 8 -1.990977 -0.186153 -0.636526 8 -1.552170 -1.397193 -0.533666 8 -1.107976 -1.659782 0.649996	3073.0656, 3083.7123, 3090.4455, 3098.6306, 3116.4479, 3124.0163, 3162.3047

IRC:



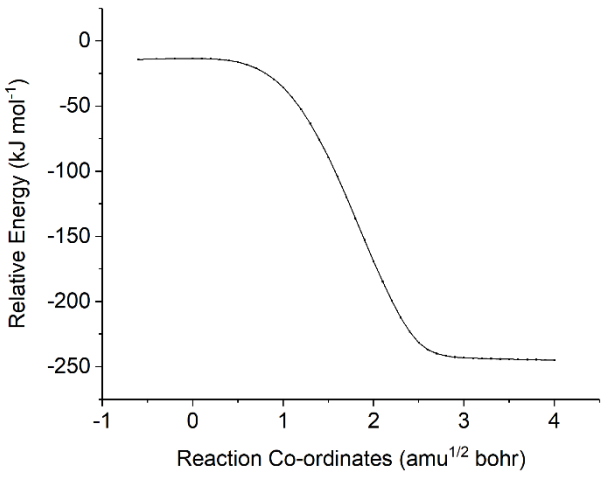
Compound: $EtCHCMe_2 + O_3$ POZ 2.1	**Energy (Hartree)** -460.843501343655
Reaction Coordinates: 6 1.667493 -0.828110 0.248072 6 0.364867 -0.541504 -0.492456 6 -0.521618 0.659809 -0.010703 6 -0.453937 1.856948 -0.948252 1 -1.173513 2.616647 -0.644264 1 0.539922 2.302516 -0.920321 1 -0.674248 1.557802 -1.971927 6 -0.321935 1.057974 1.448917 1 -1.041917 1.834302 1.706092 1 -0.481736 0.209219 2.110144 1 0.678056 1.452318 1.624326 8 -1.843077 0.102884 -0.179027 8 -1.674264 -1.216978 0.320601 8 -0.513746 -1.683048 -0.425510 1 0.577979 -0.405180 -1.556139 1 1.987376 -1.825477 -0.058793 1 1.482791 -0.882786 1.321102 6 2.784283 0.169736 -0.063184 1 2.545179 1.179939 0.270611 1 3.709224 -0.125741 0.431749 1 2.984664 0.214458 -1.135451	**Frequencies (cm^{-1}):** 47.4534, 126.4152, 192.5844, 207.5033, 219.7459, 254.4629, 273.7822, 299.043, 334.8363, 349.228, 429.6521, 481.6655, 507.1535, 616.1306, 684.515, 741.1934, 764.233, 832.789, 872.5007, 911.836, 934.2853, 943.4107, 964.3483, 989.8548, 1024.021, 1051.7533, 1097.6096, 1139.996, 1190.2706, 1228.5345, 1247.518, 1292.2529, 1329.372, 1363.5998, 1400.8704, 1404.7698, 1417.9464, 1423.8806, 1480.2859, 1489.7912, 1493.3749, 1501.5444, 1501.712, 1510.1692, 1515.7845, 3020.5767, 3028.9326, 3041.7889, 3043.3856, 3048.8662, 3071.5452, 3092.9159, 3095.1476, 3106.1513, 3112.3338, 3115.3751, 3125.813

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 2.2	**Energy (Hartree)** -460.739223263807
Reaction Coordinates: 6 2.471674 -0.371705 0.413611 6 1.565857 -1.194268 -0.516112	**Frequencies (cm^{-1}):** -210.381, 64.1734, 78.7749, 144.4476, 152.7367, 168.0899, 178.485, 199.2285,

6 0.229373 -0.599878 -0.885614 6 -0.923128 -0.706495 -0.128596 6 -2.251413 -0.437599 -0.770653 6 -0.954805 -1.452280 1.177614 1 -2.149359 0.205804 -1.642041 1 -2.940437 0.034657 -0.071257 1 -2.704924 -1.381829 -1.090402 1 -1.749325 -1.078267 1.820557 1 -0.016942 -1.388890 1.722906 1 -1.160883 -2.511743 0.988926 1 0.100554 -0.317922 -1.920912 1 1.394114 -2.171246 -0.054085 1 2.111499 -1.388760 -1.440557 1 2.750496 0.571745 -0.050663 1 3.380587 -0.934139 0.629029 1 1.987581 -0.143141 1.362637 8 -0.943726 1.401001 0.806164 8 0.239578 1.811944 0.479121 8 0.475608 1.671689 -0.784740	224.9638, 238.2085, 291.5851, 336.3554, 394.844, 458.776, 508.2422, 606.2353, 736.6651, 741.9745, 825.4385, 880.9332, 898.2541, 956.9904, 1010.4448, 1023.0714, 1057.7753, 1070.4666, 1088.8278, 1101.6903, 1111.7485, 1131.7605, 1235.1962, 1304.1358, 1356.3034, 1366.5303, 1409.1368, 1411.9132, 1420.3169, 1470.5815, 1474.4364, 1480.2292, 1490.1934, 1497.1972, 1506.0978, 1513.2282, 1562.894, 3004.8635, 3008.4611, 3010.6017, 3039.3617, 3056.5642, 3077.4097, 3087.8548, 3097.769, 3118.7522, 3119.9338, 3130.1692, 3175.0173
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ 2.2	**Energy (Hartree)** -460.840392867891
Reaction Coordinates: 6 -1.629032 -0.759939 -0.705251 6 -0.322266 0.029848 -0.857520 6 0.920513 -0.342683 0.035470 6 2.037185 -0.970964 -0.789100 1 2.932028 -1.101438 -0.181324 1 1.728418 -1.953174 -1.148652 1 2.284552 -0.345550 -1.645490 6 0.622602 -1.160980 1.288302 1 1.559527 -1.387722 1.796436 1 -0.009530 -0.603086 1.973249 1 0.133418 -2.104515 1.047289 8 1.396478 0.966349 0.419174 8 0.181882 1.684007 0.617377 8 -0.509332 1.438771 -0.634396 1 -0.006483 -0.041134 -1.899851 1 -1.388793 -1.826859 -0.722673	**Frequencies (cm^{-1}):** 33.2038, 94.3935, 192.1587, 217.787, 227.7734, 266.1785, 278.2379, 287.9476, 312.593, 361.7135, 438.1265, 503.8548, 554.0692, 634.154, 683.3027, 747.6194, 773.2159, 807.8858, 859.3256, 902.9729, 929.6835, 941.4005, 949.6806, 969.7482, 1025.4588, 1083.6496, 1091.9296, 1123.255, 1189.0178, 1221.0166, 1245.5609, 1297.0915, 1351.0727, 1359.2106, 1401.0082, 1404.5703, 1419.7757, 1426.7973, 1480.5737, 1483.3825, 1493.0461, 1498.3334, 1505.3499, 1511.8922, 1517.0094, 3018.5421, 3037.2543, 3039.2362,

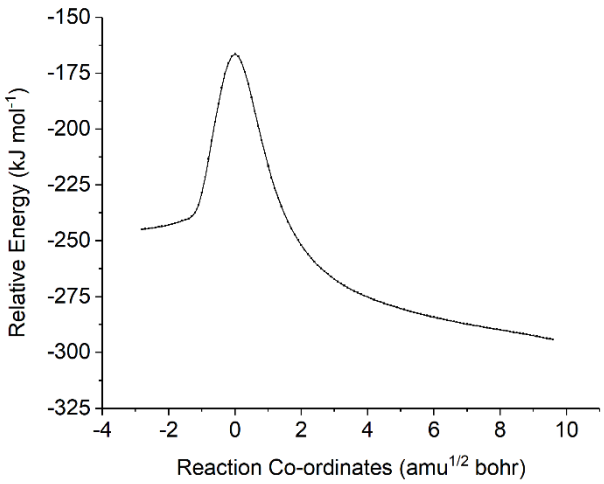
1 -2.205700 -0.575836 -1.614361 6 -2.515267 -0.422626 0.494516 1 -2.702283 0.648812 0.544259 1 -3.477021 -0.926320 0.392618 1 -2.082768 -0.732126 1.442758	3046.0323, 3047.9443, 3051.4913, 3099.815, 3102.2491, 3105.9589, 3114.9782, 3123.0568, 3139.602

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 2.3	**Energy (Hartree)** -460.744562310228
Reaction Coordinates: 6 -2.940131 -0.498997 0.192076 6 -1.580485 -0.804563 -0.430586 6 -0.431965 -0.610759 0.510496 6 0.889236 -0.809358 0.181562 6 1.942728 -0.756866 1.244621 6 1.303424 -1.395740 -1.140571 1 2.295133 -1.767314 1.475906 1 2.806458 -0.184736 0.904273 1 1.569521 -0.302992 2.160392 1 2.312160 -1.085961 -1.408047 1 0.634233 -1.118090 -1.951319 1 1.305209 -2.488907 -1.070018 1 -0.671360 -0.463757 1.555443 1 -1.568342 -1.833872 -0.807885 1 -1.428106 -0.176186 -1.315750 1 -3.130187 -1.139886 1.054960 1 -3.744101 -0.661319 -0.525717 1 -2.985733 0.537508 0.525673 8 1.306422 1.398360 -0.555729 8 0.106342 1.873917 -0.539670 8 -0.474230 1.720624 0.602462	**Frequencies (cm^{-1}):** -155.9795, 65.8628, 79.7094, 125.0189, 144.5644, 155.7207, 167.4377, 187.0588, 207.5286, 217.3186, 291.1199, 330.7988, 420.4388, 452.9391, 506.7389, 517.5295, 737.4264, 761.4205, 814.1708, 870.1303, 931.0773, 960.9485, 1008.0967, 1037.6528, 1067.2787, 1079.2626, 1086.3053, 1098.115, 1112.1505, 1138.5875, 1232.7408, 1287.0828, 1337.5211, 1377.4321, 1409.2684, 1415.9508, 1419.4432, 1466.0984, 1471.3071, 1477.6821, 1482.4807, 1499.4956, 1500.3425, 1507.9302, 1580.9457, 2986.8401, 3002.4501, 3006.8086, 3012.3662, 3030.4233, 3071.1719, 3083.8721, 3088.3992, 3102.507, 3115.8668, 3124.479, 3164.8054
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ 2.3	**Energy (Hartree)** -460.844901066989

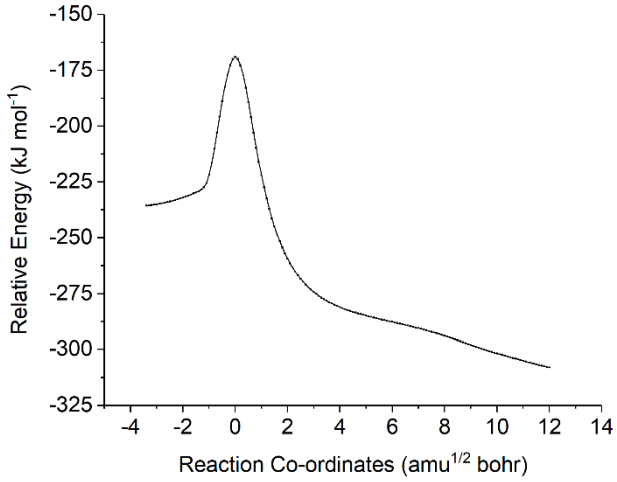
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.608994 -0.691290 0.381261 6 -0.506994 -0.049396 -0.451245 6 0.980740 -0.372674 -0.049653 6 1.711809 -1.158509 -1.129623 1 2.767087 -1.262012 -0.878330 1 1.286842 -2.158935 -1.217035 1 1.630206 -0.656781 -2.092727 6 1.150152 -1.006620 1.328265 1 2.213037 -1.132768 1.531758 1 0.726096 -0.373767 2.104785 1 0.676955 -1.986669 1.380867 8 1.572688 0.945357 -0.043607 8 0.514314 1.751675 0.470474 8 -0.576638 1.388640 -0.408813 1 -0.652831 -0.298266 -1.505013 1 -1.516220 -0.362457 1.417020 1 -1.462241 -1.774885 0.376739 6 -3.004380 -0.361941 -0.147967 1 -3.133577 -0.718363 -1.172004 1 -3.772830 -0.831357 0.466415 1 -3.179431 0.713459 -0.143127	37.7871, 105.7857, 190.8539, 219.5431, 222.7744, 258.1937, 285.9021, 290.4856, 321.0124, 341.2438, 464.8371, 490.2754, 506.3945, 610.0883, 703.2477, 740.3268, 769.374, 835.4526, 874.2226, 910.4849, 931.7367, 942.3624, 964.0713, 974.8783, 1023.5637, 1059.0311, 1099.5441, 1138.8188, 1188.8782, 1221.8449, 1244.8372, 1296.7898, 1322.7599, 1354.1272, 1402.6848, 1404.9084, 1416.2299, 1422.515, 1473.8661, 1483.5697, 1490.9123, 1499.5985, 1501.3279, 1508.9773, 1512.1057, 3021.9935, 3027.8837, 3033.3401, 3038.2292, 3047.0145, 3069.1242, 3089.9786, 3100.9758, 3103.4849, 3108.3195, 3113.9712, 3124.397

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 1	**Energy (Hartree)** -460.811539072716
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.761296 0.142974 -0.273923 6 1.730179 -0.815328 0.320875 6 0.355126 -0.733891 -0.293151 6 -0.727340 0.828886 0.053570 6 -0.292233 1.786076 -1.065222 6 -0.353458 1.257299 1.475071 1 -0.582893 1.382800 -2.033404 1 -0.818916 2.731962 -0.925774 1 0.775882 1.993371 -1.061481 1 0.693505 1.544724 1.568555 1 -0.962657 2.122327 1.743400 1 -0.578011 0.460195 2.181322 1 0.287241 -0.669948 -1.375421 1 2.075802 -1.842114 0.166635 1 1.656004 -0.680008 1.400193 1 2.548232 1.181808 -0.028932 1 3.750159 -0.089653 0.119490 1 2.808765 0.055607 -1.360181 8 -1.915600 0.349406 -0.083706 8 -1.661477 -1.590896 -0.366806 8 -0.484739 -1.631906 0.238297	-479.1659, 74.237, 84.0426, 187.0363, 194.4555, 209.3752, 225.7804, 263.1228, 272.7625, 288.9553, 354.1889, 403.9203, 444.9637, 483.4066, 515.2923, 566.7698, 617.3961, 766.3513, 789.4478, 910.0444, 924.2431, 979.7504, 1000.2722, 1039.4269, 1061.2736, 1070.1991, 1117.0657, 1150.1401, 1163.1063, 1189.3258, 1243.9402, 1302.3482, 1329.4567, 1375.6091, 1387.3813, 1403.5334, 1411.8623, 1425.2802, 1474.0566, 1482.9939, 1489.0423, 1493.334, 1501.6197, 1505.9289, 1513.7988, 3017.9122, 3032.4811, 3037.6761, 3040.1015, 3071.491, 3090.9851, 3099.6783, 3099.7627, 3110.531, 3116.7395, 3119.5251, 3128.892
IRC:	

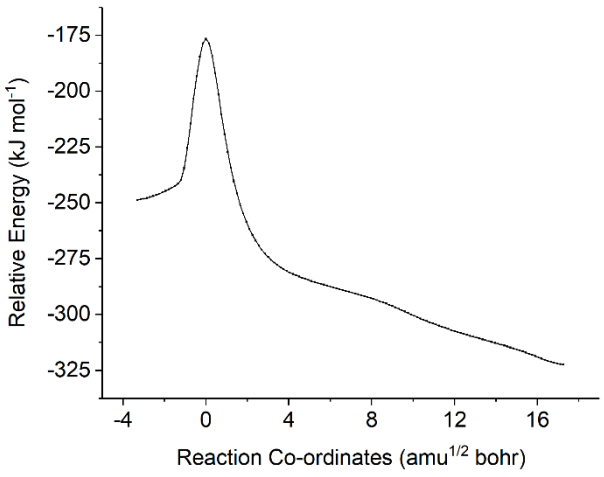


Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 1	**Energy (Hartree)** -460.864209176868
Reaction Coordinates: 6 -2.746572 -1.436900 -0.022976 6 -2.698950 0.093773 0.107491 6 -1.421595 0.658712 -0.382478 6 1.702731 -0.666516 0.009300 6 2.229291 -0.354244 1.389015 6 2.576816 -0.267518 -1.153963 1 1.628590 -0.853930 2.144791 1 3.274886 -0.652361 1.484713 1 2.175828 0.725306 1.538179 1 2.866290 0.779073 -1.065490 1 3.491250 -0.866794 -1.141119 1 2.054689 -0.428275 -2.093123 1 -1.008064 0.434117 -1.360372 1 -3.503362 0.530905 -0.496221 1 -2.855358 0.413215 1.137389 1 -1.957731 -1.900600 0.564735 1 -3.712220 -1.803948 0.322173 1 -2.615627 -1.748006 -1.059184 8 0.641492 -1.240803 -0.153890 8 0.420770 1.947482 -0.148486 8 -0.773448 1.444254 0.345526	**Frequencies (cm^{-1}):** 33.6457, 46.2326, 64.6811, 68.837, 80.8736, 93.4359, 105.0318, 139.3042, 145.6334, 200.6471, 227.2482, 321.4662, 384.8229, 421.2239, 485.633, 533.207, 536.2094, 773.9371, 788.5223, 891.6848, 901.2894, 902.674, 915.2185, 938.0514, 1022.5082, 1087.011, 1097.0075, 1117.6295, 1180.9584, 1242.8227, 1275.5046, 1325.1152, 1373.467, 1380.7905, 1388.5091, 1420.9052, 1458.2684, 1467.1285, 1468.123, 1470.9394, 1488.6784, 1496.2215, 1505.25, 1581.4933, 1749.075, 2996.7655, 3027.7843, 3035.9727, 3045.1524, 3084.8294, 3092.3543, 3097.7201, 3108.5523, 3128.7554, 3132.9936, 3140.2787, 3160.1392

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -460.813267916166
Reaction Coordinates: 6 -2.658095 -0.438840 0.413683 6 -1.672636 -0.577437 -0.747518 6 -0.443365 0.295819 -0.685945 6 1.090682 -0.423924 0.134999 6 1.625603 -1.325198 -0.989511 6 0.627738 -1.174306 1.386509 1 1.959700 -0.721056 -1.830512 1 2.484894 -1.878200 -0.607272	**Frequencies (cm^{-1}):** -466.3664, 82.1596, 98.5159, 184.1872, 199.4772, 212.44, 239.6671, 244.564, 249.7741, 306.4548, 362.9335, 410.1543, 442.0656, 484.479, 559.8324, 582.5296, 646.4352, 766.794, 786.865, 895.9897, 911.6849, 977.9318, 997.4033, 1044.8329, 1065.1108, 1076.9716, 1109.593,

1 0.885475 -2.050850 -1.328766 1 0.174912 -0.484580 2.095225 1 1.504707 -1.615617 1.863715 1 -0.069551 -1.981349 1.161706 1 0.036369 0.521708 -1.633061 1 -2.184905 -0.346862 -1.686364 1 -1.344368 -1.614215 -0.846498 1 -2.199718 -0.675262 1.371508 1 -3.054642 0.573268 0.476457 1 -3.495551 -1.119701 0.264124 8 1.783162 0.644963 0.353707 8 0.521620 2.130115 0.004566 8 -0.569393 1.381928 0.095031	1129.4466, 1168.9152, 1193.1954, 1249.9746, 1295.5509, 1367.2143, 1374.785, 1388.2109, 1393.1462, 1403.0975, 1427.864, 1474.7754, 1479.9962, 1488.7833, 1491.8261, 1503.0639, 1505.4831, 1510.3453, 3019.634, 3029.9611, 3034.704, 3049.6204, 3053.0351, 3087.0973, 3093.0151, 3108.7163, 3118.4941, 3122.2832, 3124.1391, 3125.5211
IRC:  	

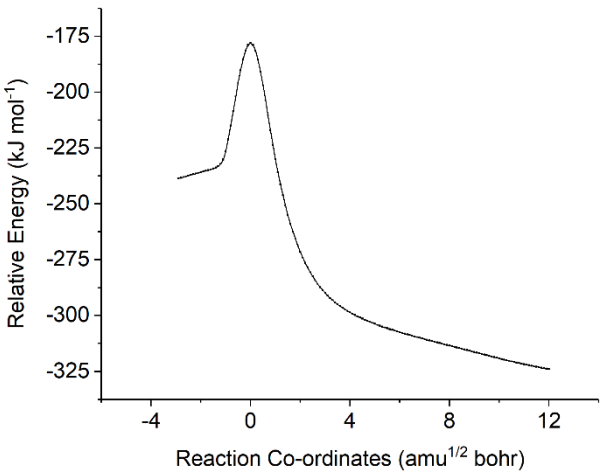
Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 2	**Energy (Hartree)** -460.861089237022
Reaction Coordinates: 6 -3.351808 -1.417482 -0.306008 6 -2.149754 -0.889328 0.493746 6 -1.483951 0.244468 -0.185015 6 2.176266 -0.407651 -0.020780 6 3.445724 -1.229661 -0.013609 6 2.331722 1.089590 0.039143 1 3.212973 -2.288251 0.064721 1 4.000555 -1.047661 -0.937139 1 4.096235 -0.925974 0.808424 1 2.729623 1.363638 1.020551 1 3.067427 1.424067 -0.695437 1 1.379951 1.596996 -0.116866 1 -1.083099 0.179235 -1.191020 1 -2.446748 -0.580228 1.495372 1 -1.401021 -1.680251 0.592891 1 -3.055857 -1.723214 -1.309867 1 -3.777666 -2.285516 0.195668 1 -4.130316 -0.660561 -0.396249 8 1.086472 -0.946040 -0.070669 8 -0.748029 2.383866 -0.273575 8 -1.388598 1.348187 0.397255	**Frequencies (cm^{-1}):** 23.9309, 35.6761, 46.5341, 69.9858, 77.4838, 94.4675, 98.5761, 142.0988, 155.4303, 205.0905, 221.0893, 331.0307, 395.5124, 417.9723, 498.7341, 534.2013, 545.5193, 777.4413, 791.8485, 889.4822, 893.0189, 904.4087, 910.6318, 940.0194, 1018.4545, 1092.5708, 1093.5578, 1125.6242, 1181.2031, 1246.6976, 1276.2185, 1324.046, 1373.2371, 1387.8472, 1402.1745, 1415.8393, 1462.5369, 1466.7706, 1472.8464, 1476.8279, 1496.5605, 1500.5129, 1505.5468, 1582.7457, 1756.4078, 3009.952, 3031.1276, 3031.3437, 3037.8114, 3069.9628, 3084.5503, 3086.4508, 3103.3832, 3106.1436, 3108.5046, 3136.8146, 3162.6793

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 3	**Energy (Hartree)** -460.815150365172
Reaction Coordinates: 6 -3.044257 -0.388912 -0.206862 6 -1.641666 -0.726048 0.316530 6 -0.586348 0.173317 -0.257533 6 1.208680 -0.382996 -0.023896 6 1.336254 -1.427883 -1.143975 6 1.297574 -0.944140 1.397884 1 1.276785 -0.945506 -2.117389 1 2.316476 -1.899817 -1.059722 1 0.581952 -2.212035 -1.073665 1 0.654244 -1.810476 1.550768 1 2.327827 -1.255570 1.578871 1 1.049927 -0.172990 2.124634 1 -0.545417 0.274780 -1.338291 1 -1.616308 -0.656224 1.404187 1 -1.393005 -1.755535 0.055297 1 -3.091941 -0.469447 -1.293537 1 -3.779588 -1.075585 0.212346 1 -3.331603 0.625274 0.069131 8 1.841179 0.720631 -0.230354 8 0.408585 2.121097 -0.224276 8 -0.483610 1.349908 0.378940	**Frequencies (cm^{-1}):** -457.3233, 71.7136, 88.4465, 163.3415, 198.7008, 207.7597, 223.3457, 239.4381, 264.134, 296.7229, 353.4822, 409.9526, 470.2056, 485.5686, 527.8649, 582.21, 622.0962, 770.3444, 784.3912, 910.532, 920.1128, 978.157, 994.6453, 1025.2795, 1055.252, 1066.4819, 1125.1303, 1152.2629, 1161.0383, 1189.0801, 1241.532, 1305.2837, 1339.3799, 1376.2074, 1390.4667, 1404.4123, 1406.2823, 1423.7964, 1473.6081, 1479.0223, 1490.3864, 1493.175, 1499.4556, 1503.9026, 1506.5505, 3030.8716, 3033.8539, 3035.5343, 3048.1488, 3080.4791, 3089.4359, 3094.3687, 3098.6311, 3106.8316, 3117.101, 3121.3381, 3122.8082
IRC:  	

Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 3	**Energy (Hartree)** -460.861089255396
Reaction Coordinates: 6 -3.351813 -1.417477 -0.305998 6 -2.149736 -0.889338 0.493730 6 -1.483949 0.244470 -0.185023 6 2.176261 -0.407650 -0.020787 6 3.445719 -1.229662 -0.013571 6 2.331718 1.089592 0.039120 1 3.212962 -2.288251 0.064756 1 4.000582 -1.047668 -0.937082	**Frequencies (cm^{-1}):** 23.9286, 35.6741, 46.5332, 69.9871, 77.4824, 94.4603, 98.5729, 142.0974, 155.4277, 205.0889, 221.0885, 331.0311, 395.5133, 417.9716, 498.7342, 534.202, 545.5198, 777.4416, 791.849, 889.4825, 893.019, 904.4071, 910.6328, 940.021, 1018.4558, 1092.5708, 1093.5582,

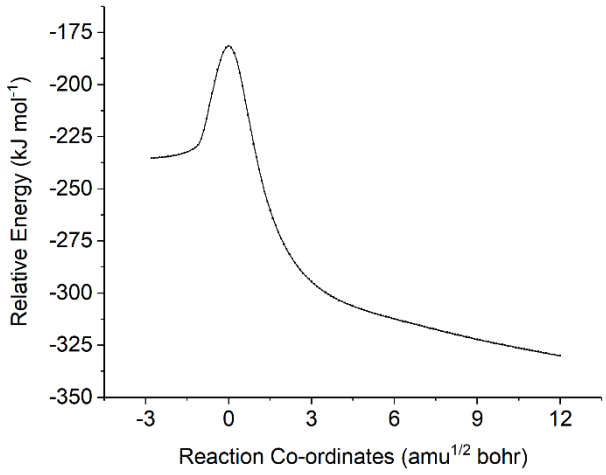
1 4.096202 -0.925975 0.808484 1 2.729623 1.363653 1.020522 1 3.067421 1.424058 -0.695468 1 1.379947 1.596995 -0.116893 1 -1.083112 0.179262 -1.191036 1 -2.446701 -0.580257 1.495370 1 -1.401001 -1.680264 0.592843 1 -3.055893 -1.723189 -1.309872 1 -3.777653 -2.285522 0.195675 1 -4.130325 -0.660556 -0.396200 8 1.086469 -0.946039 -0.070698 8 -0.748036 2.383873 -0.273557 8 -1.388590 1.348179 0.397264	1125.624, 1181.2031, 1246.6977, 1276.2193, 1324.0474, 1373.2389, 1387.8484, 1402.1758, 1415.8404, 1462.5368, 1466.7707, 1472.8474, 1476.828, 1496.5594, 1500.5123, 1505.5467, 1582.747, 1756.4072, 3009.954, 3031.1301, 3031.3461, 3037.8137, 3069.9643, 3084.5529, 3086.4509, 3103.3856, 3106.1455, 3108.5063, 3136.8158, 3162.6752

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 1.1	**Energy (Hartree)** -460.816959471184
Reaction Coordinates: 6 2.901085 0.305717 0.163324 6 1.774784 -0.577887 -0.370812 6 0.531142 -0.612527 0.525616 6 -0.730164 0.665562 0.005819 6 -1.671779 0.763298 1.182401 6 -0.134478 1.960941 -0.478165 1 -1.892354 -0.212801 1.599566 1 -2.606461 1.219490 0.846748 1 -1.234615 1.402020 1.947899 1 0.472551 2.409846 0.304950 1 -0.933776 2.664214 -0.721681 1 0.477696 1.815707 -1.365057 1 0.674958 -0.156917 1.520388 1 2.119367 -1.610622 -0.439598 1 1.499112 -0.289120 -1.386766 1 3.784935 0.230017 -0.470464 1 3.192816 0.000922 1.170406 1 2.620864 1.358569 0.205994 8 -1.164787 -0.071166 -1.054583 8 -1.689613 -1.218826 -0.650348 8 -0.170430 -1.692752 0.532246	**Frequencies (cm^{-1}):** -471.0743, 81.6386, 105.4888, 168.6498, 180.2379, 210.585, 225.8014, 257.8719, 276.5099, 318.6966, 352.7581, 383.2011, 413.3991, 492.6395, 543.5212, 622.5578, 656.414, 774.7803, 797.3925, 881.9389, 953.2105, 969.8193, 990.7369, 1008.2743, 1031.8374, 1080.8487, 1113.3007, 1129.4713, 1161.8987, 1275.4081, 1280.812, 1282.7783, 1304.4924, 1331.83, 1403.1779, 1409.8112, 1418.9948, 1423.5344, 1470.9732, 1480.7155, 1487.7482, 1496.6431, 1503.4551, 1506.004, 1507.362, 2908.6421, 3028.2587, 3033.7609, 3039.3049, 3041.2397, 3065.4527, 3087.3637, 3094.1067, 3101.7185, 3105.7787, 3136.6371, 3161.8636
IRC:	

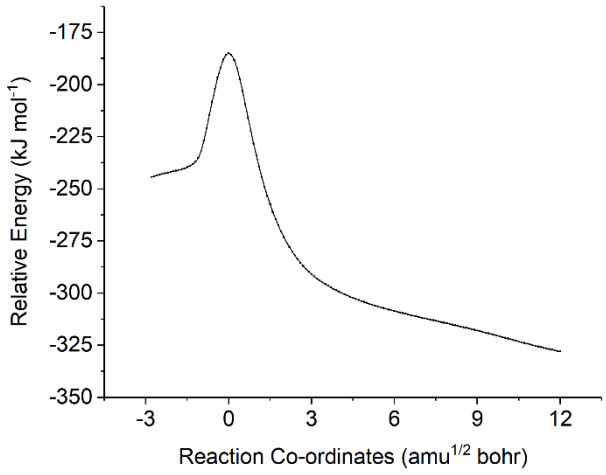


Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 1.1	**Energy (Hartree)** -460.867934905695
Reaction Coordinates: 6 -3.860828 0.009408 -0.201594 6 -2.484954 0.188240 0.451376 6 -1.419492 -0.589281 -0.267965 6 2.036072 0.062166 -0.002279 6 1.890844 0.356893 1.433660 6 2.967888 -0.957952 -0.544586 1 0.885814 0.069186 1.749641 1 1.952682 1.437238 1.581681 1 2.635139 -0.172647 2.022421 1 2.689492 -1.939727 -0.153941 1 3.987489 -0.753232 -0.210793 1 2.932745 -0.979827 -1.630559 1 -1.359773 -0.396613 -1.355782 1 -2.494664 -0.111798 1.499261 1 -2.184831 1.238131 0.397528 1 -4.601675 0.639258 0.289721 1 -4.201922 -1.024429 -0.134572 1 -3.836715 0.288896 -1.256078 8 1.353300 0.690848 -0.858834 8 0.427084 1.615774 -0.390671 8 -0.678004 -1.395532 0.248231	**Frequencies (cm^{-1}):** 27.8053, 37.1247, 44.6573, 75.4092, 86.3917, 92.1706, 148.1384, 158.2367, 160.2278, 213.9424, 292.7054, 308.851, 345.7128, 367.8171, 480.7424, 511.2775, 594.1502, 761.2436, 812.6567, 875.9366, 913.8521, 919.1078, 930.4521, 988.1959, 1007.2752, 1073.3832, 1097.5459, 1129.2985, 1162.7426, 1271.5519, 1306.0831, 1327.8363, 1387.813, 1405.6697, 1409.7397, 1427.9857, 1443.8341, 1458.6885, 1469.9351, 1470.432, 1479.5184, 1501.8644, 1505.3573, 1570.5704, 1773.3791, 2910.3032, 3026.9668, 3029.736, 3033.954, 3034.6784, 3075.3711, 3077.3872, 3082.2355, 3097.806, 3098.6158, 3137.4983, 3138.8749

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 1.2	**Energy (Hartree)** -460.818460392725
Reaction Coordinates: 6 -2.482014 0.195109 -0.616668 6 -1.765611 0.611426 0.665055 6 -0.474827 -0.155666 0.969705 6 0.948746 0.432245 -0.056953 6 2.172628 -0.047299 0.689677 6 0.899750 1.903822 -0.372714 1 3.024931 -0.040831 0.005930 1 2.039876 -1.054190 1.069659	**Frequencies (cm^{-1}):** -454.0009, 77.2587, 109.644, 181.412, 188.1209, 213.2111, 243.3287, 248.0009, 276.7827, 317.0274, 342.2381, 376.3952, 420.8202, 537.4465, 547.0684, 641.5719, 686.8183, 776.8888, 792.7865, 855.6644, 954.351, 970.9598, 991.9732, 1006.9882, 1033.3206, 1072.4483, 1104.3095,

1 2.387783 0.632272 1.512548 1 0.076604 2.140958 -1.042518 1 1.834369 2.214248 -0.844098 1 0.785292 2.479088 0.544599 1 -0.005626 0.159922 1.917110 1 -2.422140 0.422336 1.520232 1 -1.570342 1.685863 0.676726 1 -1.905006 0.448058 -1.505661 1 -2.648089 -0.880716 -0.629143 1 -3.449286 0.692895 -0.690222 8 0.600410 -0.295432 -1.158244 8 0.617203 -1.591063 -0.889689 8 -0.460163 -1.430721 0.772462	1128.8541, 1168.0884, 1274.614, 1277.5031, 1290.9043, 1301.1546, 1346.6058, 1402.8714, 1404.6547, 1419.2349, 1436.3834, 1472.1008, 1476.9934, 1492.1135, 1494.358, 1496.4221, 1506.543, 1510.7876, 2907.6912, 3014.0588, 3034.5399, 3039.5029, 3040.2522, 3049.2946, 3096.7606, 3099.0988, 3104.4754, 3113.962, 3131.967, 3160.1674
IRC:  	

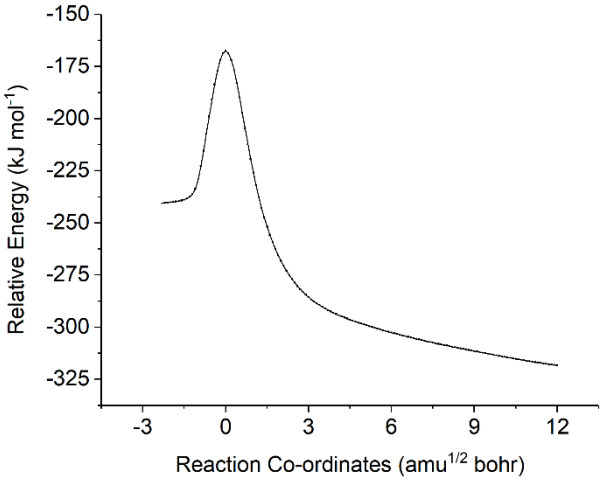
Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 1.2	**Energy (Hartree)** -460.869579166621
Reaction Coordinates: 6 3.094760 -0.026109 0.958873 6 2.628573 0.208301 -0.470480 6 1.407488 -0.565369 -0.878563 6 -1.907478 0.055573 0.160776 6 -1.474003 0.271010 1.551733 6 -2.937231 -0.936399 -0.237909 1 -1.492487 1.341455 1.767465 1 -0.429138 -0.034337 1.641431 1 -2.090183 -0.290583 2.248848 1 -3.119725 -0.900022 -1.308646 1 -3.868120 -0.751728 0.302736 1 -2.595661 -1.937172 0.037322 1 1.059744 -0.363464 -1.908113 1 3.412017 -0.047966 -1.194710 1 2.397571 1.260964 -0.656543 1 2.332832 0.287166 1.671906 1 3.301313 -1.080478 1.139912 1 4.002086 0.541643 1.164166 8 -1.405804 0.732593 -0.780139 8 -0.398443 1.635168 -0.458308 8 0.831383 -1.376202 -0.188097	**Frequencies (cm^{-1}):** 32.5771, 36.0513, 52.0089, 87.0383, 91.2122, 96.6722, 156.7307, 161.4639, 170.7772, 243.2004, 254.8985, 292.5509, 309.469, 367.7152, 481.215, 593.934, 666.6772, 676.7098, 812.8249, 851.4518, 909.0247, 913.0981, 930.7797, 988.1837, 1006.2303, 1073.2807, 1097.6846, 1110.2357, 1142.8199, 1285.0888, 1306.0627, 1368.4862, 1387.7171, 1405.7078, 1410.4635, 1423.8994, 1443.6497, 1449.0725, 1458.7549, 1470.4144, 1479.5275, 1494.4236, 1501.1051, 1570.2078, 1774.5573, 2918.3955, 2999.3505, 3026.8341, 3033.706, 3040.5998, 3046.8548, 3075.1883, 3081.4609, 3101.0818, 3104.2373, 3137.3909, 3138.6957

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 1.3	**Energy (Hartree)** -460.819507452064
Reaction Coordinates: 6 3.119465 0.176826 0.127878 6 1.711089 0.576835 -0.321015 6 0.652339 -0.122017 0.525816 6 -1.054162 0.443223 0.043124 6 -1.931376 0.009719 1.193558 6 -1.121954 1.898147 -0.338379 1 -2.969687 -0.013578 0.853531 1 -1.661510 -0.977346 1.552174 1 -1.851911 0.732009 2.004272 1 -0.588252 2.090867 -1.265873 1 -2.163325 2.201506 -0.464576 1 -0.691657 2.512299 0.451093 1 0.565807 0.266576 1.555238 1 1.598611 1.660425 -0.246825 1 1.561585 0.295866 -1.364586 1 3.256243 -0.900581 0.042897 1 3.876571 0.668840 -0.483497 1 3.297697 0.457271 1.168124 8 -1.097852 -0.337085 -1.073576 8 -1.024456 -1.620126 -0.757813 8 0.561985 -1.404109 0.432906	**Frequencies (cm^{-1}):** -451.6284, 74.3251, 117.8385, 166.8116, 183.6887, 208.2467, 237.6444, 255.616, 275.2332, 309.65, 351.0906, 372.9184, 410.0775, 512.6074, 540.196, 643.8212, 651.8946, 780.6727, 807.6634, 880.5007, 953.9002, 970.4386, 992.6413, 1006.3586, 1016.2658, 1076.6189, 1117.7308, 1138.0936, 1165.0822, 1275.7393, 1279.0241, 1290.0328, 1295.6164, 1351.53, 1403.6186, 1406.1474, 1416.8627, 1432.5928, 1472.0785, 1478.636, 1484.565, 1493.9877, 1498.3776, 1504.5138, 1506.6789, 2907.9268, 3026.3595, 3030.4917, 3034.2701, 3039.1643, 3070.8277, 3087.6606, 3098.7651, 3104.4819, 3106.063, 3132.6655, 3162.141
IRC:  	

Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 1.3	**Energy (Hartree)** -460.866786927255
Reaction Coordinates: 6 3.185611 0.672167 0.637887 6 2.236185 0.217307 -0.478639 6 1.839433 -1.220027 -0.316682 1 2.685884 -1.929675 -0.194829 8 0.706502 -1.643333 -0.307602 1 2.760119 0.285191 -1.440239 1 1.346357 0.846252 -0.527436 1 3.528903 1.687757 0.447627	**Frequencies (cm^{-1}):** 26.4289, 39.7216, 59.5485, 66.1879, 77.3031, 92.8913, 103.0281, 156.5794, 161.8554, 208.2951, 287.8481, 308.3365, 330.22, 366.9893, 480.2665, 521.0254, 593.4122, 763.9939, 812.1858, 881.7843, 911.1396, 924.4177, 929.0942, 989.0809, 1007.9408, 1072.5339, 1096.726,

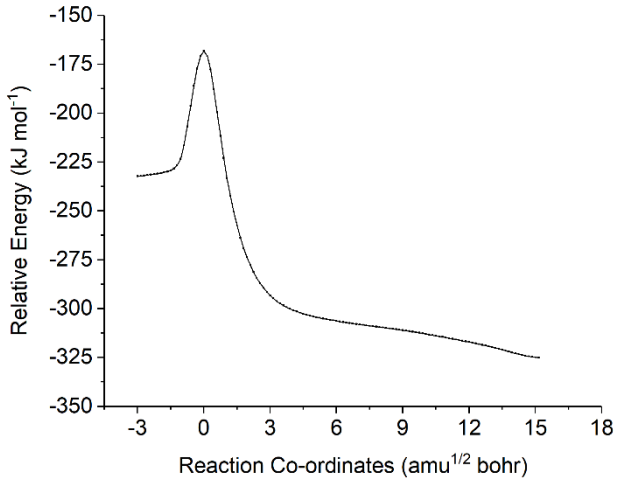
1 4.064740 0.028801 0.709845 1 2.680786 0.668516 1.603938 6 -1.834425 0.019159 0.163504 6 -2.149032 0.018241 -1.275153 1 -1.213972 0.003420 -1.838064 1 -2.629602 0.965232 -1.533147 1 -2.771266 -0.830635 -1.544799 6 -2.265024 -1.044677 1.103741 1 -1.810694 -1.990298 0.799945 1 -3.349182 -1.170199 1.060147 1 -1.962993 -0.810073 2.121165 8 -1.166437 0.965286 0.666931 8 -0.715761 1.962133 -0.193340	1135.8189, 1170.3004, 1281.2302, 1305.8977, 1350.1376, 1388.1302, 1403.5358, 1410.5875, 1428.4456, 1442.0338, 1459.5666, 1471.3934, 1477.1977, 1478.5579, 1500.5376, 1505.715, 1569.6299, 1782.4593, 2857.0609, 2992.1677, 3028.0053, 3029.7568, 3033.8826, 3070.3747, 3078.8762, 3080.9003, 3092.6217, 3107.1726, 3136.3707, 3140.5222

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 2.1	**Energy (Hartree)** -460.812591422153
Reaction Coordinates: 6 2.761406 0.290513 -0.053894 6 1.769555 -0.824458 0.267236 6 0.449639 -0.810641 -0.525072 6 -0.603053 0.711152 0.014606 6 -0.266192 1.944545 -0.781369 6 -0.472474 0.791800 1.514324 1 -0.522015 1.806018 -1.830068 1 -0.821312 2.803365 -0.396984 1 0.793094 2.173044 -0.706880 1 0.480620 1.234730 1.791603 1 -1.269745 1.442067 1.885382 1 -0.578599 -0.179946 1.983484 1 0.579386 -0.513781 -1.580150 1 1.554544 -0.875021 1.333552 1 2.226887 -1.782774 0.011426 1 3.740797 0.053727 0.362478 1 2.888478 0.412426 -1.131570 1 2.462825 1.254010 0.358735 8 -1.763005 0.185681 -0.449485 8 -2.067728 -0.941366 0.169193 8 -0.340298 -1.799982 -0.306708	**Frequencies (cm^{-1}):** -488.0994, 76.6912, 104.4884, 151.4119, 201.2416, 218.3989, 231.0198, 244.0531, 274.444, 327.3185, 351.3859, 398.7746, 416.0491, 489.5555, 530.7337, 580.5624, 646.675, 763.2517, 799.302, 874.7799, 953.0059, 988.0134, 998.2711, 1022.0807, 1035.2307, 1060.9173, 1103.8592, 1141.844, 1182.1691, 1272.8841, 1279.5604, 1289.5145, 1332.9465, 1348.1638, 1401.7346, 1410.7662, 1421.1893, 1424.2433, 1470.5881, 1479.8346, 1485.5512, 1495.2903, 1500.362, 1507.3689, 1511.3193, 2902.4321, 3028.7355, 3029.9501, 3036.9281, 3037.8088, 3077.539, 3091.106, 3098.2902, 3106.4894, 3113.6332, 3146.3587, 3162.8553
IRC:	

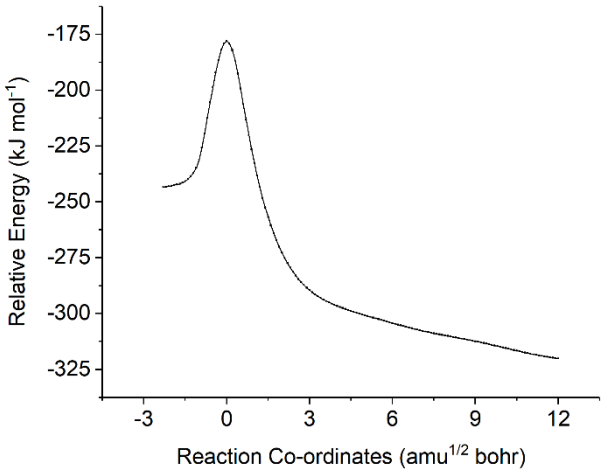


Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 2.1	**Energy (Hartree)** -460.868574244763
Reaction Coordinates: 6 3.130956 -0.790899 -0.262324 6 2.448340 0.561704 -0.456522 6 1.422964 0.884328 0.598264 6 -1.842686 -0.177379 -0.159311 6 -2.614315 0.573285 -1.181012 6 -2.155216 -0.155974 1.279937 1 -2.227703 0.384012 -2.178843 1 -3.670114 0.297588 -1.133746 1 -2.547522 1.641981 -0.964073 1 -3.089740 0.364271 1.472483 1 -2.179144 -1.181848 1.653331 1 -1.335366 0.337646 1.805770 1 1.611010 0.438478 1.593666 1 1.970844 0.646007 -1.433268 1 3.189959 1.369230 -0.402901 1 3.897941 -0.947004 -1.020712 1 3.616313 -0.849961 0.713840 1 2.401327 -1.596253 -0.326432 8 -0.880128 -0.867605 -0.598291 8 -0.093994 -1.538536 0.330724 8 0.476864 1.621824 0.430903	**Frequencies (cm^{-1}):** 31.3421, 45.6193, 47.5088, 83.8815, 87.7596, 95.8092, 153.9235, 158.7132, 178.3563, 218.3773, 297.1738, 312.566, 320.2917, 368.4028, 480.055, 522.6356, 595.0632, 692.6976, 812.7758, 882.5456, 914.2083, 917.6329, 930.3352, 988.2781, 1029.4331, 1073.8301, 1097.126, 1128.6589, 1155.8921, 1278.4194, 1306.4992, 1332.2185, 1385.3263, 1405.421, 1412.6147, 1427.8829, 1444.8958, 1450.4783, 1458.531, 1470.0813, 1479.6599, 1497.0407, 1513.8315, 1570.4154, 1768.2816, 2903.031, 2991.699, 3027.7864, 3030.7221, 3035.6716, 3071.0709, 3076.3986, 3085.1692, 3090.3481, 3115.0263, 3137.7983, 3139.246

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 2.2	**Energy (Hartree)** -460.813275099648
Reaction Coordinates: 6 -2.696225 0.079311 0.531770 6 -1.764794 0.653589 -0.529954 6 -0.526831 -0.210149 -0.875449 6 0.935294 0.471211 0.088976 6 1.489255 1.689982 -0.598145 6 0.503046 0.632032 1.524650 1 1.916557 1.429147 -1.564470 1 2.262021 2.157796 0.014828	**Frequencies (cm^{-1}):** -479.53, 86.2827, 109.2833, 165.107, 181.3241, 210.3598, 233.15, 248.0362, 266.2619, 326.0068, 341.8753, 393.4658, 400.9406, 524.6673, 553.8027, 641.6015, 645.3993, 762.728, 794.6158, 846.5084, 950.1201, 985.7957, 994.1469, 1011.2631, 1055.6358, 1063.795, 1095.3492,

1 0.699523 2.424286 -0.751310 1 -0.158574 1.487499 1.633889 1 1.397655 0.818907 2.125071 1 0.018289 -0.261847 1.898151 1 -0.146412 0.014081 -1.885625 1 -1.465962 1.673831 -0.280777 1 -2.312092 0.732030 -1.473489 1 -3.577640 0.714136 0.631347 1 -3.021223 -0.922714 0.258517 1 -2.224235 0.011299 1.509731 8 1.722068 -0.607849 -0.169861 8 1.207434 -1.709203 0.351117 8 -0.557799 -1.454736 -0.552126	1139.5666, 1200.2413, 1274.3023, 1282.2251, 1294.8333, 1315.3799, 1355.1976, 1402.0768, 1409.5581, 1417.0971, 1443.3523, 1471.6155, 1478.9567, 1488.1808, 1491.1732, 1500.0457, 1506.9508, 1507.5315, 2908.4522, 3021.6706, 3032.0116, 3038.0869, 3044.8708, 3049.0216, 3097.8013, 3104.3348, 3114.3172, 3121.9948, 3124.9729, 3172.8571
IRC:  	

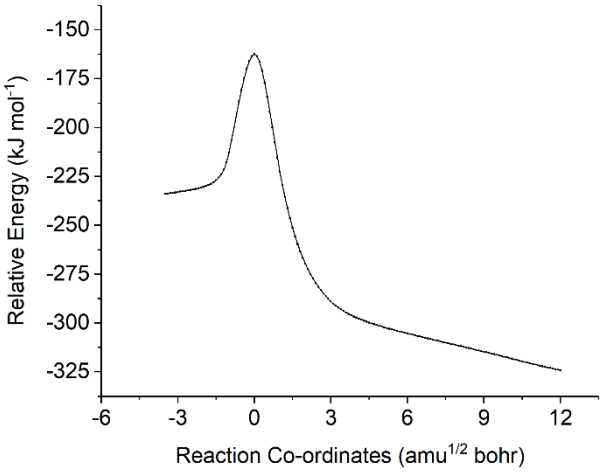
Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 2.2	**Energy (Hartree)** -460.869923564643
Reaction Coordinates: 6 -2.760207 1.174688 -0.310228 6 -2.567204 -0.332304 -0.220746 6 -1.503050 -0.781838 0.739179 6 1.785844 0.234548 -0.114556 6 2.214631 1.634680 0.128547 6 2.279746 -0.917619 0.658517 1 1.744004 2.314919 -0.576265 1 3.301190 1.714602 0.050387 1 1.941134 1.921790 1.146640 1 3.089198 -0.628483 1.323543 1 2.585592 -1.705379 -0.032954 1 1.448801 -1.328813 1.236108 1 -1.362554 -1.876950 0.788672 1 -2.299826 -0.765240 -1.189139 1 -3.492364 -0.839560 0.079785 1 -3.562405 1.417264 -1.006950 1 -3.009576 1.600201 0.661443 1 -1.850217 1.661386 -0.658912 8 0.954095 0.070986 -1.051274 8 0.485864 -1.217139 -1.279836 8 -0.843901 -0.048680 1.442781	**Frequencies (cm^{-1}):** 32.0791, 36.3885, 50.3062, 81.7583, 93.3164, 95.5359, 156.5819, 160.791, 176.1345, 247.3597, 254.8558, 294.8025, 311.7278, 367.6771, 481.1739, 594.3187, 669.5543, 673.4792, 812.6998, 851.1821, 906.6049, 914.6816, 930.349, 988.0072, 1006.3988, 1073.25, 1097.1092, 1110.4828, 1141.317, 1286.5316, 1306.504, 1368.703, 1385.7386, 1405.8651, 1410.897, 1424.3268, 1444.4487, 1449.4016, 1458.8081, 1470.1997, 1479.4604, 1494.4387, 1501.5803, 1569.3955, 1772.4071, 2917.6717, 3000.3105, 3027.1148, 3034.623, 3040.7016, 3044.8829, 3075.2249, 3083.146, 3101.118, 3105.2648, 3137.4639, 3138.933

Compound: $EtCHCMe_2 + O_3$ TS_{AO} 2.3	**Energy (Hartree)** -460.816015668238
Reaction Coordinates: 6 -3.138942 0.095211 -0.113837 6 -1.736875 0.475855 0.368585 6 -0.675680 -0.292764 -0.432019 6 0.978314 0.515635 -0.015367 6 1.167989 1.780052 -0.808105 6 1.040514 0.622005 1.487917 1 1.262785 1.560811 -1.869863 1 2.064339 2.307843 -0.476128 1 0.319764 2.446664 -0.661366 1 0.468483 1.480248 1.831217 1 2.085866 0.772627 1.770880 1 0.681899 -0.279619 1.971660 1 -0.705991 -0.055231 -1.509972 1 -1.629261 0.229970 1.423793 1 -1.591489 1.552132 0.250922 1 -3.897609 0.663143 0.426281 1 -3.262314 0.303515 -1.178121 1 -3.325894 -0.966306 0.044698 8 1.704217 -0.491510 -0.565947 8 1.506898 -1.629954 0.074677 8 -0.496427 -1.527506 -0.127111	**Frequencies (cm^{-1}):** -464.5056, 85.9277, 100.2104, 167.2365, 187.1582, 201.5997, 233.4101, 246.1573, 281.9128, 319.6402, 338.0145, 387.4977, 398.206, 494.8809, 531.9622, 612.8663, 644.2466, 781.3726, 801.9247, 885.7056, 955.5296, 988.2384, 995.1731, 1004.9783, 1042.4614, 1069.6011, 1116.8607, 1142.4611, 1181.7165, 1276.7344, 1281.8838, 1289.3677, 1330.362, 1351.7667, 1402.8039, 1408.8579, 1418.3662, 1430.5735, 1469.4775, 1480.26, 1482.1232, 1494.279, 1495.7028, 1502.6158, 1504.6885, 2897.2873, 3026.8312, 3028.3065, 3032.2072, 3037.7245, 3079.0827, 3094.5078, 3098.6077, 3107.3115, 3113.2645, 3126.2524, 3163.1099
IRC:  	

Compound: $EtCHCMe_2 + O_3$ CPr_{AO} 2.3	**Energy (Hartree)** -460.868053456462
Reaction Coordinates: 6 3.802266 0.065135 -0.156918 6 2.333210 -0.115135 -0.555308 6 1.448611 -0.349126 0.635888 6 -1.971417 0.017075 -0.158115 6 -2.638197 -1.052440 -0.942193 6 -2.243131 0.278430 1.265507 1 -2.303265 -1.044503 -1.976008 1 -3.722636 -0.927640 -0.903237	**Frequencies (cm^{-1}):** 29.9627, 39.6791, 45.4127, 77.2831, 83.7118, 92.3951, 153.8323, 158.8319, 160.0159, 213.5014, 294.1901, 311.7773, 344.7388, 367.649, 481.4676, 513.1831, 594.1278, 754.5233, 812.7161, 875.1885, 913.7388, 918.2885, 930.2463, 988.1077, 1009.8716, 1073.2731, 1097.2736,

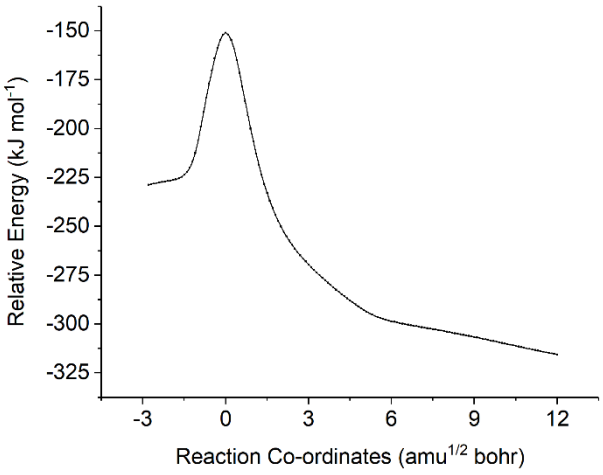
1 -2.407081 -2.021774 -0.494239 1 -3.079633 -0.316032 1.623138 1 -2.417668 1.347376 1.404090 1 -1.343211 0.043157 1.838307 1 1.572677 0.382251 1.456855 1 2.202535 -0.937626 -1.258574 1 1.962519 0.800181 -1.025893 1 4.407781 0.309019 -1.029162 1 3.919362 0.876501 0.563295 1 4.208929 -0.843045 0.289950 8 -1.135107 0.720570 -0.791925 8 -0.448027 1.699177 -0.083508 8 0.659589 -1.261184 0.747723	1128.7074, 1162.2264, 1273.7171, 1306.4198, 1329.8785, 1385.7028, 1405.8328, 1410.351, 1429.0087, 1444.4131, 1458.5106, 1469.8437, 1470.2111, 1479.2547, 1501.797, 1505.421, 1569.353, 1771.8207, 2907.6319, 3027.17, 3028.0697, 3031.0588, 3034.2387, 3075.5306, 3076.5069, 3082.4138, 3096.4445, 3098.4116, 3137.5747, 3138.999

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 1	**Energy (Hartree)** -460.811969201101
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.766294 0.656071 0.244958 6 -1.686819 -0.292571 -0.273798 6 -0.463627 -0.353130 0.616626 6 0.967812 0.574308 -0.139113 6 2.020934 0.671890 0.970137 6 0.361194 1.937839 -0.517259 1 2.368213 -0.318482 1.253711 1 1.647090 1.192033 1.853386 1 2.875803 1.231887 0.586721 1 -0.369883 1.843504 -1.314475 1 -0.083965 2.438595 0.341508 1 1.177379 2.562253 -0.883015 1 -0.584166 0.007879 1.635698 1 -1.405411 -0.055842 -1.296933 1 -2.072976 -1.315500 -0.311077 1 -2.431885 1.692819 0.257461 1 -3.648659 0.603925 -0.392684 1 -3.075949 0.390956 1.257376 8 1.261356 -0.192352 -1.137221 8 0.422866 -1.951663 -0.573251 8 0.191430 -1.536043 0.660850	-468.7864, 91.5167, 107.1496, 186.3395, 193.1488, 223.8092, 232.0664, 257.3948, 275.8856, 315.3557, 350.5433, 378.4904, 426.0326, 487.3212, 550.8395, 575.6686, 703.5794, 777.721, 809.4047, 909.9975, 915.2302, 970.4371, 991.9742, 1026.3256, 1057.2693, 1069.8646, 1080.6486, 1130.8532, 1163.854, 1183.4241, 1186.8126, 1281.7509, 1334.7916, 1363.9778, 1393.4132, 1405.54, 1416.2593, 1425.6041, 1475.7756, 1479.1219, 1490.1092, 1494.3606, 1503.032, 1507.7117, 1508.6434, 3027.8691, 3030.0223, 3033.1197, 3040.9776, 3084.9336, 3086.0788, 3097.6576, 3102.0145, 3107.0016, 3113.9528, 3129.3519, 3142.0922
IRC	

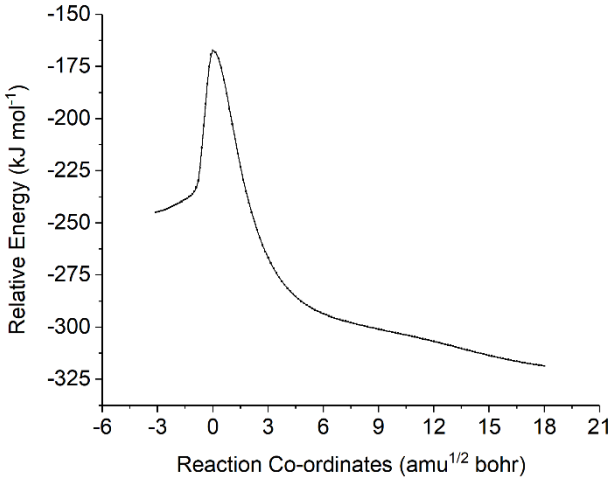


Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 1	**Energy (Hartree)** -460.865444864793
Reaction Coordinates: 6 2.313223 -2.059251 -0.283387 6 2.056536 -0.571305 -0.497913 6 1.649440 0.138040 0.722103 1 1.570697 -0.333872 1.695478 8 1.372699 1.364057 0.748030 8 1.412859 2.046732 -0.454403 1 2.930792 -0.041116 -0.896041 1 1.279028 -0.384930 -1.244577 1 1.411920 -2.562737 0.065213 1 2.619799 -2.528879 -1.216862 1 3.105965 -2.229536 0.446756 6 -2.077242 -0.222504 0.018359 6 -2.000176 1.209916 -0.448212 1 -0.971658 1.521747 -0.618596 1 -2.443742 1.854512 0.315914 1 -2.594761 1.349164 -1.353278 6 -3.453803 -0.846706 0.077326 1 -4.146322 -0.202821 0.622435 1 -3.850234 -0.948346 -0.935845 1 -3.406178 -1.826154 0.545627 8 -1.089705 -0.855311 0.336888	**Frequencies (cm^{-1}):** 25.9622, 34.5316, 46.2082, 70.1313, 71.1642, 84.5992, 99.073, 111.5629, 152.662, 209.0405, 222.5433, 361.4854, 392.1321, 455.9351, 497.2504, 540.9262, 684.3924, 702.1492, 788.2835, 843.9204, 868.0986, 887.9738, 902.0967, 936.558, 1048.0589, 1089.2291, 1103.9213, 1123.3178, 1142.0878, 1242.569, 1253.6461, 1324.53, 1377.723, 1387.8906, 1399.5746, 1421.5018, 1424.9074, 1462.305, 1466.199, 1475.8167, 1494.869, 1502.9655, 1508.8689, 1577.3807, 1761.5253, 3002.9158, 3018.9968, 3030.9491, 3034.897, 3040.7278, 3073.2313, 3083.9126, 3095.6327, 3108.6934, 3122.1549, 3137.0069, 3164.5409

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 2	**Energy (Hartree)** -460.807123410423
Reaction Coordinates: 6 2.296440 0.740451 -0.498059 6 1.545684 0.644466 0.830353 6 0.308918 -0.222550 0.964218 6 -1.085418 0.288186 -0.212874 6 -2.348219 -0.303185 0.426079 6 -1.043272 1.825474 -0.167163 1 -2.276054 -1.386996 0.477108 1 -3.202816 -0.051792 -0.204675 1 -2.537008 0.096709 1.423345	**Frequencies (cm^{-1}):** -466.2744, 87.1898, 119.8976, 184.6315, 203.936, 243.855, 252.2109, 267.7604, 282.2899, 297.1045, 316.3958, 388.2188, 428.6042, 489.3294, 547.0559, 563.4913, 721.8044, 786.3065, 810.7037, 850.1438, 907.977, 976.7008, 989.6317, 1008.422, 1051.8707, 1068.6455, 1087.3559,

1 -0.162819 2.216389 -0.667533 1 -1.923265 2.186912 -0.701710 1 -1.092603 2.208665 0.851772 1 -0.125798 -0.187020 1.960980 1 2.227707 0.265120 1.601401 1 1.257334 1.639029 1.172700 1 2.761801 -0.204886 -0.760665 1 1.639401 1.017360 -1.318281 1 3.079390 1.495159 -0.406351 8 -0.704661 -0.252372 -1.318021 8 0.672407 -1.627328 -0.694219 8 0.320996 -1.511761 0.576813	1129.5116, 1159.2621, 1180.4836, 1215.4094, 1304.4489, 1367.5289, 1374.1183, 1395.399, 1408.2357, 1418.8115, 1440.8961, 1470.094, 1481.6797, 1487.1251, 1491.9741, 1498.449, 1504.6923, 1512.3972, 2992.1801, 3030.2445, 3038.5553, 3042.9547, 3064.8386, 3086.9193, 3094.8031, 3109.3773, 3114.7553, 3127.5551, 3141.2108, 3146.3303
IRC  	

Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 2	**Energy (Hartree)** -460.862748738498
Reaction Coordinates: 6 1.767600 -1.416121 1.100665 6 2.502338 -0.881574 -0.147928 6 1.646632 -0.059934 -1.022496 6 -2.139357 -0.146426 -0.022942 6 -1.802637 0.997537 0.903038 6 -3.608179 -0.398606 -0.283023 1 -0.737827 1.216115 0.898148 1 -2.113572 0.733728 1.917795 1 -2.365846 1.891438 0.628641 1 -3.740105 -1.317633 -0.847704 1 -4.163758 -0.450915 0.655055 1 -4.025097 0.437621 -0.849551 1 1.221544 -0.413499 -1.954300 1 3.325217 -0.240760 0.179797 1 2.894719 -1.711512 -0.735837 1 1.417513 -0.587607 1.710041 1 0.917032 -2.033476 0.819828 1 2.460195 -2.017161 1.688768 8 -1.283676 -0.838567 -0.536191 8 1.780618 1.693167 0.405984 8 1.342008 1.135950 -0.779113	**Frequencies (cm^{-1}):** 23.7473, 34.5367, 40.1218, 53.3533, 75.3019, 76.0034, 93.7949, 112.6496, 140.6921, 198.2996, 243.1058, 317.524, 389.5487, 496.0073, 530.7907, 538.6688, 650.005, 786.2135, 810.9969, 843.0581, 870.3721, 888.3579, 898.5125, 906.5406, 1018.6502, 1086.9217, 1087.1552, 1122.5299, 1147.4445, 1239.7194, 1291.7765, 1335.0154, 1376.8092, 1387.6644, 1398.0328, 1403.2297, 1460.7673, 1462.1854, 1466.1347, 1474.692, 1490.9435, 1491.9057, 1514.3318, 1573.5704, 1765.6965, 3022.5206, 3027.9573, 3031.1668, 3050.2596, 3075.4424, 3083.8373, 3083.9844, 3116.5354, 3136.1728, 3137.0479, 3140.4147, 3177.0273

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 3	**Energy (Hartree)** -460.812859521795
Reaction Coordinates: 6 -2.894842 0.528923 0.215677 6 -1.448353 0.874680 -0.164163 6 -0.466543 0.059363 0.640370 6 1.252531 0.208094 -0.106273 6 2.196983 -0.324172 0.977091 6 1.399673 1.719280 -0.359981 1 1.981166 -1.368369 1.190210 1 2.138234 0.254693 1.900040 1 3.220937 -0.260908 0.604414 1 1.187775 2.311187 0.530337 1 2.438176 1.899166 -0.642121 1 0.767129 2.042486 -1.181168 1 -0.387095 0.306381 1.696775 1 -1.283901 0.701721 -1.224275 1 -1.259403 1.927502 0.039396 1 -3.085048 0.705076 1.275500 1 -3.584487 1.150298 -0.355561 1 -3.120853 -0.513340 -0.003528 8 1.132282 -0.519531 -1.164770 8 -0.515864 -1.639559 -0.745219 8 -0.522584 -1.285023 0.529195	**Frequencies (cm^{-1}):** -463.4298, 72.9943, 112.9906, 177.5762, 199.7273, 220.3099, 230.072, 267.5653, 276.9306, 304.3164, 347.9416, 388.5291, 438.8609, 486.0667, 553.9463, 595.6396, 675.0687, 786.7642, 817.9969, 896.219, 911.0528, 970.4132, 986.6603, 995.2966, 1054.9554, 1062.8364, 1082.8149, 1125.3399, 1171.5634, 1181.9626, 1199.8501, 1304.4136, 1344.1312, 1371.2267, 1392.7722, 1404.9442, 1407.3881, 1430.2224, 1476.4057, 1482.1159, 1489.7158, 1497.0901, 1498.6225, 1505.3896, 1506.6735, 3029.3874, 3033.7466, 3037.0537, 3070.4136, 3086.0046, 3090.3532, 3094.1983, 3108.4188, 3111.8246, 3127.1662, 3131.5909, 3142.4878
IRC  	

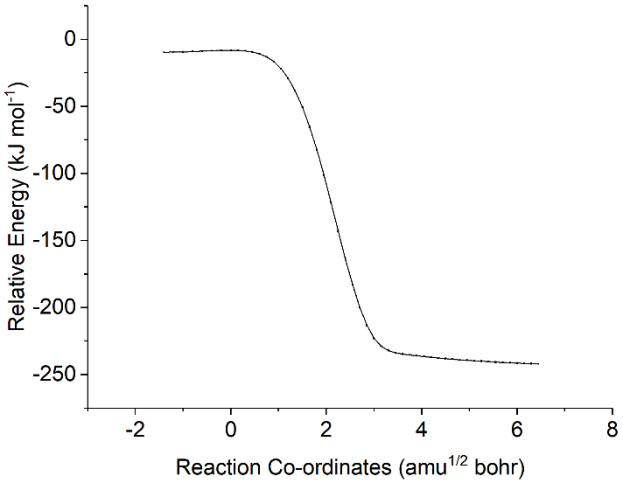
Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 3	**Energy (Hartree)** -460.863846029253
Reaction Coordinates: 6 3.310736 -0.890412 -0.598063 6 1.794289 -0.994246 -0.326007 6 1.406572 -0.224853 0.868737 6 -2.238351 -0.207423 -0.029653 6 -1.994924 1.192657 -0.535701 6 -3.666151 -0.705674 -0.065598 1 -0.932232 1.410371 -0.622199 1 -2.446903 1.903936 0.161341 1 -2.492805 1.342282 -1.495867 1 -4.338213 0.016067 0.402107	**Frequencies (cm^{-1}):** 26.1077, 35.0579, 54.5098, 69.0616, 72.9627, 78.7581, 96.8273, 111.5316, 152.656, 203.8266, 247.9063, 327.4773, 392.5347, 497.4806, 531.3288, 541.8035, 646.2076, 788.4496, 808.9049, 847.2536, 868.9046, 888.3579, 901.4048, 907.0536, 1008.7598, 1083.7553, 1089.5371, 1123.4939, 1150.8493, 1242.4352, 1283.8716, 1329.8784, 1376.6785,

1 -3.989019 -0.808814 -1.104381 1 -3.744462 -1.667709 0.433597 1 1.226561 -0.674734 1.838371 1 1.251145 -0.575540 -1.173041 1 1.496242 -2.031356 -0.180234 1 3.892779 -1.309414 0.222793 1 3.552946 -1.447602 -1.502202 1 3.596879 0.148662 -0.742777 8 -1.341792 -0.911586 0.391444 8 1.463499 1.719162 -0.296210 8 1.285050 1.026618 0.889790	1387.7664, 1399.7869, 1401.8019, 1462.1527, 1463.8635, 1466.6525, 1475.9937, 1494.975, 1496.6873, 1511.2746, 1575.4999, 1761.322, 3018.824, 3030.9988, 3040.9223, 3057.0563, 3073.0566, 3083.9463, 3098.2405, 3109.5749, 3121.5949, 3130.4695, 3137.1968, 3171.3473

S10.10 Ozonolysis of 2,4-dimethyl-2-pentene (Alkene 8)

Compound: $iPrCHCMe_2 + O_3$ PRC1.1	**Energy (Hartree)** -500.007113422271
Reaction Coordinates: 6 1.789066 -0.540930 0.209110 6 0.691449 0.188997 -0.510722 6 0.072421 1.333862 -0.162440 6 -0.984184 1.926673 -1.047708 1 -0.738110 2.958755 -1.312374 1 -1.947715 1.964452 -0.528697 1 -1.115377 1.357790 -1.966598 6 0.374635 2.123768 1.078151 1 -0.540095 2.299762 1.648949 1 0.770648 3.107827 0.810908 1 1.094297 1.639131 1.732249 1 0.397567 -0.261315 -1.455879 1 1.827149 -0.207269 1.247501 6 3.150653 -0.223281 -0.436954 1 3.373438 0.843012 -0.392070 1 3.161334 -0.523623 -1.486853 1 3.951292 -0.762288 0.072998 6 1.529884 -2.053945 0.207590 1 0.577787 -2.292084 0.678838 1 2.322619 -2.579291 0.742499 1 1.503787 -2.441055 -0.813594 8 -1.606325 -0.525700 1.009654 8 -2.596484 -0.611275 0.227196 8 -2.594962 -1.567358 -0.611854	**Frequencies (cm^{-1}):** 27.8278, 29.2216, 45.9838, 65.3306, 75.6581, 100.4951, 121.7797, 150.9946, 192.9192, 198.7622, 225.6153, 247.5404, 258.0208, 304.2647, 394.2712, 406.0228, 450.0984, 492.5071, 519.9401, 731.3498, 810.2753, 856.3753, 878.1828, 933.4397, 954.9176, 963.794, 967.212, 1005.536, 1088.8867, 1096.3883, 1108.2361, 1143.9595, 1147.8041, 1167.9505, 1193.7938, 1242.7709, 1329.6569, 1338.4878, 1393.5271, 1398.3223, 1410.2661, 1419.2407, 1421.0412, 1470.5019, 1480.9241, 1489.1324, 1489.5877, 1490.9299, 1494.0547, 1502.5791, 1511.9795, 1672.5912, 3003.5462, 3017.0545, 3018.2329, 3023.3437, 3036.1177, 3043.5051, 3057.1064, 3075.7103, 3083.3054, 3089.9149, 3102.7315, 3109.162, 3111.5439, 3124.6474

Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 1.1	**Energy (Hartree)** -500.002540642203
Reaction Coordinates: 6 1.652522 -0.123063 -0.232942 6 0.397910 0.123429 0.559559 6 -0.613245 0.998264 0.234188 6 -0.579277 1.876934 -0.983838 1 -1.585538 2.047879 -1.363889	**Frequencies (cm^{-1}):** -140.3775, 55.1427, 60.9761, 113.6625, 142.4228, 148.0175, 175.2576, 178.9401, 187.3695, 207.1642, 221.1691, 258.7806, 320.992, 357.0901, 403.2545, 432.4468,

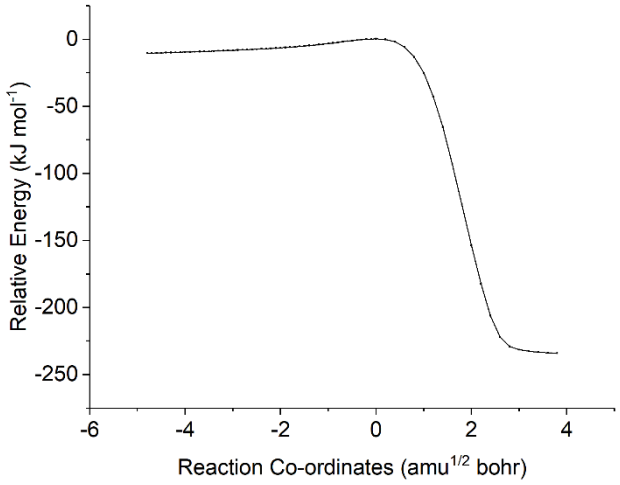
1 0.021240 1.453718 -1.785075 1 -0.160601 2.854966 -0.727730 6 -1.652512 1.334790 1.267529 1 -1.759586 0.539729 2.004774 1 -2.623864 1.521251 0.811658 1 -1.364585 2.244973 1.803977 1 0.389200 -0.282884 1.565219 1 1.379312 -0.209606 -1.287922 6 2.624432 1.066466 -0.086852 1 2.927376 1.191294 0.954585 1 2.181987 2.003230 -0.422060 1 3.525114 0.888526 -0.676692 6 2.350254 -1.418992 0.191797 1 1.706602 -2.284379 0.053586 1 2.639121 -1.374458 1.244752 1 3.258361 -1.571853 -0.392682 8 -1.934213 -0.548831 -0.926881 8 -1.858444 -1.511919 -0.075220 8 -0.659174 -1.960418 0.067209	449.2924, 514.6342, 547.5262, 742.3748, 808.5065, 852.412, 873.6855, 933.1688, 950.9906, 962.0323, 967.4818, 1012.0507, 1071.7007, 1079.9289, 1088.7246, 1107.2123, 1118.4429, 1144.2462, 1195.7415, 1239.2319, 1314.5562, 1339.6123, 1381.8199, 1398.498, 1405.6976, 1418.397, 1419.5167, 1473.3818, 1480.9278, 1481.6195, 1489.0515, 1493.1165, 1498.8006, 1504.7293, 1514.1185, 1580.1926, 3008.8715, 3018.2182, 3020.2265, 3023.4512, 3029.3938, 3073.3521, 3077.9048, 3082.5571, 3085.1281, 3103.2035, 3110.6042, 3124.8174, 3126.4142, 3138.9563
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ POZ1.1	**Energy (Hartree)** -500.103746557038
Reaction Coordinates: 6 -1.603222 0.137923 -0.282162 6 -0.268423 -0.295439 0.327009 6 1.047886 0.490716 -0.044729 6 1.566968 1.286676 1.148293 1 2.500289 1.788293 0.893985 1 0.843779 2.044035 1.455538 1 1.748756 0.623658 1.993298 6 0.999528 1.322803 -1.320747 1 0.604907 0.743331 -2.152706 1 0.396046 2.219440 -1.189189 1 2.010417 1.637342 -1.580237 8 1.971942 -0.586522 -0.356533 8 1.398479 -1.747305 0.277168 8 0.023037 -1.628724 -0.096052 1 -0.358710 -0.298481 1.418918 6 -2.065444 1.472128 0.315512	**Frequencies (cm^{-1}):** 63.6589, 86.5072, 177.0466, 208.9956, 220.2053, 232.3028, 248.8889, 257.8465, 291.9742, 314.8425, 327.3908, 362.761, 426.6376, 455.3196, 478.5584, 507.0613, 607.2296, 702.6973, 774.7755, 784.1627, 854.0398, 882.5222, 936.0491, 938.3434, 942.2629, 945.7903, 968.7018, 997.2557, 1015.0405, 1036.869, 1124.0657, 1161.8836, 1180.7941, 1198.7893, 1217.8898, 1257.2328, 1321.2756, 1346.6698, 1358.0091, 1401.9258, 1403.9789, 1406.197, 1423.4607, 1429.2298, 1480.633, 1487.9205, 1492.1182, 1493.901, 1498.5589,

1 -3.008005 1.778112 -0.139003 1 -2.233584 1.377082 1.390432 1 -1.349526 2.277985 0.159672 1 -1.466709 0.260216 -1.358278 6 -2.674225 -0.937656 -0.058471 1 -2.825894 -1.121644 1.007537 1 -3.626131 -0.610360 -0.478630 1 -2.401698 -1.881508 -0.526237	1505.0623, 1511.8973, 1515.1472, 2994.9806, 3024.8671, 3028.6253, 3033.7306, 3042.8795, 3047.8159, 3081.1784, 3089.7995, 3096.6685, 3100.8306, 3108.5891, 3111.0904, 3114.0488, 3125.2335

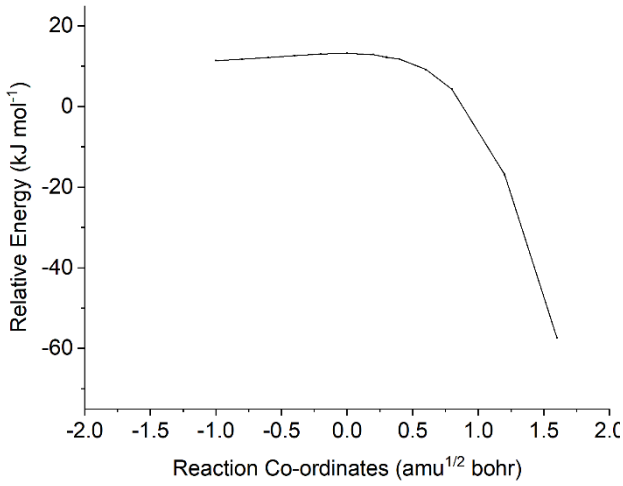
Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 1.2	**Energy (Hartree)** -499.999722430240
Reaction Coordinates: 6 -1.703144 -0.459322 -0.075252 6 -0.357254 -0.394851 0.608653 6 0.809859 -0.969072 0.150276 6 0.875651 -1.783654 -1.109930 1 1.851275 -1.683168 -1.583583 1 0.114547 -1.503913 -1.832178 1 0.740680 -2.843630 -0.870458 6 1.972489 -1.105333 1.093699 1 1.988422 -0.300628 1.828194 1 2.922294 -1.110850 0.561483 1 1.896988 -2.048845 1.643928 1 -0.366421 -0.074408 1.643113 1 -1.796345 -1.472922 -0.481927 6 -1.878085 0.512112 -1.256805 1 -1.057946 0.445957 -1.968948 1 -1.920540 1.541717 -0.908606 1 -2.809563 0.283861 -1.777383 6 -2.828457 -0.267756 0.947785 1 -2.781800 0.730064 1.388413 1 -2.763620 -0.997094 1.756842 1 -3.804458 -0.378250 0.474034 8 1.618578 0.923209 -0.860878 8 1.465230 1.711600 0.152125 8 0.221209 1.892612 0.455818	**Frequencies (cm^{-1}):** -181.9004, 40.6923, 84.8475, 111.0838, 137.3917, 147.3002, 163.0879, 179.3852, 192.9297, 213.4243, 238.5445, 259.973, 309.013, 342.5862, 401.2038, 445.2885, 454.5781, 522.1027, 576.1944, 735.5201, 807.7162, 844.0254, 877.2215, 936.658, 957.8157, 963.8347, 969.2325, 1011.4797, 1062.1522, 1071.9462, 1083.6464, 1111.7856, 1116.981, 1135.0843, 1205.9489, 1236.5869, 1327.2139, 1343.211, 1381.0615, 1402.1624, 1408.1371, 1419.7364, 1423.2549, 1471.3536, 1480.2638, 1482.8981, 1487.6355, 1493.5459, 1501.2248, 1503.927, 1512.6591, 1571.9391, 2981.7844, 3010.299, 3014.4989, 3022.5091, 3037.597, 3075.0265, 3082.9765, 3084.406, 3089.5256, 3103.6992, 3112.9175, 3122.3164, 3137.4358, 3152.3962

IRC:



Compound: iPrCHCMe$_2$ + O$_3$ POZ1.2	**Energy (Hartree)** -500.100633245354
Reaction Coordinates: 6 -1.579866 -0.488964 -0.147913 6 -0.252033 0.195836 -0.517318 6 1.121406 -0.456400 -0.079655 6 2.052393 -0.569653 -1.286569 1 3.022802 -0.959020 -0.979808 1 1.630679 -1.244647 -2.033460 1 2.196557 0.405343 -1.749080 6 1.059819 -1.769307 0.687110 1 2.065341 -2.056200 0.993992 1 0.440112 -1.697577 1.575670 1 0.670373 -2.561535 0.048192 8 1.633398 0.522032 0.847804 8 1.180982 1.755304 0.277922 8 -0.225112 1.493110 0.090875 1 -0.213898 0.317082 -1.603752 6 -2.697674 -0.022361 -1.090566 1 -3.632188 -0.536259 -0.862079 1 -2.872785 1.049660 -0.986785 1 -2.451704 -0.224012 -2.134326 1 -1.428952 -1.557767 -0.324103 6 -2.001167 -0.288295 1.313406 1 -2.297405 0.744506 1.490603 1 -2.853872 -0.929083 1.541759 1 -1.206478 -0.519184 2.019399	**Frequencies (cm^{-1}):** 31.6172, 84.6341, 173.9468, 198.7875, 210.498, 245.1068, 251.1748, 261.6889, 268.9748, 297.7303, 330.7913, 356.335, 408.5799, 446.2319, 524.1109, 560.2077, 627.1684, 698.6341, 760.4209, 789.4613, 849.0477, 882.6398, 928.4741, 933.1168, 934.3884, 951.6687, 965.5118, 983.2591, 1015.4834, 1036.9377, 1118.2199, 1136.3719, 1185.6572, 1203.7652, 1207.6023, 1258.6658, 1320.0919, 1337.9736, 1372.5351, 1395.0445, 1404.0821, 1407.8154, 1424.3239, 1432.4554, 1480.4201, 1487.2623, 1489.6693, 1494.3251, 1500.0487, 1505.3406, 1509.8258, 1518.2389, 3007.5589, 3016.628, 3024.9876, 3033.4966, 3041.5448, 3050.5396, 3086.3557, 3089.7461, 3095.4829, 3101.7082, 3105.7937, 3116.4162, 3117.0179, 3144.8173

Compound: iPrCHCMe$_2$ + O$_3$ PRC1.3	**Energy (Hartree)** -500.000279409791
Reaction Coordinates: 6 -1.581704 -0.853239 -0.074931 6 -0.501052 0.044195 -0.621235 6 -0.024825 1.264297 -0.294607 6 -0.497222 2.170694 0.805981 1 0.339661 2.429376 1.460213 1 -1.288449 1.755620 1.415307 1 -0.854377 3.112141 0.378269 6 1.111824 1.839523 -1.094025 1 1.373260 1.218469 -1.948580 1 2.003745 1.946860 -0.466960 1 0.868464 2.842564 -1.454595 1 -0.027500 -0.408139 -1.488867 1 -1.091962 -1.828882 0.026150 6 -2.198247 -0.532966 1.287533 1 -2.827605 0.357236 1.255442 1 -1.439136 -0.396251 2.056628 1 -2.834974 -1.363650 1.596115 6 -2.682702 -1.026288 -1.140101 1 -3.227057 -0.091949 -1.289197 1 -3.398077 -1.789421 -0.829474 1 -2.265302 -1.328050 -2.101395 8 1.495968 -0.624229 1.100531 8 2.551814 -0.730428 0.411051 8 2.566327 -1.631996 -0.489174	**Frequencies (cm^{-1}):** 26.3037, 33.5148, 48.9675, 52.7549, 67.208, 94.4654, 106.116, 152.5217, 194.4247, 224.8505, 260.011, 266.1376, 311.202, 330.8835, 361.1903, 411.0278, 428.6266, 502.324, 612.6817, 731.7053, 772.6249, 845.6366, 883.3978, 933.6116, 956.1644, 961.2719, 976.7021, 1009.8951, 1083.7224, 1095.3977, 1101.8301, 1141.7438, 1143.4608, 1164.4526, 1212.8486, 1234.8538, 1316.17, 1381.0462, 1396.671, 1403.5019, 1411.7191, 1422.049, 1429.6012, 1471.0963, 1478.8542, 1489.0387, 1494.1607, 1496.4895, 1498.495, 1513.0226, 1517.1128, 1669.2032, 2985.4365, 3000.8004, 3016.683, 3021.0501, 3029.4016, 3043.0184, 3050.0982, 3079.4505, 3085.22, 3088.2076, 3102.2087, 3104.1973, 3112.3794, 3186.0958

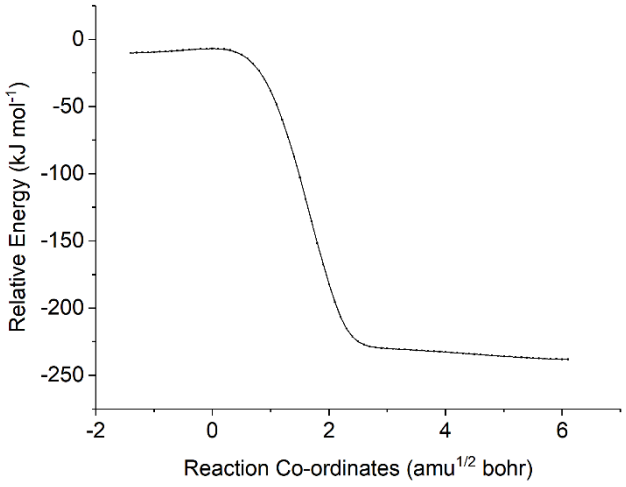
Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 1.3	**Energy (Hartree)** -499.997549805376
Reaction Coordinates: 6 -1.659128 -0.515511 -0.280310 6 -0.375304 0.147878 -0.714132 6 0.441881 1.055031 -0.080558 6 0.191077 1.655128 1.276569 1 1.102049 2.108589 1.664377 1 -0.156326 0.925521 1.998965 1 -0.561593 2.446237 1.207057 6 1.511490 1.733931 -0.893758 1 1.736673 1.189227 -1.809527 1 2.430726 1.850025 -0.320587 1 1.180957 2.738915 -1.177735 1 -0.190358 0.032111 -1.776572 1 -1.688261 -1.455265 -0.838086 6 -1.810009 -0.882316 1.199227 1 -2.032465 -0.014332 1.819222 1 -0.913847 -1.366476 1.582326 1 -2.643622 -1.577227 1.311920 6 -2.855817 0.325531 -0.768453 1 -2.797887 0.524172 -1.839446 1 -2.898802 1.284757 -0.249669 1 -3.790938 -0.202724 -0.574769 8 1.874765 -0.605230 0.886236 8 2.024209 -1.294142 -0.192312 8 0.920844 -1.800824 -0.622547	**Frequencies (cm^{-1}):** -135.7049, 45.1373, 63.3076, 80.9731, 108.6585, 135.3715, 153.5909, 173.9194, 182.8777, 215.4375, 257.6404, 300.3867, 310.67, 351.9971, 403.3407, 414.3216, 442.3494, 547.2437, 620.2243, 739.3489, 768.9937, 842.0089, 887.1343, 936.3834, 956.3107, 959.1164, 972.7979, 1014.2406, 1067.9408, 1082.6807, 1087.5722, 1100.2618, 1114.8221, 1145.2171, 1212.8139, 1234.3849, 1325.8879, 1383.1348, 1393.1328, 1401.4308, 1407.1826, 1419.4109, 1420.3396, 1476.0525, 1480.0688, 1484.0549, 1492.233, 1495.6422, 1501.5882, 1511.4496, 1521.7091, 1584.1, 3006.1583, 3015.2255, 3019.3736, 3021.4137, 3035.7223, 3072.2013, 3082.0836, 3086.0162, 3087.2944, 3089.444, 3110.5665, 3117.0969, 3134.3315, 3158.5257
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ POZ1.3	**Energy (Hartree)** -500.100633245354
Reaction Coordinates: 6 1.671337 -0.359944 -0.363183 6 0.154212 -0.342494 -0.612159 6 -0.862847 0.595918 0.156085 6 -1.463616 1.615129 -0.809602 1 -2.207219 2.227837 -0.301001 1 -0.688875 2.274072 -1.206307 1 -1.943414 1.108428 -1.645895	**Frequencies (cm^{-1}):** 46.4824, 89.9275, 187.4685, 201.508, 219.6827, 228.3401, 247.01, 261.9967, 293.8336, 316.7897, 347.0211, 368.982, 388.1407, 454.8979, 480.5243, 576.9602, 611.1634, 700.3137, 745.449, 772.236, 846.5201, 875.432, 931.4424, 937.4582, 939.944, 953.6238, 968.3482, 996.9119,

6 -0.408015 1.255759 1.452114 1 -1.256387 1.771364 1.902932 1 -0.043997 0.521584 2.163971 1 0.368210 1.996224 1.266525 8 -1.882651 -0.346614 0.577434 8 -1.757831 -1.439340 -0.350854 8 -0.341461 -1.655682 -0.348177 1 0.010590 -0.138213 -1.677799 6 2.327888 0.941390 -0.836801 1 3.413445 0.848311 -0.794591 1 2.055942 1.178301 -1.866650 1 2.050707 1.790366 -0.210976 1 2.019293 -1.149047 -1.037420 6 2.129599 -0.757133 1.044713 1 1.559499 -1.602421 1.426668 1 3.180108 -1.049721 1.012380 1 2.046287 0.064251 1.753940	1025.6649, 1040.2321, 1107.7954, 1168.5579, 1175.8131, 1205.877, 1226.6813, 1259.1471, 1337.5697, 1365.9729, 1372.4108, 1402.7308, 1404.7239, 1409.7452, 1426.8378, 1433.9203, 1480.6848, 1488.4707, 1493.6447, 1496.9913, 1500.3666, 1510.8525, 1513.4241, 1522.0331, 2996.7406, 3008.1548, 3029.0776, 3032.3352, 3040.3454, 3049.9615, 3087.8367, 3091.1481, 3094.9858, 3096.154, 3107.1995, 3112.8581, 3118.0372, 3147.2337

Compound: iPrCHCMe$_2$ + O$_3$ PRC 2.1	**Energy (Hartree)** -500.009406834231
Reaction Coordinates: 6 1.788255 -0.403335 -0.247965 6 0.696610 0.305405 0.504068 6 -0.039400 1.365684 0.124722 6 -1.044615 1.974826 1.059001 1 -0.809113 3.027230 1.243330 1 -2.044454 1.945835 0.618280 1 -1.081588 1.454670 2.014012 6 0.088630 2.071376 -1.195952 1 -0.888187 2.149436 -1.678736 1 0.441762 3.095264 -1.041948 1 0.769404 1.581309 -1.886752 1 0.525757 -0.077805 1.507342 1 1.846199 -0.012087 -1.264662 6 3.145324 -0.149222 0.431575 1 3.380503 0.914935 0.460471 1 3.139914 -0.518414 1.459554 1 3.946892 -0.662299 -0.103164 6 1.509290 -1.911502 -0.340578 1 0.590149 -2.115256 -0.889419 1 2.325645 -2.422672 -0.853664 1 1.411762 -2.351909 0.653977 8 -2.117246 -0.407449 -0.977107 8 -2.109078 -1.460781 -0.280099 8 -2.076078 -1.322723 0.976225	**Frequencies (cm^{-1}):** 18.981, 26.1882, 43.2357, 56.759, 71.7588, 82.1701, 133.2563, 153.8705, 197.3768, 202.9195, 221.6348, 226.0821, 255.998, 305.9665, 400.4669, 404.5636, 449.2833, 503.9504, 516.1791, 737.9668, 808.5246, 856.8971, 874.3888, 930.4028, 951.6773, 962.0714, 964.7791, 1009.0885, 1089.3386, 1099.5493, 1108.4234, 1141.2138, 1163.7013, 1181.7893, 1191.5402, 1240.8429, 1331.9012, 1337.6577, 1392.1902, 1396.439, 1409.2418, 1418.4163, 1420.0185, 1469.5077, 1482.2037, 1487.8275, 1488.7227, 1490.3843, 1494.6795, 1502.9823, 1510.9899, 1675.7558, 3009.2858, 3016.8792, 3017.7218, 3022.8519, 3041.0768, 3051.5577, 3056.8417, 3075.2803, 3083.7303, 3090.0323, 3095.4343, 3106.6313, 3112.3412, 3123.0306

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{OZO}$ 2.1	**Energy (Hartree)** -500.002253312432
Reaction Coordinates: 6 -1.608263 0.029661 -0.224264 6 -0.364743 -0.183322 0.596962 6 0.726083 -0.948687 0.231877 6 0.781749 -1.741291 -1.046546	**Frequencies (cm^{-1}):** -180.9287, 56.2153, 62.8728, 128.8376, 153.9729, 164.2228, 184.5153, 193.0556, 204.0999, 218.4721, 229.1815, 263.4276,

1 1.809187 -1.855607 -1.387040 1 0.204116 -1.288910 -1.849278 1 0.384116 -2.746395 -0.873661 6 1.751719 -1.304045 1.266434 1 1.710601 -0.630633 2.120096 1 2.757464 -1.269332 0.847894 1 1.582877 -2.325347 1.623634 1 -0.432586 0.102863 1.639466 1 -1.311533 0.209328 -1.262280 6 -2.489461 -1.237972 -0.202733 1 -2.815583 -1.460756 0.814943 1 -1.965337 -2.111486 -0.586603 1 -3.381025 -1.084147 -0.812614 6 -2.419237 1.235104 0.260264 1 -2.736088 1.095028 1.296648 1 -3.317802 1.359422 -0.345269 1 -1.835144 2.151120 0.208219 8 2.056531 0.739913 -0.637969 8 1.200940 1.708639 -0.672658 8 0.627486 1.896219 0.469861	323.3701, 359.1357, 404.3638, 446.5766, 456.5301, 522.6237, 563.1585, 740.0163, 807.5006, 853.439, 880.6008, 935.5041, 954.7114, 962.3628, 966.6474, 1012.6059, 1068.2445, 1074.4047, 1079.7941, 1108.1044, 1117.4222, 1143.1772, 1192.7951, 1240.5507, 1316.7084, 1336.3124, 1375.2911, 1398.7555, 1409.361, 1420.5825, 1421.0733, 1471.6174, 1478.5808, 1482.2321, 1489.8056, 1491.9585, 1499.8325, 1503.5811, 1515.58, 1567.7408, 3006.4669, 3009.0039, 3014.7146, 3023.2432, 3028.4457, 3074.6233, 3078.4428, 3084.4401, 3085.6671, 3106.3357, 3117.3085, 3120.1299, 3123.327, 3152.0532
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ POZ 2.1	**Energy (Hartree)** -500.100633245354
Reaction Coordinates: 6 1.574337 0.089491 0.304225 6 0.281080 -0.250497 -0.447646 6 -1.045484 0.475715 -0.031317 6 -1.447157 1.584092 -0.994170 1 -2.434937 1.965380 -0.736718 1 -0.740911 2.411024 -0.938929 1 -1.472784 1.214323 -2.018140 6 -1.107218 0.923040 1.427250 1 -2.104643 1.309439 1.635104 1 -0.915766 0.089424 2.099038 1 -0.388138 1.712352 1.638984 8 -2.002832 -0.584264 -0.243244 8 -1.336044 -1.701431 0.324712 8 -0.033516 -1.654471 -0.328195 1 0.441693 -0.080458 -1.516901	**Frequencies (cm^{-1}):** 50.4531, 93.3355, 179.8159, 200.6646, 215.7982, 226.5486, 242.3165, 265.6575, 281.1236, 304.078, 329.7536, 351.7206, 403.0925, 463.2806, 487.6588, 512.3638, 614.9535, 702.4236, 752.3579, 812.375, 857.4392, 885.2058, 918.9238, 937.7959, 939.3218, 946.3204, 967.9881, 997.2897, 1001.0016, 1027.6671, 1116.0032, 1152.7003, 1190.2494, 1192.783, 1228.5787, 1248.1367, 1320.9337, 1335.2542, 1350.7611, 1400.2939, 1402.532, 1405.7611, 1422.4386, 1427.3866, 1482.003, 1488.0895,

6 2.684698 -0.899357 -0.071372 1 3.599001 -0.665783 0.475772 1 2.400762 -1.924110 0.158570 1 2.913263 -0.842818 -1.138561 1 1.382779 -0.009236 1.374967 6 2.029428 1.523191 0.006245 1 1.306735 2.274449 0.322202 1 2.966516 1.734163 0.522303 1 2.207469 1.659128 -1.063170	1491.664, 1495.7339, 1500.2557, 1505.0807, 1513.854, 1516.7735, 3007.0368, 3021.5804, 3025.0275, 3039.2277, 3044.2819, 3050.4058, 3077.969, 3086.0478, 3098.0634, 3108.6054, 3113.9024, 3115.6127, 3118.8761, 3127.8143

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{OZO}$ 2.2	**Energy (Hartree)** -499.998901097346
Reaction Coordinates: 6 -1.647352 -0.491510 -0.187702 6 -0.328037 -0.510170 0.554178 6 0.879437 -0.942757 0.036709 6 1.014188 -1.453737 -1.372024 1 2.032540 -1.328350 -1.735174 1 0.341062 -0.960908 -2.067971 1 0.791151 -2.526243 -1.394060 6 1.992789 -1.299732 0.976582 1 1.882687 -0.795399 1.934244 1 2.963527 -1.037255 0.557388 1 1.993641 -2.380470 1.154001 1 -0.392999 -0.448772 1.632114 1 -1.657371 -1.376817 -0.833778 6 -1.866060 0.726996 -1.100905 1 -1.052159 0.869029 -1.810700 1 -1.952533 1.637873 -0.510448 1 -2.787479 0.594579 -1.669582 6 -2.809321 -0.627542 0.802713 1 -2.707644 -1.522449 1.418504 1 -3.761822 -0.689420 0.275314 1 -2.850277 0.237103 1.468032 8 1.865598 1.101511 -0.351266 8 0.853410 1.889982 -0.178046 8 0.248968 1.673284 0.944912	**Frequencies (cm^{-1}):** -206.2337, 48.3375, 77.2884, 143.3548, 147.4371, 164.0839, 169.6774, 199.1707, 203.7144, 220.6669, 243.8215, 277.3659, 310.8946, 337.0919, 403.2166, 446.2786, 463.2756, 517.6724, 596.0347, 736.8243, 807.1903, 847.1062, 883.3437, 935.2766, 956.7314, 964.2363, 970.0326, 1013.747, 1062.2978, 1069.8668, 1083.085, 1111.5553, 1118.5845, 1133.7831, 1205.6172, 1235.7641, 1328.5416, 1341.2537, 1374.9208, 1401.2988, 1408.8557, 1419.3688, 1422.6629, 1470.007, 1473.9273, 1482.0141, 1491.0436, 1493.6054, 1500.6361, 1505.419, 1514.308, 1560.722, 2983.0405, 3005.1057, 3010.5308, 3023.0533, 3035.3184, 3077.3005, 3084.1586, 3088.1752, 3089.6386, 3096.4546, 3110.6873, 3120.0723, 3132.9801, 3164.4379
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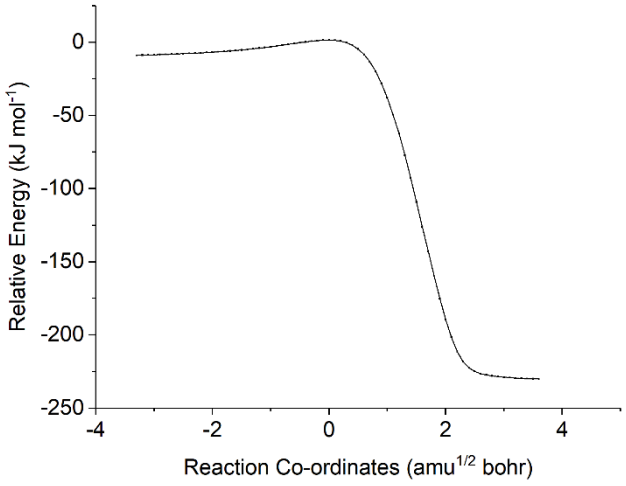
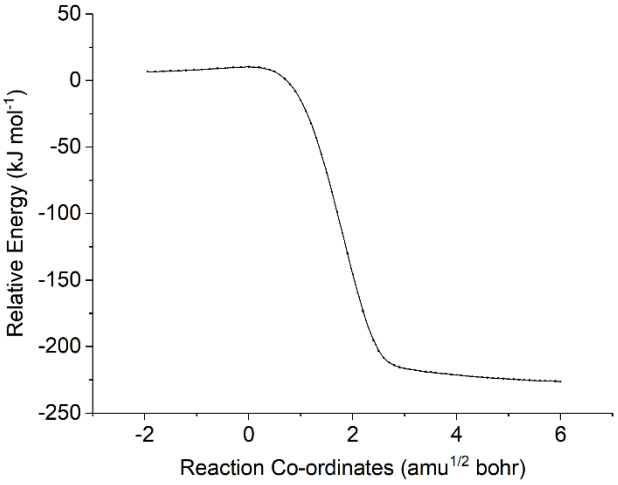


Compound: $iPrCHCMe_2 + O_3$ POZ 2.2	**Energy (Hartree)** -500.099560637349
Reaction Coordinates: 6 1.511226 0.541820 0.208904 6 0.236883 0.191002 -0.586858 6 -1.181507 0.391005 0.080941 6 -2.044347 1.357910 -0.723975 1 -3.065988 1.361543 -0.344586 1 -1.650488 2.371569 -0.641457 1 -2.065075 1.071532 -1.774355 6 -1.185916 0.754121 1.562760 1 -2.217875 0.854166 1.897963 1 -0.709791 -0.015737 2.162803 1 -0.681759 1.702839 1.745642 8 -1.786352 -0.912297 -0.098992 8 -0.667687 -1.799552 -0.062133 8 0.216302 -1.176976 -1.020841 1 0.248233 0.763110 -1.515969 6 1.951610 -0.536631 1.205267 1 2.842258 -0.201214 1.738036 1 1.190859 -0.774050 1.944216 1 2.200934 -1.459144 0.682124 1 1.301660 1.463763 0.758617 6 2.655344 0.839774 -0.770554 1 2.401460 1.656463 -1.448704 1 3.561309 1.121365 -0.232816 1 2.886402 -0.039611 -1.374698	**Frequencies (cm^{-1}):** 19.7529, 66.68, 184.6829, 201.3522, 217.0809, 235.7174, 241.2649, 261.5466, 284.4967, 311.8119, 325.9465, 357.2385, 406.5973, 480.7434, 496.2725, 570.0217, 645.4632, 706.6525, 751.4539, 811.9241, 843.4929, 888.7217, 920.7518, 930.026, 938.2038, 941.1205, 964.2786, 973.9224, 1015.3362, 1030.6448, 1113.2067, 1120.435, 1182.7668, 1200.7552, 1218.7763, 1243.0849, 1311.1311, 1325.0125, 1365.515, 1391.1997, 1403.3744, 1406.4317, 1422.8857, 1429.6434, 1480.1074, 1487.5858, 1489.2818, 1497.0927, 1500.165, 1507.0239, 1510.4919, 1517.8574, 3016.3181, 3021.9496, 3036.3651, 3042.7333, 3047.0783, 3050.7718, 3082.8316, 3088.7794, 3098.5789, 3099.8779, 3105.7524, 3114.1895, 3124.4814, 3143.1334

Compound: $iPrCHCMe_2 + O_3$ PRC 2.3	**Energy (Hartree)** -500.005090090309
Reaction Coordinates: 6 -1.623834 -0.854408 -0.484766 6 -0.579881 0.196663 -0.819377 6 -0.155354 1.257177 -0.105273 6 0.847048 2.210841 -0.691280 1 0.423649 3.217763 -0.756724	**Frequencies (cm^{-1}):** 30.4237, 36.3336, 45.8848, 57.6055, 74.3464, 100.6906, 139.6606, 159.5093, 195.2367, 203.4711, 225.0322, 233.2679, 239.1553, 313.096, 378.2277, 397.2372,

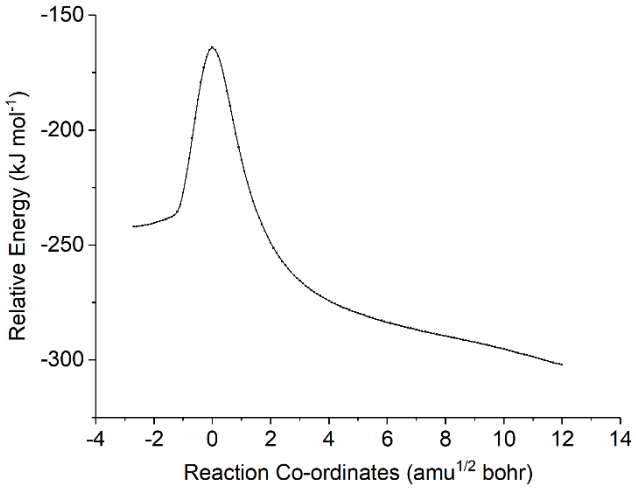
1 1.731981 2.279413 -0.054002 1 1.168544 1.905268 -1.684706 6 -0.650258 1.651402 1.259145 1 0.191459 1.795822 1.939958 1 -1.170550 2.612213 1.201408 1 -1.326818 0.930277 1.704588 1 -0.153600 0.099368 -1.811710 1 -1.650124 -1.521284 -1.350314 6 -1.274529 -1.741300 0.722059 1 -0.309826 -2.229514 0.587277 1 -1.233538 -1.177658 1.653133 1 -2.027085 -2.523138 0.840649 6 -3.038696 -0.261137 -0.358557 1 -3.298879 0.322316 -1.242278 1 -3.775402 -1.059990 -0.252939 1 -3.130134 0.392160 0.508915 8 2.186168 -0.250005 1.003876 8 2.274712 -1.235036 0.216485 8 2.215790 -0.989764 -1.022231	407.2777, 501.8941, 621.163, 737.5982, 768.0594, 838.4163, 854.8978, 930.7721, 958.6408, 962.4473, 975.9139, 1007.3822, 1074.562, 1099.2991, 1117.797, 1131.6367, 1162.1776, 1179.6282, 1205.4712, 1230.8193, 1356.1323, 1382.7233, 1385.4314, 1398.9969, 1411.0293, 1418.5159, 1423.9129, 1470.1953, 1480.7417, 1486.2552, 1490.0982, 1491.2978, 1500.0878, 1505.2301, 1513.1099, 1665.6227, 3009.2798, 3012.868, 3017.8091, 3025.4197, 3032.412, 3053.4266, 3058.8581, 3083.0867, 3088.8068, 3097.3399, 3105.1244, 3111.407, 3135.9647, 3148.2124

Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 2.3	**Energy (Hartree)** -499.996366433202
Reaction Coordinates: 6 -1.665814 -0.441125 -0.342935 6 -0.364275 0.229217 -0.728482 6 0.479681 1.050826 -0.009683 6 0.281690 1.445193 1.430372 1 1.214227 1.812606 1.855395 1 -0.073292 0.630344 2.051069 1 -0.447766 2.259059 1.496489 6 1.479690 1.880723 -0.763808 1 1.647782 1.498212 -1.768368 1 2.436014 1.913101 -0.242255 1 1.119094 2.911907 -0.844348 1 -0.220796 0.264138 -1.801304 1 -1.790563 -1.251322 -1.064738 6 -1.767432 -1.078144 1.048365 1 -1.896621 -0.336531 1.835558 1 -0.896806 -1.687049 1.285744 1 -2.642096 -1.729680 1.077364 6 -2.827505 0.545098 -0.578511 1 -2.775075 1.386553 0.114418 1 -3.784815 0.043439 -0.425709 1 -2.815515 0.943379 -1.593769 8 2.166364 -0.558785 0.476619 8 1.501459 -1.631027 0.208765 8 0.985929 -1.616299 -0.973816	**Frequencies (cm^{-1}):** -162.6441, 42.626, 53.8993, 117.6566, 126.5366, 151.4485, 155.1816, 181.475, 195.1166, 209.3387, 252.6882, 298.5906, 309.7401, 347.7951, 405.1941, 414.0097, 446.3455, 563.2313, 619.9793, 738.1627, 768.0798, 840.8062, 893.259, 936.158, 954.8705, 959.3061, 971.7796, 1016.0146, 1064.7336, 1081.7593, 1082.2415, 1099.6062, 1115.3371, 1144.5755, 1212.0356, 1233.3561, 1332.3875, 1381.1193, 1393.2182, 1401.5779, 1409.4948, 1420.3684, 1422.739, 1473.0324, 1479.0256, 1482.0782, 1491.3118, 1494.5322, 1500.3068, 1511.5857, 1519.5704, 1571.4045, 3006.3802, 3012.5716, 3020.8165, 3024.9599, 3038.0158, 3073.8912, 3082.3013, 3087.1173, 3088.4959, 3092.1226, 3114.3353, 3117.4812, 3149.9853, 3155.7495
IRC:	



Compound: $iPrCHCMe_2 + O_3$ POZ 2.3	**Energy (Hartree)** -500.098143883523
Reaction Coordinates: 6 1.670392 -0.238455 -0.390414 6 0.170788 -0.185791 -0.742297 6 -0.883799 0.578490 0.130335 6 -1.238380 1.940238 -0.453036 1 -2.069761 2.379545 0.097310 1 -0.387829 2.616343 -0.376717 1 -1.522161 1.851419 -1.500526 6 -0.614874 0.661932 1.629794 1 -1.473104 1.130663 2.111274 1 -0.476068 -0.325168 2.060851 1 0.264310 1.266518 1.845256 8 -2.043338 -0.254419 -0.098331 8 -1.504717 -1.559558 0.045966 8 -0.349594 -1.526806 -0.847109 1 0.096510 0.234619 -1.749128 6 2.313800 1.151485 -0.446731 1 3.398379 1.066019 -0.373281 1 2.086864 1.664160 -1.383334 1 1.983000 1.788622 0.374822 1 2.094939 -0.812723 -1.220062 6 2.039035 -0.998356 0.887311 1 1.484689 -1.932695 0.962261 1 3.102214 -1.242573 0.868837 1 1.857444 -0.415743 1.788464	**Frequencies (cm^{-1}):** 44.6921, 104.3266, 189.4513, 210.6007, 217.1462, 239.7434, 249.0825, 269.3811, 277.9811, 296.3378, 324.534, 361.5894, 386.3785, 455.3301, 496.9549, 577.6385, 617.1396, 687.9109, 748.7095, 783.3638, 843.4096, 879.4662, 924.8332, 936.7227, 945.2614, 950.0748, 969.7543, 992.7414, 1011.2932, 1029.3371, 1108.2063, 1153.4811, 1183.502, 1220.285, 1229.7507, 1255.1683, 1333.6474, 1358.8002, 1368.6897, 1402.6724, 1404.9038, 1410.9872, 1426.1544, 1432.4832, 1481.3745, 1489.5617, 1493.3653, 1495.3651, 1502.8971, 1512.7125, 1512.9408, 1520.7649, 2997.9491, 3015.6902, 3025.9247, 3039.9615, 3043.7288, 3050.8246, 3083.4268, 3088.4833, 3094.6311, 3106.8354, 3112.9882, 3117.3468, 3118.8233, 3142.077

Compound: $iPrCHCMe_2 + O_3$ TS_{ANTI} 1	**Energy (Hartree)** -500.070492661337
Reaction Coordinates: 6 -1.621157 -0.207910 0.293868 6 -0.356163 0.380047 -0.297068 6 1.354416 -0.460175 0.052671 6 1.457646 -1.500084 -1.071548 1 0.638332 -2.215126 -1.074934	**Frequencies (cm^{-1}):** -471.1801, 57.9601, 88.0866, 163.1743, 186.4835, 204.171, 216.8057, 222.3976, 242.3326, 265.1519, 281.4379, 294.9007, 349.5894, 426.1388, 453.9438, 479.3616,

1 2.387821 -2.054518 -0.933896 1 1.509562 -0.999213 -2.036406 6 1.239055 -1.018898 1.473698 1 0.471697 -1.786104 1.568335 1 1.038562 -0.214324 2.178666 1 2.196495 -1.468145 1.743994 1 -0.260713 0.369224 -1.380034 1 -1.490448 -0.261313 1.376675 6 -1.928798 -1.610525 -0.238054 1 -2.893122 -1.942087 0.146779 1 -1.185803 -2.345229 0.063020 1 -1.990224 -1.616010 -1.328045 6 -2.802790 0.738111 0.003463 1 -2.631213 1.729664 0.417997 1 -2.965488 0.841778 -1.071202 1 -3.716031 0.334757 0.442195 8 -0.052772 1.567173 0.247708 8 0.999172 2.105251 -0.347528 8 2.158265 0.540481 -0.077095	484.7667, 539.3743, 585.7889, 617.239, 774.6216, 864.2835, 912.7329, 935.5245, 943.2124, 973.5274, 985.5904, 1005.1832, 1065.3997, 1088.4899, 1121.1091, 1151.9518, 1169.4564, 1187.5874, 1191.5036, 1243.1903, 1317.7933, 1336.8421, 1372.3582, 1388.2665, 1399.065, 1403.3356, 1409.9566, 1431.3369, 1477.4686, 1485.7221, 1489.726, 1494.6302, 1494.9663, 1502.8035, 1509.4269, 1518.3202, 3027.7162, 3032.8072, 3035.2257, 3039.9833, 3041.293, 3086.6453, 3093.9118, 3095.0956, 3101.2777, 3108.5995, 3114.3751, 3117.6017, 3122.5213, 3133.5451
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ C_{ANTI} 1	**Energy (Hartree)** -500.123510392293
Reaction Coordinates: 6 -2.305770 -0.171141 -0.319203 6 -1.088537 0.505103 0.197996 1 -0.722785 0.370435 1.211703 8 -0.454580 1.292134 -0.540027 8 0.670377 1.912091 -0.013305 1 -2.373074 0.051551 -1.385397 6 -3.548971 0.400340 0.390957 1 -4.443148 -0.097686 0.015564 1 -3.653671 1.470524 0.215661 1 -3.498956 0.231606 1.467879 6 -2.191952 -1.691303 -0.117136 1 -1.307294 -2.090984 -0.607671 1 -2.126407 -1.939929 0.943082 1 -3.077873 -2.178657 -0.524714 6 2.164393 -0.577026 0.088517 6 2.922223 -0.024784 1.270626	**Frequencies (cm^{-1}):** 29.3556, 33.946, 63.9613, 67.1364, 77.8482, 90.4112, 102.9606, 122.2043, 139.4607, 204.9024, 209.7612, 224.9697, 267.4681, 320.0664, 384.9399, 429.9275, 477.4483, 485.446, 521.9341, 536.3316, 788.5174, 850.4705, 892.0988, 902.082, 910.6877, 939.6556, 948.7239, 957.6358, 970.5887, 1087.0823, 1100.6954, 1117.4863, 1184.0228, 1202.5914, 1242.708, 1326.0712, 1331.0379, 1372.3638, 1380.6734, 1388.3722, 1402.6001, 1425.4602, 1458.1037, 1468.148, 1470.7619, 1487.9195, 1488.8987, 1489.4387, 1501.2361,

1 3.128891 1.034726 1.123568 1 3.881997 -0.541295 1.357856 1 2.353142 -0.166571 2.185232 6 2.754277 -0.312600 -1.275612 1 2.627138 0.746795 -1.503384 1 2.245543 -0.908470 -2.029171 1 3.823930 -0.529839 -1.286627 8 1.147777 -1.232192 0.228275	1511.0797, 1579.3058, 1749.793, 3027.4826, 3030.1211, 3035.5321, 3035.8033, 3052.7572, 3092.3544, 3092.733, 3097.739, 3099.0019, 3104.7283, 3125.1317, 3132.9509, 3140.2823, 3151.7939

Compound: $iPrCHCMe_2 + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -500.072336326532
Reaction Coordinates: 6 -1.552772 0.482412 0.024310 6 -0.304991 -0.278943 0.425705 6 1.361765 0.468572 -0.022401 6 1.495756 1.551813 1.060298 1 0.654724 2.246304 1.060609 1 2.402162 2.125597 0.861522 1 1.594547 1.093943 2.042323 6 1.258943 1.007423 -1.451484 1 0.488147 1.769782 -1.563233 1 1.075047 0.194244 -2.150053 1 2.216281 1.461794 -1.713435 1 -0.109340 -0.346865 1.491776 1 -1.270494 1.537878 -0.020608 6 -2.619975 0.341811 1.123163 1 -3.498072 0.938222 0.873627 1 -2.247865 0.680199 2.090715 1 -2.937322 -0.697022 1.226741 6 -2.114697 0.074893 -1.341937 1 -1.377587 0.163944 -2.136600 1 -2.465961 -0.956787 -1.327832 1 -2.961189 0.714380 -1.592134 8 -0.141384 -1.460464 -0.194501 8 0.911234 -2.089880 0.309753 8 2.141743 -0.551343 0.128579	**Frequencies (cm^{-1}):** -462.2543, 63.6016, 81.1371, 162.9494, 200.1402, 207.9409, 216.0407, 235.5798, 241.7963, 251.3711, 270.7694, 310.6758, 375.4883, 404.1233, 420.2776, 484.4743, 520.2483, 575.2814, 591.815, 630.2075, 776.0971, 847.7494, 910.8123, 929.6322, 958.5321, 967.7949, 992.1435, 1033.6567, 1060.0104, 1076.9625, 1121.3748, 1127.5066, 1169.9828, 1192.505, 1205.2895, 1252.9394, 1326.5249, 1352.5479, 1370.9894, 1388.061, 1390.1849, 1404.0971, 1406.6844, 1432.9231, 1475.8925, 1486.6406, 1491.2632, 1492.1053, 1495.8642, 1504.2979, 1506.603, 1514.073, 3019.175, 3027.3429, 3029.4878, 3035.1462, 3043.4231, 3087.347, 3091.8211, 3092.4273, 3093.7615, 3101.5168, 3113.3553, 3121.3541, 3122.3969, 3125.246

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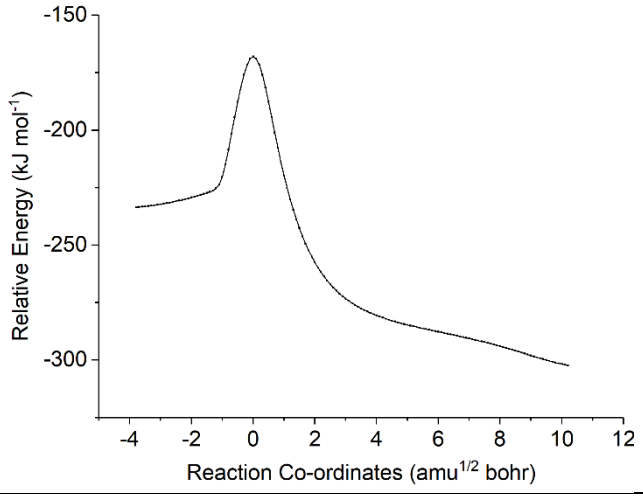
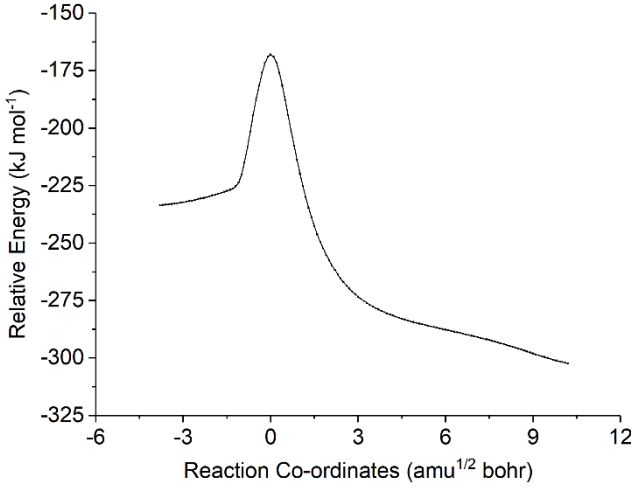


Compound: $iPrCHCMe_2 + O_3$ C_{ANTI} 2	**Energy (Hartree)** -500.120499876249
Reaction Coordinates: 6 -1.953916 -0.779032 0.036276 6 -1.177695 0.386127 -0.462423 6 2.440269 -0.441445 -0.015306 6 3.672341 -1.317526 0.031582 1 4.268530 -1.095985 0.918514 1 4.303938 -1.101715 -0.833500 1 3.392922 -2.367657 0.021310 6 2.649270 1.040898 0.153592 1 2.985806 1.235593 1.176059 1 1.731591 1.597712 -0.035401 1 3.448742 1.388134 -0.504542 1 -0.688610 0.381245 -1.431150 1 -1.230113 -1.602144 0.044249 6 -3.047186 -1.138466 -0.990205 1 -3.536986 -2.065680 -0.693818 1 -2.631532 -1.281929 -1.987934 1 -3.804408 -0.355455 -1.044340 6 -2.513759 -0.586934 1.444217 1 -1.723811 -0.365922 2.160238 1 -3.232192 0.232500 1.475436 1 -3.021736 -1.496249 1.764533 8 -1.083677 1.431909 0.215709 8 -0.338281 2.484565 -0.312113 8 1.337198 -0.926996 -0.180602	**Frequencies (cm^{-1}):** 20.882, 27.3247, 45.1603, 60.3496, 74.0044, 91.552, 97.7926, 138.3232, 156.8233, 193.0098, 217.9741, 224.1083, 257.4163, 336.2253, 395.5306, 439.0949, 445.7254, 498.7131, 545.3482, 601.4094, 791.7709, 826.622, 889.4105, 893.8463, 904.1785, 931.792, 946.4897, 971.6223, 975.1344, 1092.8839, 1111.693, 1125.7724, 1141.1876, 1205.4969, 1246.6721, 1303.8298, 1352.1113, 1378.8007, 1387.6804, 1402.3032, 1406.6338, 1427.9046, 1462.5708, 1467.0079, 1476.8716, 1489.0684, 1492.8779, 1496.8961, 1504.4592, 1511.4612, 1579.2211, 1756.6969, 3006.0507, 3009.1656, 3030.9345, 3031.4219, 3040.4566, 3069.4844, 3084.2886, 3096.5046, 3099.9138, 3102.178, 3103.6423, 3111.3342, 3136.5723, 3158.0452

Compound: $iPrCHCMe_2 + O_3$ TS_{ANTI} 3	**Energy (Hartree)** -500.066952645815
Reaction Coordinates: 6 1.713991 -0.264797 -0.393055 6 0.219904 -0.458719 -0.609011 6 -1.136865 0.636744 0.218607 6 -1.205039 1.849808 -0.721417 1 -0.265416 2.393961 -0.783511 1 -1.964443 2.531785 -0.334931 1 -1.515422 1.538181 -1.716951 6 -0.671689 0.944062 1.644410 1 0.244516 1.531503 1.673346 1 -0.534724 0.023476 2.206942 1 -1.455565 1.522708 2.137375 1 -0.125666 -0.261829 -1.620154 1 2.154859 -0.929015 -1.148058 6 2.242116 -0.729786 0.968285 1 1.920202 -0.073885 1.774657 1 1.916709 -1.741130 1.204054 1 3.332365 -0.723163 0.951098 6 2.188513 1.149720 -0.739064 1 1.859892 1.880346 -0.000923 1 3.278059 1.170874 -0.758551 1 1.833612 1.470769 -1.718741 8 -0.218576 -1.636266 -0.134683 8 -1.468648 -1.852334 -0.515298	**Frequencies (cm^{-1}):** -482.4731, 72.424, 84.1642, 181.1988, 190.084, 209.7179, 219.247, 241.3283, 250.125, 265.0202, 281.6505, 320.8835, 338.3924, 414.182, 425.3494, 465.3799, 483.6881, 566.3456, 594.4233, 644.3468, 771.4695, 838.2625, 911.7703, 935.9893, 955.5541, 979.2762, 993.9721, 1025.6364, 1064.5484, 1092.1581, 1099.104, 1151.1831, 1163.1748, 1191.5638, 1220.3509, 1245.614, 1334.0414, 1352.5278, 1373.3171, 1381.3922, 1388.8319, 1403.9838, 1410.6919, 1432.8136, 1476.9238, 1487.406, 1488.8329, 1493.6328, 1502.7808, 1504.3049, 1512.258, 1518.5451, 2968.5141, 3033.6618, 3036.1891, 3040.0265, 3046.6242, 3092.8349, 3096.3311, 3100.7053, 3102.8949, 3106.1854, 3109.6152, 3124.1121, 3128.7563, 3131.9885

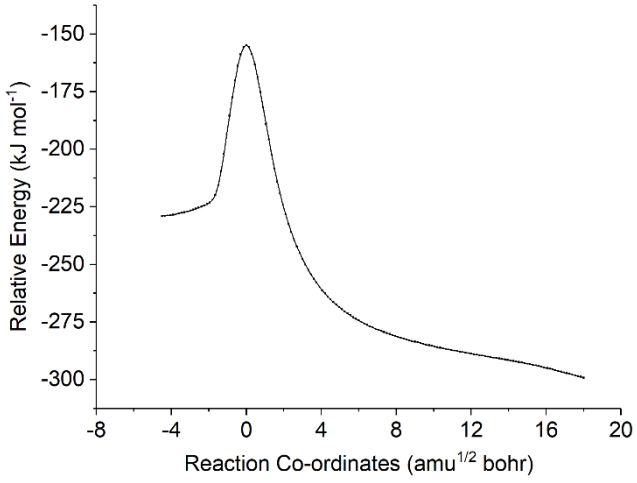
8 -2.160847 -0.148496 0.140208	

IRC:



Compound: $iPrCHCMe_2 + O_3$ C_{ANTI} 3	**Energy (Hartree)** -500.124303990849
Reaction Coordinates: 6 -2.382824 -0.129443 -0.325221 6 -1.074251 0.432787 -0.751514 1 -0.543188 0.067282 -1.624800 8 -0.545806 1.371952 -0.117074 8 0.677653 1.851322 -0.570847 1 -3.077699 0.133670 -1.136237 6 -2.906238 0.460969 0.983052 1 -2.240562 0.217551 1.811105 1 -2.994263 1.545009 0.931188 1 -3.889438 0.046977 1.204245 6 -2.294814 -1.667732 -0.291939 1 -1.599147 -1.995787 0.478198 1 -3.280485 -2.082536 -0.083052 1 -1.950079 -2.069680 -1.244474 6 2.046895 -0.595206 0.208409 6 2.411775 0.005829 1.544183 1 2.288138 1.087741 1.475728 1 3.455593 -0.195639 1.791440 1 1.762267 -0.383898 2.323941 6 3.018452 -0.366376 -0.923120 1 3.248923 0.694685 -1.012306 1 2.604985 -0.734401 -1.858054 1 3.952873 -0.892228 -0.708919 8 1.036667 -1.258738 0.061533	**Frequencies (cm^{-1}):** 27.4213, 34.0516, 65.4931, 70.1959, 82.0788, 93.6496, 105.4779, 138.7385, 147.3152, 191.6971, 214.2501, 227.3651, 257.012, 336.7136, 384.9264, 441.1124, 447.3466, 486.0142, 536.2614, 596.0506, 788.3514, 828.4378, 891.9183, 902.5857, 904.9527, 931.8615, 939.7318, 975.3256, 978.1187, 1087.0022, 1110.7904, 1117.3594, 1146.4621, 1207.1281, 1242.5396, 1296.9603, 1347.2716, 1375.1951, 1380.6564, 1388.3723, 1410.0425, 1429.8317, 1458.2797, 1468.3225, 1470.9759, 1488.3255, 1488.8198, 1490.9387, 1502.6203, 1511.2647, 1576.4281, 1749.5251, 2957.4457, 3027.5773, 3035.8616, 3039.8724, 3042.7367, 3092.4506, 3097.7545, 3103.345, 3105.5396, 3111.7179, 3121.0061, 3132.6058, 3140.1532, 3156.321

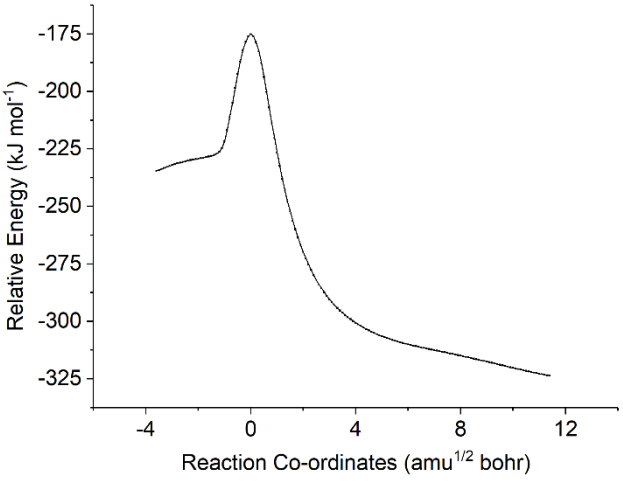
Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 1.1	**Energy (Hartree)** -500.075670013921
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.602448 0.162377 -0.230437 6 -0.374052 -0.224118 0.625084 6 1.201839 0.497909 -0.064928 6 2.195689 0.382226 1.067093 1 3.205468 0.461226 0.656755 1 2.104403 -0.566201 1.584325 1 2.046471 1.201070 1.768749 6 1.059448 1.866798 -0.677118 1 0.704766 2.576102 0.067126 1 2.034825 2.213110 -1.025608 1 0.374551 1.863386 -1.521488 1 -0.295309 0.339946 1.570342 1 -1.267229 0.356233 -1.252408 6 -2.267054 1.427454 0.319742 1 -1.584963 2.277212 0.357886 1 -3.117619 1.716962 -0.298463 1 -2.640030 1.256131 1.332467 6 -2.602166 -0.997047 -0.295294 1 -3.444840 -0.730418 -0.935181 1 -2.135266 -1.896023 -0.690682 1 -2.992869 -1.234102 0.696358 8 1.300638 -0.440812 -1.050155 8 1.430554 -1.654665 -0.532006 8 -0.063679 -1.470552 0.735282	-462.8351, 49.0125, 95.177, 162.3988, 176.1447, 201.5902, 209.2841, 233.1641, 248.1251, 267.9689, 303.7398, 338.6916, 343.3215, 381.8714, 413.0056, 427.1393, 534.9081, 573.8174, 644.6694, 665.3672, 786.0754, 831.7373, 917.4204, 935.3415, 952.3717, 966.8606, 972.5306, 990.427, 1011.9406, 1097.5121, 1125.5317, 1138.4621, 1163.9922, 1195.2854, 1273.7237, 1280.8368, 1297.8542, 1326.0099, 1349.9759, 1397.2951, 1401.4685, 1403.89, 1419.3568, 1429.5839, 1470.9667, 1481.5396, 1488.7819, 1490.7186, 1494.1225, 1504.1951, 1505.7506, 1511.8159, 2907.5713, 3019.39, 3022.5946, 3028.7693, 3034.043, 3039.8467, 3077.5167, 3084.1178, 3091.1681, 3101.8077, 3106.2256, 3120.7541, 3137.6264, 3162.1852
IRC:  	

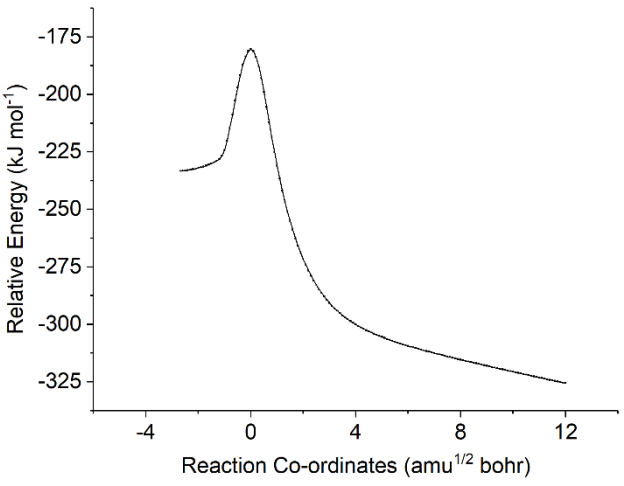
Compound: $iPrCHCMe_2 + O_3$ CPr_{AO} 1.1	**Energy (Hartree)** -500.127738386250
Reaction Coordinates: 6 2.280766 0.020421 0.243743 6 1.109599 0.555313 -0.543903 6 -2.323608 -0.021283 0.041788 6 -2.091733 -1.453139 0.296797 1 -2.172812 -1.640091 1.369793 1 -1.059885 -1.691467 0.029636 1 -2.779744 -2.072448 -0.272484 6 -3.261608 0.492055 -0.987693 1 -2.933548 0.150741 -1.972518 1 -4.262540 0.087818 -0.821339 1 -3.296468 1.578227 -0.976401	**Frequencies (cm^{-1}):** 28.8479, 31.4456, 40.2345, 64.9932, 84.6148, 87.6478, 149.2758, 157.7152, 162.9258, 198.9538, 229.2595, 272.9603, 291.9476, 310.2365, 351.4906, 367.6751, 410.5925, 481.2188, 593.8979, 641.1227, 796.501, 812.8661, 913.0078, 913.9669, 926.0007, 930.5531, 946.387, 973.8385, 988.2613, 1073.135, 1097.5548, 1126.9288, 1152.0461, 1199.3392, 1305.2502, 1306.1502, 1362.7537,

1 0.883849 1.621234 -0.352219 1 1.987305 0.163926 1.289487 6 3.509359 0.906887 -0.021959 1 3.290226 1.960692 0.156855 1 4.330060 0.621777 0.636141 1 3.853062 0.801596 -1.052817 6 2.550689 -1.456469 -0.017103 1 3.377788 -1.806660 0.601384 1 1.675390 -2.063341 0.210636 1 2.809138 -1.629282 -1.062549 8 -1.714356 0.856717 0.715048 8 -0.785716 0.419401 1.652778 8 0.457246 -0.069297 -1.349530	1387.6256, 1401.6335, 1405.6884, 1412.1562, 1433.8316, 1443.9564, 1458.7778, 1470.4252, 1479.1982, 1486.9531, 1490.4176, 1504.6272, 1508.9443, 1570.0899, 1772.3351, 2909.4477, 3012.5999, 3024.1472, 3026.7341, 3033.9029, 3034.6161, 3075.0393, 3081.4913, 3084.128, 3091.8887, 3095.3449, 3103.1073, 3137.4614, 3138.7634

Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 1.2	**Energy (Hartree)** -500.078148008237
Reaction Coordinates: 6 1.605736 0.474029 0.043317 6 0.385443 -0.084251 -0.710002 6 -1.225552 0.483084 0.006953 6 -2.219779 0.283943 -1.114693 1 -3.227158 0.274591 -0.691494 1 -2.053057 -0.652487 -1.635364 1 -2.149961 1.113589 -1.816100 6 -1.175807 1.863190 0.607770 1 -0.772694 2.571100 -0.114530 1 -2.184533 2.191571 0.866272 1 -0.561661 1.886447 1.504761 1 0.214125 0.433561 -1.670200 1 1.434240 1.537709 0.229910 6 2.822926 0.363942 -0.888755 1 2.651465 0.875523 -1.837958 1 3.703652 0.809319 -0.423894 1 3.044068 -0.681997 -1.106136 6 1.870115 -0.235115 1.371458 1 2.778861 0.155098 1.831818 1 1.051085 -0.105210 2.077355 1 1.999388 -1.305084 1.212042 8 -1.249451 -0.457558 0.995545 8 -1.273338 -1.677557 0.483650 8 0.234499 -1.364468 -0.769540	**Frequencies (cm^{-1}):** -442.9627, 61.036, 103.4755, 167.1876, 185.9858, 204.0616, 217.6061, 243.5371, 248.6403, 262.369, 296.049, 310.3756, 343.0872, 377.9881, 402.0569, 425.3787, 538.9022, 630.5345, 648.3162, 683.9385, 775.6779, 820.9131, 919.8382, 936.3115, 955.6347, 969.0862, 983.068, 1000.8802, 1024.5609, 1092.9989, 1107.4285, 1133.5826, 1169.3909, 1197.6573, 1274.7883, 1278.8809, 1296.2285, 1342.4837, 1348.9773, 1399.4069, 1403.0968, 1404.8225, 1420.2185, 1436.5624, 1471.9546, 1483.5098, 1488.489, 1492.7339, 1495.0027, 1502.9817, 1506.0707, 1514.5336, 2897.3101, 3017.8808, 3020.8839, 3034.3892, 3037.3136, 3039.5797, 3079.7387, 3090.7534, 3096.6893, 3099.2351, 3104.6386, 3110.3456, 3132.5172, 3160.352
IRC:	

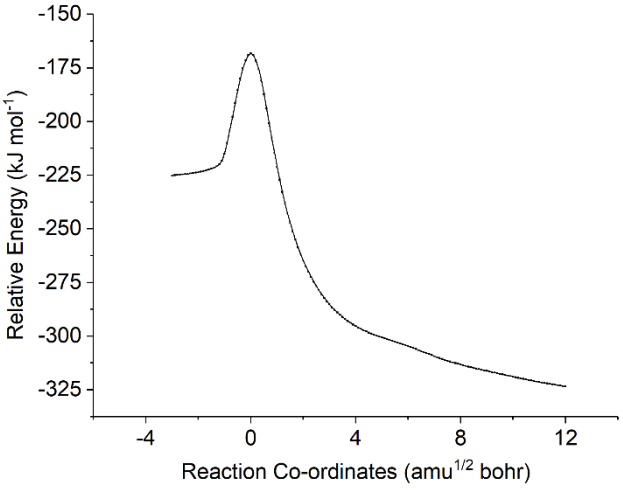


Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 1.3	**Energy (Hartree)** -500.073453434399
Reaction Coordinates: 6 1.734063 -0.296988 -0.357009 6 0.282747 -0.293658 -0.887311 6 -0.989035 0.618985 0.134630 6 -2.142086 0.812244 -0.824865 1 -3.046172 1.013763 -0.245000 1 -2.310007 -0.067894 -1.435028 1 -1.945286 1.672872 -1.461833 6 -0.511315 1.869807 0.825928 1 -0.065558 2.551858 0.105963 1 -1.363800 2.378697 1.281564 1 0.214363 1.648250 1.603125 1 0.147663 0.378533 -1.752875 1 2.218581 -0.983042 -1.060353 6 1.894080 -0.916225 1.032220 1 1.340233 -1.850919 1.103271 1 2.946150 -1.127537 1.229111 1 1.539371 -0.252690 1.821363 6 2.453884 1.046786 -0.497991 1 2.167472 1.759633 0.274164 1 3.532058 0.902911 -0.416653 1 2.261301 1.506047 -1.470523 8 -1.133322 -0.387451 1.044675 8 -1.583379 -1.487204 0.461543 8 -0.279599 -1.447368 -1.022457	**Frequencies (cm^{-1}):** -461.1451, 75.975, 108.3295, 177.1786, 186.2279, 211.4554, 235.119, 235.7138, 249.4934, 262.2912, 279.2264, 326.1872, 342.5325, 376.6126, 410.2419, 483.624, 514.0737, 555.2316, 644.8178, 682.8027, 773.4254, 824.5874, 919.8837, 933.8156, 952.7748, 975.0733, 981.0583, 1000.1476, 1020.9794, 1094.8482, 1126.6398, 1140.4738, 1168.0175, 1208.2899, 1272.7923, 1278.3631, 1297.9258, 1343.92, 1350.6298, 1397.4681, 1401.2057, 1404.6278, 1420.1886, 1430.2874, 1471.4806, 1481.4577, 1487.9063, 1493.832, 1500.6531, 1504.4551, 1511.9914, 1512.9309, 2900.7525, 2995.3514, 3024.4398, 3034.3336, 3034.865, 3039.4472, 3078.1385, 3087.3881, 3099.2106, 3103.8642, 3110.2417, 3113.234, 3146.441, 3163.9564
IRC:	



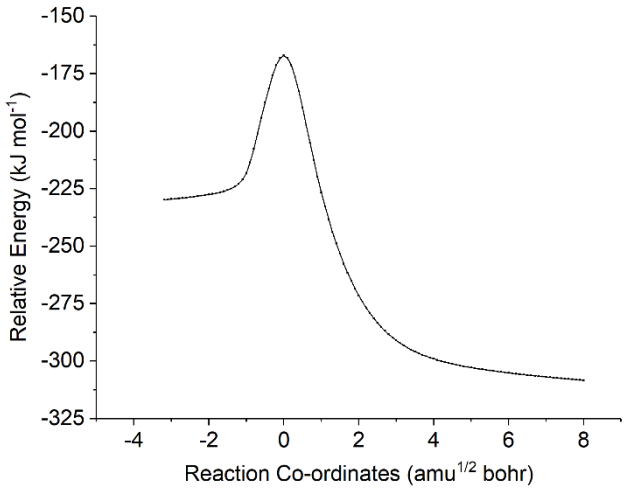
Compound: $iPrCHCMe_2 + O_3$ CPr_{AO} 1.3	**Energy (Hartree)** -500.122385192186
Reaction Coordinates: 6 2.889427 -0.222678 0.318605 6 1.423575 -0.529923 0.137027 6 -2.698685 0.038082 0.007238 6 -2.253383 -1.207135 -0.633565 1 -1.247238 -1.455295 -0.268305 1 -2.142969 -1.037853 -1.706513 1 -2.935681 -2.026214 -0.420887 6 -3.794291 0.107003 1.009267 1 -3.935214 1.124751 1.363960 1 -4.725248 -0.259020 0.569720 1 -3.564366 -0.546310 1.854439 1 0.829207 0.242319 -0.391357 1 3.338442 -1.066159 0.846056 6 3.036907 1.054000 1.159986 1 2.610241 0.927103 2.155411 1 4.091108 1.309281 1.274035 1 2.537333 1.898687 0.681829 6 3.546611 -0.062912 -1.060376 1 4.601856 0.188337 -0.947065 1 3.478387 -0.981521 -1.643795 1 3.071519 0.737405 -1.630975 8 -2.142739 1.141594 -0.265596 8 -1.101936 1.134838 -1.184170 8 0.881132 -1.540700 0.529059	**Frequencies (cm^{-1}):** 17.997, 23.7773, 43.5708, 48.9089, 84.7219, 92.7803, 99.8405, 157.2725, 207.0856, 228.2621, 241.1585, 285.0301, 312.6748, 332.7768, 349.2666, 362.086, 369.4749, 494.1998, 545.6884, 594.2158, 816.0457, 844.6458, 913.1819, 914.6117, 935.85, 938.2155, 970.6384, 989.0403, 996.4127, 1073.4082, 1099.1939, 1149.5405, 1180.5863, 1185.9172, 1307.1448, 1323.7547, 1345.8832, 1398.6401, 1400.3225, 1408.6369, 1416.4049, 1444.9111, 1450.7741, 1459.0266, 1470.5514, 1487.0453, 1489.8751, 1491.5541, 1504.8901, 1512.3676, 1562.2399, 1765.0888, 2899.4863, 2973.506, 3024.1812, 3025.2724, 3026.6817, 3046.436, 3059.7836, 3070.1193, 3085.7628, 3091.4801, 3092.5306, 3093.8049, 3132.7889, 3136.0249

Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 2.1	**Energy (Hartree)** -500.071981948728
Reaction Coordinates: 6 -1.650163 0.044057 0.296592 6 -0.423353 -0.471638 -0.495729 6 1.157578 0.524381 -0.001306 6 1.093945 0.682655 1.496852 1 2.087476 0.981104 1.843702	**Frequencies (cm^{-1}):** -477.186, 77.0669, 86.0197, 141.6379, 177.6548, 195.4179, 223.4689, 234.2487, 248.98, 263.3514, 321.2703, 327.8648, 353.7062, 376.7076, 408.1218, 434.2736,

1 0.824783 -0.244818 1.989480 1 0.391746 1.464879 1.771911 6 1.336346 1.768980 -0.830977 1 0.463711 2.411097 -0.761241 1 2.198545 2.336451 -0.473073 1 1.499432 1.511561 -1.875762 1 -0.443823 -0.169938 -1.558332 1 -1.433074 -0.070426 1.359211 6 -2.022743 1.496271 -0.004003 1 -2.095585 1.669482 -1.080488 1 -2.998064 1.727667 0.425870 1 -1.314176 2.214168 0.406394 6 -2.831016 -0.881077 -0.040443 1 -3.718206 -0.584006 0.521230 1 -3.076829 -0.828897 -1.103860 1 -2.592996 -1.915049 0.200712 8 2.007411 -0.429102 -0.455428 8 1.849702 -1.570224 0.191261 8 -0.076676 -1.686305 -0.259790	522.822, 535.4822, 623.1601, 649.2633, 787.2981, 837.2084, 908.9541, 934.957, 952.3219, 970.8741, 987.9967, 1000.7291, 1026.9948, 1097.2154, 1129.9278, 1143.8113, 1167.9972, 1189.9358, 1275.3809, 1279.429, 1310.961, 1333.9271, 1342.748, 1397.3151, 1402.6208, 1408.7535, 1420.3127, 1427.9879, 1473.5692, 1480.9665, 1490.1072, 1491.8858, 1496.0081, 1500.6997, 1509.197, 1515.6255, 2891.115, 3019.8263, 3024.863, 3028.6869, 3036.4295, 3051.1204, 3075.1273, 3084.4341, 3096.7447, 3106.233, 3114.7852, 3116.1087, 3148.1339, 3164.6568
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{AO} 2.1	**Energy (Hartree)** -500.127134953934
Reaction Coordinates: 6 2.213869 -0.111205 -0.354076 6 1.178814 -0.510876 0.669384 6 -2.254159 -0.021929 -0.179566 6 -2.596658 -0.025953 1.252760 1 -2.857170 0.989618 1.558577 1 -1.703214 -0.290453 1.822126 1 -3.398810 -0.727657 1.465191 6 -2.824124 -0.972011 -1.167018 1 -2.540254 -1.989351 -0.887330 1 -3.915109 -0.922808 -1.152332 1 -2.458560 -0.759600 -2.168156 1 1.268061 -0.001149 1.649468 1 1.819187 -0.396448 -1.331168 6 2.487466 1.394088 -0.311747 1 2.890625 1.688511 0.660272 1 3.224416 1.663960 -1.069332	**Frequencies (cm^{-1}):** 25.2482, 31.4077, 38.5771, 66.097, 78.0186, 87.1926, 150.1874, 153.6528, 157.9164, 214.2854, 233.2662, 293.6013, 311.2542, 320.0828, 339.6151, 364.8213, 367.6549, 480.2013, 546.5744, 595.1374, 812.7628, 845.8718, 903.8044, 916.0259, 929.3499, 939.0462, 964.0933, 978.7578, 988.4704, 1073.5852, 1096.7989, 1129.0417, 1181.8969, 1186.5562, 1306.4216, 1319.0425, 1338.494, 1385.5432, 1397.0523, 1405.3266, 1413.8224, 1428.9651, 1444.1218, 1458.589, 1470.2864, 1478.6056, 1488.7266, 1493.1665, 1502.2797,

1 1.573875 1.961184 -0.482713 6 3.488531 -0.930666 -0.077519 1 4.265152 -0.662764 -0.794812 1 3.878010 -0.727045 0.922582 1 3.299357 -2.000933 -0.158947 8 -1.437062 0.823831 -0.640464 8 -0.835998 1.693746 0.260553 8 0.334561 -1.361796 0.501569	1516.939, 1570.0738, 1772.238, 2889.4607, 3020.0885, 3023.0692, 3027.342, 3035.0695, 3043.9497, 3075.8787, 3077.4889, 3083.6251, 3085.0653, 3097.9716, 3111.7213, 3137.7133, 3139.0013

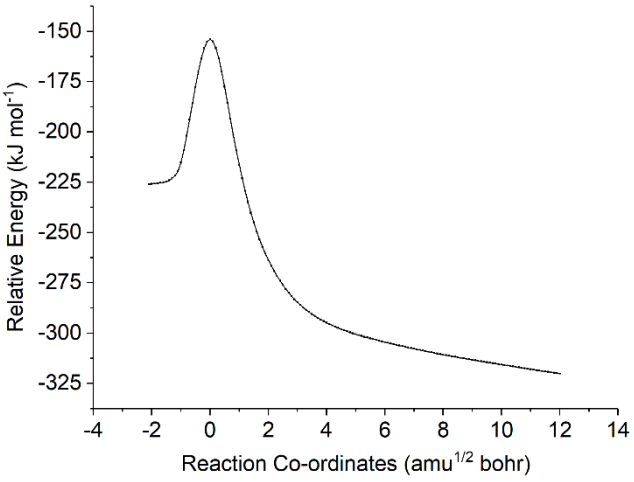
Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 2.2	**Energy (Hartree)** -500.072421952321
Reaction Coordinates: 6 -1.613862 0.303497 0.179073 6 -0.380571 -0.148710 -0.663744 6 1.161328 0.533138 0.161814 6 1.108762 0.169016 1.624537 1 2.094709 0.368056 2.053461 1 0.877228 -0.879548 1.767303 1 0.384131 0.784808 2.150706 6 1.328876 1.990711 -0.173515 1 0.431367 2.542825 0.101668 1 2.164484 2.418598 0.383618 1 1.510555 2.124881 -1.238108 1 -0.305507 0.424762 -1.602921 1 -1.345641 1.180993 0.772217 6 -2.709368 0.741931 -0.803418 1 -3.025451 -0.092765 -1.431161 1 -3.581841 1.104721 -0.257535 1 -2.367923 1.544804 -1.458308 6 -2.128346 -0.790023 1.112571 1 -1.369252 -1.135156 1.810575 1 -2.973940 -0.414224 1.690884 1 -2.459286 -1.656372 0.541144 8 2.003111 -0.219328 -0.597378 8 1.815657 -1.510737 -0.379644 8 -0.148086 -1.409152 -0.761409	**Frequencies (cm^{-1}):** -468.8294, 69.9601, 83.5466, 162.4342, 174.8974, 196.094, 202.543, 234.0363, 244.3457, 271.1151, 301.4603, 312.4394, 340.6927, 382.999, 395.7375, 425.2798, 529.4784, 608.7191, 629.581, 644.3865, 777.7042, 821.2586, 905.3799, 942.8821, 950.4471, 964.7296, 986.6206, 1003.016, 1047.9331, 1091.1513, 1118.0686, 1139.1364, 1191.9356, 1202.2983, 1276.6492, 1282.911, 1319.0373, 1343.1461, 1354.3946, 1401.2325, 1403.3469, 1409.6838, 1418.3709, 1435.0381, 1474.825, 1478.79, 1486.7251, 1488.8021, 1495.6582, 1499.7402, 1505.6081, 1509.6282, 2905.077, 3021.4644, 3023.2365, 3031.6685, 3038.1925, 3039.3135, 3085.0392, 3089.9928, 3097.9203, 3100.3187, 3114.7259, 3121.4946, 3125.064, 3173.2694
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{AO} 2.2	**Energy (Hartree)** -500.124259822023
Reaction Coordinates: 6 2.123726 -0.353472 0.069736 6 1.573618 0.816086 -0.704554 6 -2.364186 0.114129 0.001670 6 -3.532380 -0.758643 0.210934 1 -3.323993 -1.436757 1.043081 1 -3.647544 -1.412811 -0.657536 1 -4.435674 -0.182705 0.391451 6 -2.403284 1.598194 0.037296 1 -3.086317 1.969614 -0.731226 1 -2.798886 1.934455 0.998978 1 -1.412259 2.018154 -0.116874 1 1.481845 0.633903 -1.796124 1 1.349856 -1.126174 -0.042725 6 3.398473 -0.874216 -0.612387 1 4.214584 -0.154134 -0.524841 1 3.721243 -1.805307 -0.147297 1 3.233501 -1.073331 -1.672510 6 2.321988 -0.045625 1.549514 1 1.399292 0.310203 2.005092 1 2.644503 -0.940398 2.082456 1 3.078430 0.727865 1.691498 8 -1.232023 -0.400199 -0.225072 8 -1.139276 -1.782916 -0.263202 8 1.230509 1.877953 -0.241310	**Frequencies (cm^{-1}):** 14.4891, 21.2726, 35.2289, 43.2848, 58.8272, 68.3785, 108.3498, 164.3416, 175.8775, 194.2761, 224.3244, 269.2932, 279.2299, 306.6837, 347.0984, 368.1928, 401.4177, 485.8981, 594.8197, 631.9608, 795.9861, 812.7106, 920.0257, 921.407, 931.9275, 932.1064, 948.4987, 975.5994, 989.3746, 1073.5879, 1097.6623, 1135.909, 1156.5968, 1203.8476, 1306.9287, 1323.7128, 1368.1208, 1392.7404, 1402.6293, 1410.9566, 1411.3325, 1432.5452, 1440.3432, 1457.4661, 1474.9388, 1476.2167, 1486.2944, 1490.8627, 1505.0435, 1508.7512, 1565.8231, 1781.2541, 2863.9563, 2973.5848, 3019.9088, 3023.4853, 3025.9787, 3034.2256, 3063.5348, 3065.6795, 3082.0888, 3090.9894, 3096.1639, 3106.9785, 3135.6667, 3140.3932

Compound: $iPrCHCMe_2 + O_3$ TS_{AO} 2.3	**Energy (Hartree)** -500.066795839265
Reaction Coordinates: 6 -1.766469 -0.217341 -0.394559 6 -0.288191 -0.411231 -0.855008 6 0.988521 0.607271 0.162316 6 0.671406 0.420317 1.624173 1 1.547158 0.741576 2.196303 1 0.467403 -0.615216 1.866160 1 -0.169125 1.042702 1.916852 6 1.109037 2.022144 -0.341169 1 0.160684 2.543584 -0.253740 1 1.846096 2.566879 0.253281 1 1.425108 2.036662 -1.382465 1 -0.110415 0.110985 -1.811761 1 -2.287256 -0.684552 -1.238326 6 -2.238497 1.235400 -0.358987 1 -1.934648 1.782558 -1.253315 1 -3.327961 1.269262 -0.313406 1 -1.865722 1.771589 0.514600 6 -2.177136 -1.005500 0.848499 1 -1.896765 -0.501951 1.772280 1 -3.261548 -1.124897 0.863687 1 -1.725465 -1.995714 0.845332 8 2.042665 -0.114589 -0.298365 8 1.955057 -1.382438 0.063344	**Frequencies (cm^{-1}):** -495.6363, 69.6213, 100.52, 154.7337, 183.0207, 206.4045, 223.6152, 236.1763, 248.7624, 268.2419, 281.2969, 336.5263, 351.5232, 381.3227, 400.304, 490.8485, 507.3589, 539.8327, 638.715, 649.0084, 757.6566, 810.9272, 919.3114, 938.5082, 952.2078, 973.1992, 985.6012, 1003.7491, 1039.8187, 1088.8458, 1137.7089, 1143.521, 1185.7544, 1211.2596, 1273.1017, 1279.0107, 1320.7893, 1341.3197, 1358.4769, 1398.1285, 1402.113, 1410.5389, 1421.0847, 1436.3244, 1471.9642, 1481.1005, 1489.3929, 1493.5216, 1499.6349, 1508.8499, 1510.8068, 1518.8725, 2888.9119, 2986.0693, 3023.5227, 3024.8017, 3036.7874, 3040.0091, 3081.1475, 3084.6483, 3093.6675, 3105.4367, 3117.1616, 3122.8608, 3147.9095, 3177.8571

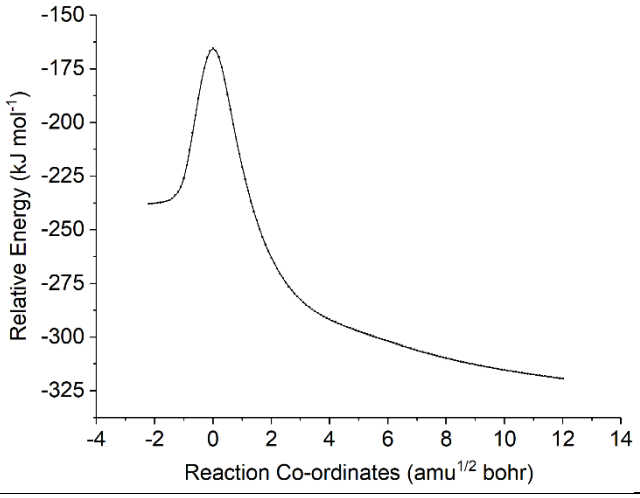
8 0.169831 -1.609201 -0.775861	

IRC:



Compound: $iPrCHCMe_2 + O_3$ CPr_{AO} 2.3	**Energy (Hartree)** -500.125832022823
Reaction Coordinates: 6 -2.691871 0.167027 -0.332935 6 -1.189100 0.017371 -0.364028 6 2.391626 -0.188751 0.188959 6 2.701365 -0.416603 -1.232175 1 3.335421 0.396556 -1.592983 1 1.775056 -0.341577 -1.806043 1 3.166721 -1.386167 -1.386937 6 2.589509 -1.205604 1.251055 1 1.946897 -2.064344 1.041832 1 3.622242 -1.560576 1.248199 1 2.341439 -0.800898 2.228794 1 -0.621108 0.961250 -0.464188 1 -2.941520 0.633575 -1.295958 6 -3.073673 1.173724 0.766129 1 -2.521148 2.108407 0.664083 1 -4.137829 1.403389 0.715889 1 -2.864377 0.763618 1.755626 6 -3.425263 -1.162864 -0.205801 1 -3.192417 -1.644685 0.744465 1 -4.503804 -1.009950 -0.254195 1 -3.138252 -1.851524 -0.999343 8 1.916931 0.918817 0.566345 8 1.669774 1.878950 -0.410943 8 -0.597064 -1.036876 -0.283711	**Frequencies (cm^{-1}):** 17.274, 27.7281, 34.4582, 48.0621, 61.4965, 75.338, 115.0368, 153.3148, 158.6065, 199.5321, 229.3104, 274.4694, 284.3913, 308.6947, 345.338, 367.0033, 403.9287, 481.2934, 592.7389, 639.1293, 793.6342, 812.2531, 908.6225, 917.3767, 926.9215, 935.5493, 953.5336, 975.1232, 988.7548, 1071.9688, 1096.6657, 1131.518, 1164.3151, 1202.0956, 1303.3236, 1305.9453, 1358.0547, 1387.1315, 1403.5097, 1404.3155, 1419.3381, 1441.9909, 1451.8918, 1459.0231, 1470.9115, 1476.7442, 1486.8526, 1491.133, 1504.9349, 1509.7574, 1569.6274, 1765.8294, 2924.2893, 2973.5082, 3026.8061, 3027.6927, 3033.5845, 3035.715, 3076.2393, 3078.5658, 3089.2776, 3094.6394, 3098.2667, 3104.8448, 3136.7657, 3139.8181

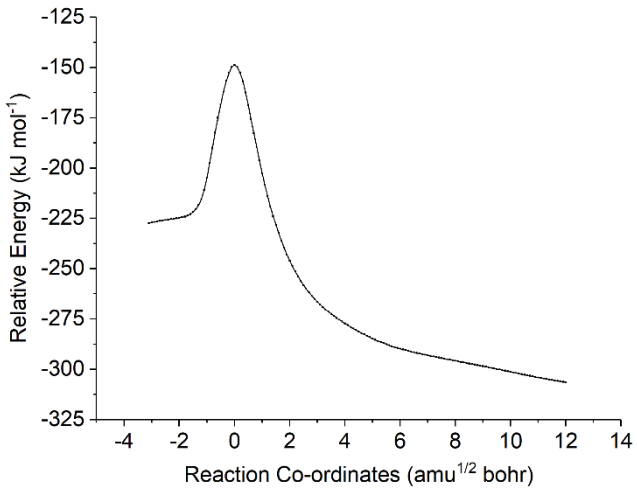
Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 1	**Energy (Hartree)** -500.068262053231

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.461709 0.350608 -0.197709 6 -0.284725 -0.121977 0.649210 6 1.392419 0.302598 -0.159282 6 2.413962 0.106669 0.965845 1 2.425423 -0.929758 1.293900 1 2.220397 0.756139 1.820707 1 3.405580 0.348078 0.578009 6 1.262599 1.764058 -0.615617 1 0.507377 1.878880 -1.387300 1 2.224545 2.048293 -1.044928 1 1.057617 2.436302 0.215569 1 -0.254526 0.259087 1.668174 1 -1.143583 0.414903 -1.237274 6 -2.618000 -0.662429 -0.124787 1 -2.975214 -0.779122 0.900135 1 -3.448816 -0.295765 -0.728307 1 -2.329505 -1.638062 -0.506128 6 -1.948660 1.722716 0.284002 1 -1.176838 2.487246 0.241914 1 -2.780523 2.058080 -0.335533 1 -2.309861 1.664220 1.313377 8 -0.012901 -1.443234 0.696773 8 0.091198 -1.932419 -0.528632 8 1.427029 -0.559594 -1.118427	-481.4162, 84.0977, 91.8708, 179.9365, 198.0151, 200.6185, 231.9471, 235.1189, 256.4753, 269.9332, 291.8698, 321.3273, 370.2625, 383.5532, 411.2257, 465.745, 484.995, 565.2111, 596.8721, 697.8948, 804.197, 858.3296, 912.2048, 927.0302, 942.4135, 963.3563, 968.7725, 992.696, 1058.5784, 1065.9338, 1098.2219, 1127.1574, 1176.3397, 1183.4883, 1187.5908, 1198.4202, 1322.7995, 1342.3393, 1369.7385, 1393.4626, 1399.8376, 1406.0983, 1411.2366, 1432.2244, 1476.6139, 1486.0965, 1487.9644, 1495.923, 1497.4666, 1506.4185, 1509.3256, 1520.4549, 3028.2824, 3029.5043, 3032.2362, 3041.5389, 3067.5458, 3084.7733, 3085.1274, 3094.8, 3098.9383, 3108.1452, 3124.09, 3129.1503, 3130.6534, 3143.6853
IRC  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 1	**Energy (Hartree)** -500.123229909559
Reaction Coordinates: 6 -1.829302 0.554246 -0.292000 6 -1.290763 -0.127721 0.903600 1 -1.179673 0.364076 1.865085 8 -0.936726 -1.333440 0.939750 8 -1.004904 -2.072778 -0.228235 1 -1.223933 0.197944 -1.128764 6 -3.279604 0.079417 -0.541795 1 -3.940642 0.398049 0.265592 1 -3.643372 0.521749 -1.469343 1 -3.318727 -1.003519 -0.633536	**Frequencies (cm^{-1}):** 15.6953, 33.0925, 47.6754, 62.3364, 69.5352, 77.8472, 84.4034, 114.2779, 150.9378, 201.1945, 214.6263, 234.6859, 278.4175, 337.0276, 392.8163, 409.5348, 498.1089, 538.604, 541.5551, 669.2494, 789.2977, 841.8158, 859.6544, 871.6625, 889.7857, 898.2679, 940.2435, 954.109, 975.4055, 1090.6197, 1112.3829, 1125.1761, 1175.5226, 1193.6934,

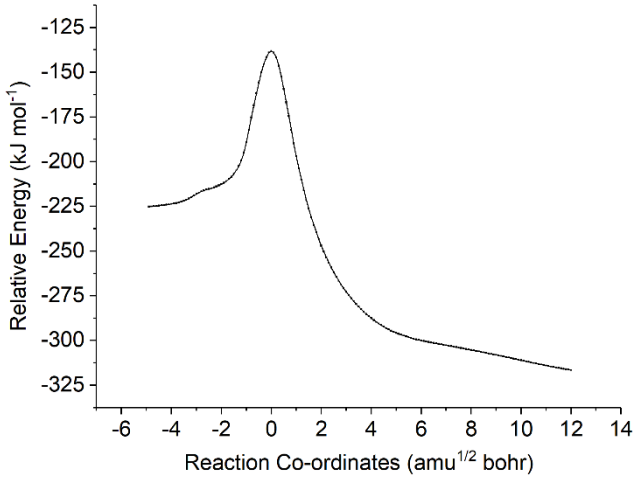
6 -1.725664 2.073407 -0.152797 1 -2.099467 2.555386 -1.056140 1 -2.325115 2.436691 0.685188 1 -0.693308 2.384070 -0.000662 6 2.435591 0.211740 -0.062963 6 2.314071 -1.156732 -0.685406 1 1.287975 -1.518078 -0.657707 1 2.971051 -1.863227 -0.173358 1 2.659494 -1.110163 -1.721890 6 3.833341 0.771718 0.085094 1 3.795138 1.793175 0.453962 1 4.363418 0.737959 -0.868567 1 4.402936 0.153791 0.783202 8 1.466406 0.845674 0.305302	1243.1204, 1303.9092, 1320.9912, 1378.9565, 1387.8324, 1392.0116, 1400.487, 1420.567, 1462.0744, 1468.8427, 1474.8476, 1487.3731, 1494.524, 1499.6487, 1501.2636, 1517.6436, 1573.5063, 1762.1163, 3017.3861, 3025.6979, 3031.1666, 3031.5407, 3044.5671, 3071.6854, 3083.9696, 3086.3412, 3094.1577, 3113.6004, 3120.6472, 3125.6497, 3136.6817, 3152.5093

Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 2	**Energy (Hartree)** -500.066213954739
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.436251 0.615092 -0.229243 6 0.248396 -0.200428 -0.726430 6 -1.404894 0.305379 0.047577 6 -2.453156 -0.216640 -0.943383 1 -2.392409 -1.299229 -1.025331 1 -2.350527 0.229965 -1.933392 1 -3.443336 0.037159 -0.560575 6 -1.326204 1.841394 0.093551 1 -0.612395 2.184258 0.835798 1 -2.314007 2.204306 0.382270 1 -1.085725 2.270411 -0.878887 1 0.101437 -0.108859 -1.800999 1 1.219958 1.637100 -0.546835 6 2.675389 0.151657 -1.023195 1 3.529161 0.779875 -0.767361 1 2.520179 0.218192 -2.100912 1 2.930532 -0.879464 -0.777343 6 1.735296 0.630487 1.273162 1 0.850094 0.830950 1.869470 1 2.138630 -0.324057 1.602648 1 2.479811 1.403096 1.474680 8 0.122456 -1.505795 -0.418611 8 0.105803 -1.692404 0.891764 8 -1.357995 -0.294970 1.186165	-460.0688, 74.5295, 108.4249, 166.6766, 199.9193, 215.9657, 228.66, 251.9497, 256.6673, 261.7352, 272.0979, 316.1321, 367.4025, 387.5567, 416.4393, 456.1983, 488.3841, 556.2803, 601.8534, 726.8905, 801.9999, 823.3968, 907.9831, 918.129, 949.0882, 967.2588, 990.2745, 992.1108, 1058.5191, 1059.9501, 1097.3907, 1116.6333, 1160.0811, 1180.1905, 1200.8988, 1219.0603, 1330.3787, 1364.7292, 1370.4011, 1393.0153, 1404.639, 1406.3964, 1420.2337, 1443.4603, 1477.7713, 1485.3411, 1487.0939, 1493.6931, 1497.0142, 1501.2564, 1504.978, 1515.6145, 3027.7507, 3029.6423, 3034.8062, 3037.6912, 3040.4626, 3086.1254, 3090.465, 3093.8947, 3098.4555, 3103.9244, 3109.4, 3127.2386, 3139.4036, 3147.5646
IRC	



Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 2	**Energy (Hartree)** -500.118357688853
Reaction Coordinates: 6 -2.080683 -0.879992 -0.149560 6 -1.229099 -0.032220 -1.026714 6 2.534282 -0.205632 -0.012512 6 2.242059 0.990637 0.860657 1 1.184172 1.241279 0.856123 1 2.829278 1.852858 0.539343 1 2.556063 0.764614 1.883670 6 3.991489 -0.506201 -0.286223 1 4.091352 -1.457032 -0.802790 1 4.564648 -0.520870 0.642563 1 4.415308 0.288446 -0.905102 1 -0.836662 -0.402449 -1.967625 1 -2.141851 -1.843095 -0.661628 6 -3.506835 -0.297320 -0.048988 1 -4.121780 -0.975472 0.543231 1 -3.968353 -0.195991 -1.031733 1 -3.485297 0.677318 0.431313 6 -1.459303 -1.121539 1.239560 1 -0.458062 -1.538944 1.151129 1 -1.405958 -0.192367 1.799596 1 -2.085873 -1.831960 1.780284 8 -0.893778 1.162494 -0.829532 8 -1.270497 1.795665 0.339763 8 1.653220 -0.902252 -0.474693	**Frequencies (cm^{-1}):** 24.5521, 32.7713, 35.56, 54.5448, 71.4591, 76.68, 95.9597, 111.1639, 141.0605, 199.3674, 209.2241, 231.7209, 238.0842, 341.6722, 389.7899, 416.9106, 496.4191, 532.427, 539.0914, 740.6541, 786.2616, 797.8643, 855.4423, 866.6592, 888.5187, 899.4939, 944.1503, 966.4917, 973.7381, 1087.1571, 1101.7275, 1122.6367, 1126.2667, 1198.7375, 1239.9997, 1335.766, 1373.6813, 1387.2059, 1387.588, 1395.3244, 1398.7111, 1419.9976, 1462.2397, 1466.3041, 1474.9142, 1480.8502, 1491.884, 1493.3312, 1505.1668, 1526.0808, 1573.8247, 1764.6775, 3021.7578, 3030.8994, 3031.0287, 3036.2914, 3041.7423, 3075.2214, 3083.8592, 3093.0048, 3107.9704, 3134.4241, 3134.6034, 3136.9303, 3141.3789, 3162.5492

Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 3	**Energy (Hartree)** -500.062771247118
Reaction Coordinates: 6 1.613477 -0.200771 -0.271594 6 0.180099 -0.219525 -0.821064 6 -1.170119 0.523144 0.234062 6 -2.381826 0.645234 -0.700128 1 -2.711636 -0.336514 -1.029528 1 -2.177890 1.271693 -1.569818	**Frequencies (cm^{-1}):** -461.0477, 54.232, 93.7044, 178.5156, 183.9439, 199.0438, 211.2799, 232.687, 251.0008, 258.9887, 278.1869, 320.5225, 362.2752, 375.6822, 413.2658, 467.3043, 518.947, 545.3978,

1 -3.197740 1.104780 -0.139222 6 -0.614079 1.899478 0.645907 1 0.207906 1.815722 1.346266 1 -1.427252 2.431039 1.142691 1 -0.309845 2.488494 -0.217718 1 0.088992 0.262931 -1.792189 1 2.027053 -1.100542 -0.746039 6 1.866153 -0.366214 1.232317 1 1.642350 0.538819 1.792694 1 1.283875 -1.178839 1.650554 1 2.926459 -0.580628 1.377790 6 2.387823 0.998648 -0.834821 1 2.060573 1.937620 -0.389685 1 3.449132 0.885360 -0.613364 1 2.283844 1.080639 -1.917967 8 -0.433703 -1.422164 -0.916930 8 -0.472784 -2.012441 0.265293 8 -1.272887 -0.352961 1.176320	580.8329, 685.7595, 806.4349, 851.2102, 906.3865, 931.1481, 942.9749, 966.7674, 988.0093, 991.944, 1055.0774, 1068.5416, 1085.375, 1146.8252, 1153.0952, 1178.855, 1194.295, 1212.1295, 1318.3241, 1346.433, 1367.5772, 1394.3539, 1405.7915, 1407.6633, 1409.6432, 1433.0077, 1476.4085, 1483.0153, 1490.1729, 1493.0785, 1497.4494, 1506.9714, 1509.3086, 1513.5409, 2973.1486, 3030.3957, 3032.0624, 3042.1619, 3044.864, 3085.9593, 3090.0437, 3098.5355, 3101.9952, 3105.609, 3107.068, 3132.7734, 3165.1651, 3173.0404
IRC  	

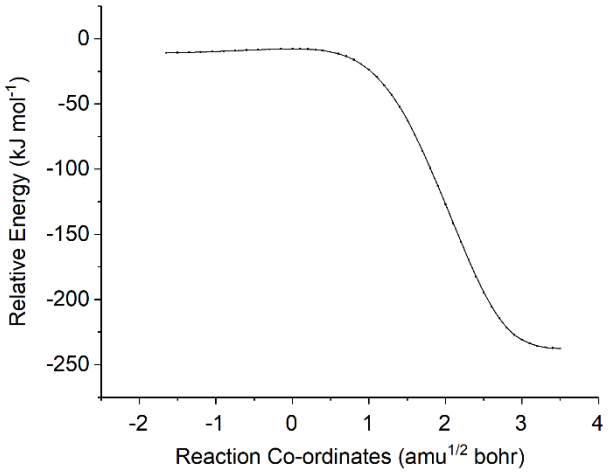
Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 3	**Energy (Hartree)** -500.121175602241
Reaction Coordinates: 6 -2.292198 -0.277602 0.166078 6 -1.341785 0.182129 -0.869528 6 2.457346 -0.344803 -0.016746 6 2.374333 1.014816 0.634794 1 1.360888 1.406887 0.613758 1 3.053479 1.716397 0.146937 1 2.707734 0.929978 1.672866 6 3.845005 -0.895311 -0.261946 1 3.788341 -1.924512 -0.606058 1 4.450862 -0.834832 0.643978 1 4.347983 -0.287703 -1.018176 1 -1.017642 -0.440086 -1.696854 1 -2.934349 0.585946 0.368122 6 -1.551636 -0.602923 1.482700 1 -0.854053 -1.427364 1.342060 1 -1.006960 0.268181 1.836996 1 -2.285095 -0.888408 2.237202	**Frequencies (cm^{-1}):** 21.6608, 25.8795, 31.0925, 47.0769, 71.8579, 72.7097, 91.4274, 103.0246, 137.507, 197.8939, 208.3724, 231.1948, 273.352, 338.7782, 388.7323, 409.3848, 495.659, 537.9287, 540.7916, 669.488, 785.7415, 842.0848, 851.4226, 877.785, 887.9959, 898.1869, 940.9245, 953.4296, 974.6768, 1086.3091, 1113.6974, 1122.2066, 1174.1187, 1193.3338, 1239.1454, 1307.6197, 1324.7563, 1379.9123, 1387.6935, 1393.8902, 1397.3693, 1422.1712, 1461.939, 1465.6463, 1474.4219, 1484.3829, 1490.9829, 1495.5498, 1502.6173, 1516.2136, 1572.5155, 1766.2766,

6 -3.113671 -1.465095 -0.342019 1 -2.476356 -2.327642 -0.545948 1 -3.843074 -1.762732 0.410866 1 -3.658249 -1.220108 -1.254848 8 -0.832563 1.331219 -0.904949 8 -1.122493 2.211534 0.120086 8 1.467822 -0.975412 -0.328999	3015.9119, 3023.0509, 3027.6426, 3031.2524, 3040.6693, 3075.7965, 3084.0213, 3087.2277, 3098.523, 3105.9891, 3133.7071, 3137.0306, 3138.1189, 3163.4736

S10.11 Ozonolysis of 2,4,4-trimethyl-2-pentene (Alkene 9)

Compound: $tBuCHCMe_2 + O_3$ PRC1	**Energy (Hartree)** -539.265745943092
Reaction Coordinates: 6 -1.644468 -0.549744 -0.088818 6 -0.420617 0.188677 -0.618756 6 0.114081 1.379140 -0.282475 6 1.316165 1.892010 -1.024629 1 1.110556 2.871959 -1.464366 1 2.162782 2.032168 -0.344745 1 1.626701 1.218470 -1.821171 6 -0.381028 2.307985 0.789253 1 0.388336 2.439636 1.555221 1 -0.569936 3.298882 0.367158 1 -1.288026 1.972026 1.278102 1 0.072809 -0.321908 -1.440114 6 -1.724088 -1.902765 -0.820978 1 -1.811237 -1.761134 -1.899900 1 -2.592682 -2.471402 -0.485859 1 -0.832585 -2.501918 -0.630543 6 -1.561776 -0.835886 1.424081 1 -0.670445 -1.415658 1.659053 1 -1.536053 0.072614 2.022315 1 -2.434648 -1.412482 1.737161 6 -2.929293 0.245965 -0.405762 1 -3.016770 0.433480 -1.476849 1 -3.807731 -0.321148 -0.090300 1 -2.952836 1.208261 0.103560 8 1.759711 -0.554546 1.054341 8 2.803442 -0.609437 0.343643 8 2.879086 -1.547785 -0.510512	**Frequencies (cm^{-1}):** 23.5497, 27.0865, 52.1706, 63.276, 72.898, 104.4801, 134.0495, 161.6554, 189.8, 202.7545, 224.1315, 236.5571, 253.3059, 289.6774, 309.8088, 326.7049, 355.0153, 377.5504, 429.1205, 447.8513, 501.0525, 564.4954, 732.6551, 763.1567, 823.6631, 860.1496, 927.5884, 931.6965, 948.1554, 960.3492, 964.695, 1003.8433, 1049.0301, 1052.8213, 1096.9679, 1102.3413, 1149.301, 1170.2271, 1183.4046, 1220.7054, 1254.0176, 1273.3372, 1392.2059, 1398.5246, 1402.5877, 1412.3159, 1422.2824, 1434.7596, 1471.6078, 1478.5623, 1481.6579, 1489.6815, 1491.5657, 1492.3093, 1497.0071, 1507.2385, 1509.4523, 1522.267, 1664.889, 3004.7658, 3017.4938, 3019.769, 3023.872, 3033.3399, 3043.5817, 3052.4394, 3078.9743, 3084.3854, 3089.2383, 3095.3166, 3101.4159, 3105.6899, 3116.2226, 3121.2693, 3155.803

Compound: $tBuCHCMe_2 + O_3$ TS_{OZO} 1	**Energy (Hartree)** -539.256954633627
Reaction Coordinates: 6 -1.578478 -0.037448 -0.043717 6 -0.200049 0.182165 -0.650181 6 0.834935 1.002310 -0.255201 6 1.966772 1.220213 -1.224944 1 2.105478 0.363613 -1.883512 1 2.903997 1.415912 -0.706039	**Frequencies (cm^{-1}):** -154.5626, 58.096, 79.6197, 102.6513, 126.5792, 146.5512, 161.3784, 173.9659, 186.2558, 193.7456, 231.4053, 247.0458, 283.054, 305.6357, 329.7352, 342.2766, 377.8088, 410.4105, 442.6905, 458.0767,

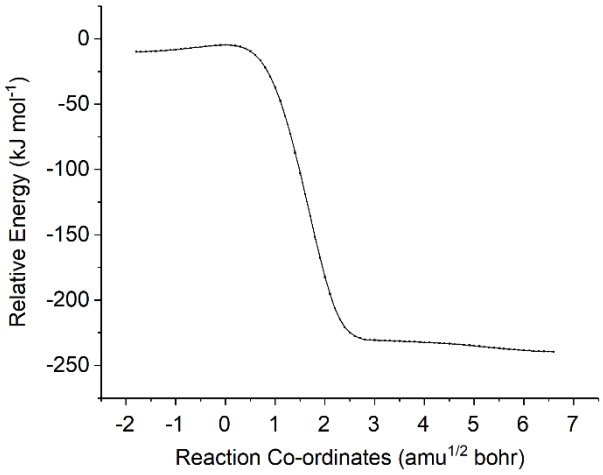
1 1.754113 2.089105 -1.856357 6 0.805101 1.959815 0.902257 1 1.783128 2.011399 1.379618 1 0.070148 1.705844 1.656209 1 0.576513 2.964607 0.533081 1 -0.106372 -0.209681 -1.656563 6 -2.280728 -1.139599 -0.859240 1 -3.294985 -1.297283 -0.490410 1 -1.741709 -2.083541 -0.786438 1 -2.347321 -0.866829 -1.914349 6 -1.563130 -0.473808 1.433825 1 -1.181285 0.295823 2.100467 1 -0.956741 -1.365493 1.569280 1 -2.584099 -0.697602 1.748738 6 -2.393912 1.268389 -0.193261 1 -2.445768 1.585134 -1.236268 1 -1.964892 2.084314 0.386835 1 -3.414905 1.107243 0.158709 8 1.950971 -0.633630 0.974591 8 1.949601 -1.536339 0.053333 8 0.762132 -1.954379 -0.235453	551.2908, 568.0049, 737.0809, 760.6, 817.6705, 874.633, 926.5463, 928.1873, 945.2539, 953.2571, 966.2232, 1009.3663, 1043.3984, 1051.4435, 1073.0755, 1079.2551, 1088.7215, 1119.9448, 1182.6554, 1215.25, 1253.7168, 1277.4695, 1388.6686, 1396.7039, 1402.3193, 1408.1939, 1421.2918, 1430.8371, 1470.6831, 1479.2151, 1482.9469, 1486.0857, 1490.4377, 1491.7719, 1498.3092, 1507.8178, 1509.6354, 1522.7248, 1572.9182, 3009.9294, 3018.1838, 3021.1309, 3025.9216, 3039.5454, 3074.9543, 3078.2198, 3081.9444, 3084.7541, 3099.7867, 3102.5979, 3105.4176, 3112.2188, 3133.7127, 3138.3895, 3167.4627
IRC:  	

Compound: $tBuCHCMe_2 + O_3$ POZ1	**Energy (Hartree)** -539.357798672299
Reaction Coordinates: 6 1.520244 0.092091 -0.038106 6 0.075647 -0.330414 -0.402213 6 -1.226627 0.486443 -0.015529 6 -1.821614 1.140277 -1.261072 1 -2.751170 1.651817 -1.013596 1 -1.129770 1.871580 -1.682681 1 -2.031330 0.388663 -2.020945 6 -1.173441 1.461350 1.155244 1 -2.183913 1.817515 1.358093 1 -0.802195 0.980098 2.054665 1 -0.558080 2.329293 0.926328 1 0.048113 -0.428985 -1.492085 6 1.797584 0.160105 1.473078 1 1.446605 -0.736978 1.981334	**Frequencies (cm^{-1}):** 54.7313, 81.5257, 186.2241, 197.1281, 219.7587, 234.5228, 242.4183, 262.4339, 269.9165, 279.8438, 305.5961, 319.4592, 353.2745, 360.7425, 383.1867, 419.6713, 466.1317, 494.9815, 547.6901, 609.6174, 697.8755, 756.5622, 777.088, 811.5459, 856.9015, 928.4238, 932.8798, 939.0355, 943.6535, 952.5398, 969.0177, 991.3728, 1014.8152, 1023.7222, 1054.8785, 1082.9622, 1167.554, 1188.6298, 1228.8164, 1241.0925, 1260.1366, 1278.5925, 1363.3752, 1394.5838,

1 2.873448 0.238285 1.637369 1 1.336163 1.024547 1.943469 6 2.457221 -0.969912 -0.652834 1 2.282605 -1.080615 -1.724565 1 3.497135 -0.672567 -0.511242 1 2.315580 -1.943919 -0.187004 6 1.831479 1.444131 -0.700163 1 1.679127 1.402793 -1.780324 1 2.876030 1.705575 -0.525298 1 1.221772 2.254257 -0.302348 8 -2.110851 -0.565604 0.457235 8 -1.573063 -1.775697 -0.111362 8 -0.176471 -1.621922 0.152676	1402.6817, 1404.4827, 1405.3334, 1426.1329, 1439.2985, 1480.1545, 1483.2597, 1490.0747, 1492.3556, 1495.3892, 1498.5639, 1507.3223, 1511.2106, 1518.4392, 1527.4549, 3000.0535, 3025.3325, 3029.7809, 3033.9887, 3041.3085, 3050.1698, 3082.1625, 3087.2705, 3096.7462, 3097.0816, 3100.0784, 3107.427, 3109.1137, 3112.4874, 3126.6405, 3147.4868

Compound: $tBuCHCMe_2 + O_3$ PRC 2	**Energy (Hartree)** -539.265526918345
Reaction Coordinates: 6 -1.632890 -0.363740 -0.038094 6 -0.429763 0.310868 -0.690752 6 0.324803 1.353600 -0.291209 6 1.418373 1.871464 -1.183497 1 1.234294 2.918002 -1.444902 1 2.382368 1.837189 -0.670266 1 1.503404 1.295242 -2.102313 6 0.151483 2.147781 0.974412 1 1.106866 2.238749 1.495350 1 -0.166968 3.165965 0.730913 1 -0.571403 1.727777 1.664577 1 -0.179903 -0.090968 -1.666889 6 -2.105296 -1.488740 -0.978040 1 -2.391733 -1.090518 -1.953151 1 -2.970370 -2.004617 -0.558701 1 -1.315719 -2.225390 -1.135074 6 -1.285835 -0.998771 1.323892 1 -0.510026 -1.756657 1.214991 1 -0.936485 -0.267384 2.049706 1 -2.168488 -1.487643 1.741639 6 -2.796493 0.636579 0.131082 1 -3.064304 1.084684 -0.826758 1 -3.678208 0.123127 0.520934 1 -2.550028 1.443510 0.818775 8 2.420046 -0.407536 0.965862 8 2.162480 -1.524162 0.431266 8 1.968776 -1.533967 -0.817827	**Frequencies (cm^{-1}):** 30.9442, 37.6476, 52.1308, 54.9747, 74.6594, 101.6515, 140.0704, 162.633, 186.5701, 205.0574, 222.9856, 232.3392, 254.2087, 289.3297, 310.2149, 326.1317, 354.682, 377.6114, 427.0166, 447.4998, 512.2073, 563.7791, 737.5549, 761.8683, 822.7831, 853.1217, 927.0167, 930.5099, 947.4473, 960.2709, 962.8428, 1007.7204, 1048.6469, 1050.061, 1099.5815, 1103.2451, 1161.5029, 1178.8357, 1181.4919, 1219.9116, 1253.0953, 1271.5368, 1390.5746, 1398.3699, 1401.8715, 1411.438, 1421.0428, 1434.0506, 1470.4054, 1480.4365, 1481.4603, 1488.3906, 1489.4895, 1490.811, 1497.8706, 1507.4661, 1509.1625, 1521.3878, 1658.9915, 3009.2608, 3017.7663, 3019.1038, 3023.7565, 3031.1639, 3053.7751, 3060.1983, 3078.6436, 3083.6565, 3083.9951, 3089.8689, 3106.6494, 3111.7127, 3112.3438, 3130.3894, 3151.8273

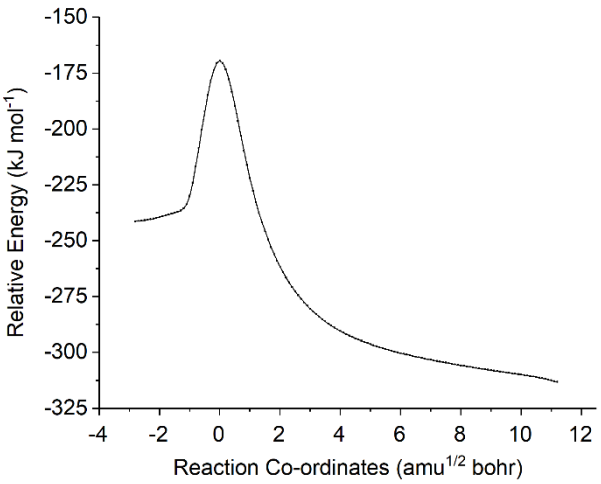
Compound: $tBuCHCMe_2 + O_3$ TS_{OZO} 2	**Energy (Hartree)** -539.256271387596
Reaction Coordinates: 6 -1.556663 0.034326 -0.034528 6 -0.181899 0.245852 -0.660636 6 0.906603 0.971816 -0.211011 6 1.977901 1.322431 -1.205159 1 1.979845 0.638888 -2.051318 1 2.964580 1.302109 -0.743414 1 1.814114 2.337744 -1.581847	**Frequencies (cm^{-1}):** -182.0827, 54.5369, 66.171, 129.4737, 139.6262, 162.4678, 180.2883, 190.7544, 202.8194, 211.4033, 224.3888, 256.0198, 285.4569, 307.5131, 330.5054, 338.9148, 378.8596, 411.6041, 448.2256, 460.3677, 558.2471, 579.3681, 736.8611, 758.9415,

6 0.963707 1.758503 1.070717 1 1.984074 1.799940 1.448299 1 0.326749 1.364436 1.854305 1 0.653123 2.789692 0.873315 1 -0.153662 0.012147 -1.717130 6 -2.373067 -0.862198 -0.983516 1 -3.380131 -1.013784 -0.592808 1 -1.899529 -1.837018 -1.097399 1 -2.463372 -0.409476 -1.972845 6 -1.537555 -0.639461 1.350960 1 -0.981308 -0.074845 2.095694 1 -1.110826 -1.638507 1.296620 1 -2.562566 -0.733551 1.713935 6 -2.266740 1.404780 0.067615 1 -2.302159 1.903691 -0.902178 1 -1.770460 2.070000 0.772433 1 -3.294344 1.262849 0.408264 8 2.210054 -0.794364 0.571826 8 1.347270 -1.755064 0.529464 8 0.767945 -1.849398 -0.622612	818.455, 882.8058, 925.2355, 927.9553, 945.6943, 953.49, 966.0294, 1012.7119, 1044.7666, 1049.0199, 1073.4436, 1075.9417, 1087.6856, 1121.045, 1182.8916, 1214.7134, 1254.4116, 1275.302, 1385.4988, 1397.3856, 1401.868, 1409.4216, 1420.8972, 1432.1767, 1469.601, 1474.791, 1482.2913, 1485.7805, 1491.0804, 1492.2271, 1498.1131, 1507.0724, 1511.5601, 1523.947, 1559.8969, 3007.648, 3014.701, 3021.6328, 3026.0458, 3040.6844, 3076.694, 3078.759, 3084.8869, 3087.0346, 3099.735, 3102.6927, 3104.9281, 3120.4962, 3126.5482, 3153.234, 3157.747
IRC:  	

Compound: $tBuCHCMe_2 + O_3$ POZ 2	**Energy (Hartree)** -539.357832299616
Reaction Coordinates: 6 1.504174 0.113384 0.003509 6 0.090722 -0.215603 -0.548228 6 -1.223360 0.474428 -0.039085 6 -1.660360 1.624919 -0.937027 1 -2.650730 1.971474 -0.643560 1 -0.969224 2.461168 -0.846156 1 -1.696361 1.311963 -1.979307 6 -1.302538 0.852251 1.437060 1 -2.312910 1.202288 1.648654 1 -1.095210 -0.001385 2.075541 1 -0.610410 1.654406 1.685189 1 0.125559 -0.024053 -1.624825 6 1.709597 -0.295208 1.470348 1 1.383256 -1.320689 1.638618 1 2.771292 -0.237952 1.715744	**Frequencies (cm^{-1}):** 51.0782, 94.5258, 186.5379, 202.5518, 211.9824, 245.5409, 248.5029, 256.5475, 274.5599, 283.5052, 296.9066, 307.8899, 324.2383, 364.6322, 386.0471, 401.5335, 475.9873, 516.099, 540.6345, 615.3699, 694.9578, 748.6247, 770.9239, 821.9376, 867.4428, 919.7046, 930.1384, 940.5628, 944.9789, 949.1961, 967.5352, 992.9131, 999.1402, 1027.7963, 1055.043, 1062.4796, 1174.5989, 1200.9098, 1235.5174, 1244.0955, 1255.5219, 1271.6656, 1353.7676, 1391.5798, 1401.3038, 1403.7077, 1407.0454,

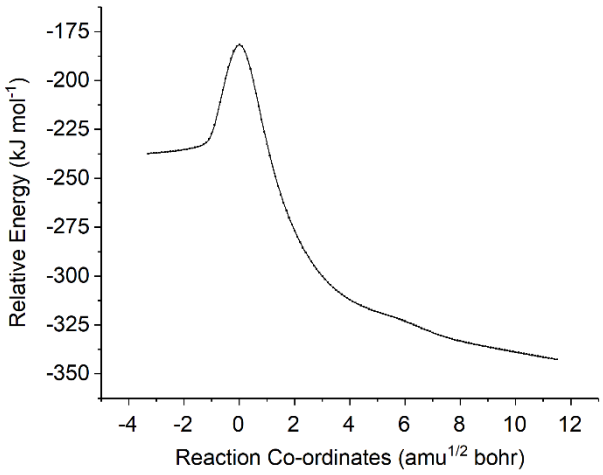
1 1.182031 0.352389 2.165963 6 2.501341 -0.688205 -0.859831 1 3.524676 -0.465335 -0.554583 1 2.341580 -1.760690 -0.753545 1 2.403973 -0.434892 -1.917308 6 1.799274 1.609643 -0.185648 1 2.836406 1.817158 0.081933 1 1.662387 1.916158 -1.224720 1 1.169384 2.240928 0.440715 8 -2.165132 -0.591648 -0.301307 8 -1.486294 -1.722143 0.219553 8 -0.170923 -1.628284 -0.412613	1425.0451, 1437.6446, 1481.1113, 1484.0114, 1489.3225, 1492.6268, 1496.2037, 1499.9662, 1508.8784, 1513.2251, 1518.6218, 1527.1226, 3005.9437, 3022.1232, 3026.7116, 3040.7109, 3045.393, 3051.8436, 3079.4364, 3084.6288, 3092.8585, 3096.331, 3102.6909, 3108.464, 3113.9793, 3121.0409, 3127.2425, 3143.0158

Compound: $tBuCHCMe_2 + O_3$ TS_{ANTI}	**Energy (Hartree)** -539.327032833075
Reaction Coordinates: 6 -1.540215 -0.155755 -0.027950 6 -0.159816 0.403136 -0.384328 6 1.525252 -0.457664 0.016289 6 1.681560 -1.452642 -1.143261 1 0.892698 -2.200318 -1.172844 1 2.633042 -1.971348 -1.014008 1 1.720427 -0.922274 -2.092893 6 1.416029 -1.088217 1.406598 1 0.668738 -1.878008 1.458407 1 1.197887 -0.327696 2.152778 1 2.384414 -1.528364 1.653253 1 0.039448 0.463635 -1.451122 6 -2.554795 0.716296 -0.807657 1 -3.567010 0.352385 -0.625743 1 -2.372473 0.676507 -1.882680 1 -2.504324 1.757976 -0.492160 6 -1.859189 -0.060194 1.472517 1 -1.206651 -0.690800 2.071408 1 -1.770562 0.961750 1.837294 1 -2.885652 -0.388315 1.641117 6 -1.688448 -1.606808 -0.508263 1 -1.050222 -2.292068 0.046260 1 -2.720538 -1.927463 -0.362790 1 -1.459021 -1.706472 -1.569932 8 2.330138 0.553885 -0.052033 8 1.198006 2.118578 -0.243541 8 0.106546 1.556532 0.253073	**Frequencies (cm^{-1}):** -477.3822, 73.794, 77.5295, 175.8847, 188.591, 208.3787, 216.5621, 231.0017, 241.3669, 251.2152, 269.3275, 282.4735, 299.1787, 341.2072, 354.7064, 381.1608, 422.5781, 440.5439, 482.9363, 509.3246, 566.091, 603.2183, 617.9604, 769.0503, 797.4205, 905.262, 913.3312, 938.4944, 948.7907, 969.7748, 991.9959, 1024.535, 1038.5257, 1054.8993, 1065.1038, 1114.9027, 1151.8488, 1188.6723, 1207.2784, 1230.0709, 1252.7153, 1283.2772, 1358.0867, 1372.0879, 1388.6172, 1400.1263, 1404.9052, 1409.1667, 1440.197, 1477.0628, 1481.1232, 1486.4694, 1493.0681, 1493.4215, 1495.0816, 1504.1499, 1508.8781, 1512.8288, 1526.4713, 3025.9577, 3033.8963, 3034.496, 3040.3172, 3044.8798, 3086.7591, 3091.9852, 3093.5652, 3100.3468, 3101.2156, 3104.6114, 3105.697, 3111.5835, 3128.8333, 3129.2424, 3133.4551
IRC:	



Compound: $tBuCHCMe_2 + O_3$ C_{ANTI}	**Energy (Hartree)** -539.384267927067
Reaction Coordinates: 6 -2.100740 -0.194484 -0.001364 6 -0.835957 0.447290 -0.468939 6 2.411503 -0.574374 0.022534 6 2.897263 -0.130974 1.381323 1 2.741645 0.945695 1.464387 1 3.965502 -0.323742 1.495964 1 2.341115 -0.638723 2.165329 6 3.250292 -0.161705 -1.161940 1 3.437067 0.911270 -1.135197 1 2.751383 -0.426683 -2.090033 1 4.217892 -0.668669 -1.113713 1 -0.391178 0.206188 -1.429981 6 -3.219112 0.272603 -0.964632 1 -4.150129 -0.231860 -0.703468 1 -2.983876 0.027694 -2.001098 1 -3.380154 1.348266 -0.893066 6 -2.440473 0.193987 1.441090 1 -1.656938 -0.121958 2.128794 1 -2.568076 1.270522 1.547880 1 -3.370662 -0.291170 1.737361 6 -1.921596 -1.722839 -0.128624 1 -1.116467 -2.078582 0.510980 1 -2.850823 -2.216487 0.158269 1 -1.685308 -2.011421 -1.153201 8 1.413369 -1.259279 -0.106467 8 0.903413 1.883363 -0.289989 8 -0.260291 1.316246 0.220720	**Frequencies (cm^{-1}):** 22.8809, 32.8118, 64.0477, 66.774, 77.6082, 91.8327, 102.7135, 120.0675, 138.4211, 192.0999, 206.5667, 227.2571, 263.2604, 265.8178, 330.1897, 340.728, 353.1951, 385.0515, 460.8436, 463.2049, 485.1919, 536.2985, 554.9666, 775.4154, 788.3248, 891.6386, 898.2931, 902.1882, 922.0936, 928.9479, 958.8792, 961.6558, 974.5545, 1045.8639, 1066.9774, 1087.0046, 1117.2707, 1211.9628, 1229.2461, 1242.393, 1298.3924, 1365.166, 1380.2487, 1388.2558, 1400.1004, 1408.9062, 1435.8529, 1458.0846, 1468.3542, 1470.6594, 1478.8787, 1487.8279, 1488.6113, 1489.3635, 1501.8179, 1503.2288, 1520.0283, 1573.6085, 1750.3308, 3027.3763, 3027.8123, 3033.9305, 3035.6951, 3040.4023, 3092.4703, 3092.8327, 3096.9914, 3097.8043, 3099.6937, 3104.0914, 3109.9575, 3121.8062, 3132.5351, 3140.1558, 3150.1772

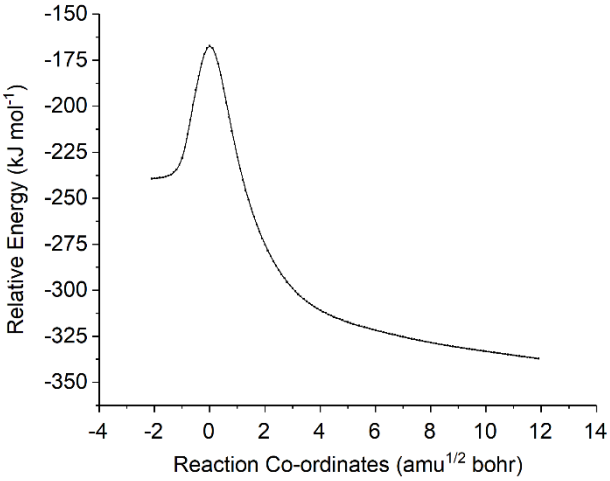
Compound: $tBuCHCMe_2 + O_3$ TS_{AO} 1	**Energy (Hartree)** -539.333201921061
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.559433 0.107331 -0.017397 6 -0.213417 -0.313093 -0.676451 1 -0.097493 0.114448 -1.688109 8 0.102828 -1.563541 -0.596582 6 -2.622827 -0.786473 -0.694098 1 -3.613134 -0.553192 -0.299153 1 -2.646430 -0.626178 -1.774276 1 -2.413369 -1.839339 -0.513818 6 -1.915117 1.569950 -0.318137 1 -1.781496 1.802480 -1.377875 1 -2.964176 1.751565 -0.079409 1 -1.327689 2.277601 0.261915 6 -1.576449 -0.166843 1.491022 1 -2.585834 -0.029412 1.882963 1 -1.267710 -1.190552 1.699382 1 -0.914418 0.501542 2.040314 6 1.364081 0.486269 -0.053608 6 1.286719 1.926320 0.384353 1 0.872265 2.542686 -0.409344 1 0.685205 2.045432 1.281063 1 2.295371 2.289671 0.594131 6 2.349704 0.213319 -1.168925 1 2.235664 -0.785789 -1.573389 1 3.361939 0.316192 -0.770377 1 2.217171 0.950048 -1.959443 8 1.467019 -0.321365 1.042753 8 1.588223 -1.588579 0.679438	-453.8957, 62.2583, 109.2404, 175.3298, 180.4832, 212.6275, 224.9261, 245.8047, 252.6287, 264.0732, 270.8779, 290.9924, 319.0619, 339.8559, 360.9034, 374.7008, 395.2826, 411.5103, 465.8846, 544.3341, 568.4464, 647.9159, 683.8495, 749.9751, 801.1489, 876.9394, 930.6561, 942.5147, 953.5123, 965.302, 981.02, 999.5584, 1015.5781, 1044.5512, 1051.1292, 1116.1606, 1150.9483, 1219.5385, 1236.9242, 1259.2227, 1271.9702, 1276.5786, 1298.0377, 1384.5961, 1396.347, 1401.3272, 1404.6069, 1420.7614, 1437.0048, 1470.6628, 1479.0805, 1485.2025, 1487.8637, 1491.4591, 1496.859, 1504.6547, 1508.0825, 1515.8569, 1522.0503, 2898.828, 3018.9973, 3024.332, 3033.5938, 3034.1468, 3039.3361, 3073.2651, 3079.0515, 3089.7142, 3102.4333, 3106.852, 3108.3556, 3111.5422, 3119.9597, 3146.2134, 3163.7718
IRC:  	

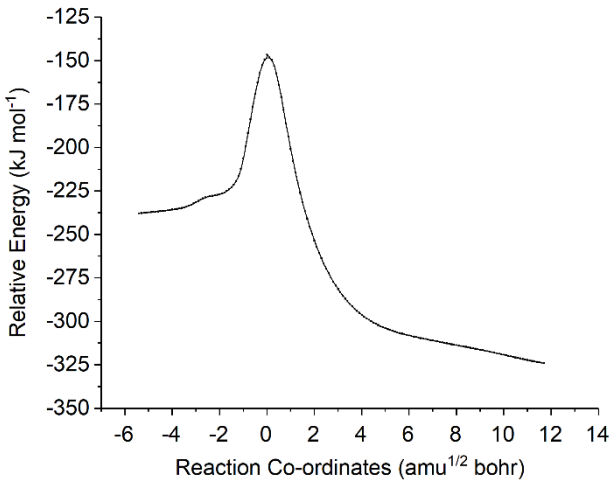
Compound: $tBuCHCMe_2 + O_3$ CPr_{AO} 1	**Energy (Hartree)** -539.386089436056
Reaction Coordinates: 6 -2.425526 -0.018182 0.014799 6 -0.918651 -0.059875 -0.164668 6 2.696933 -0.178116 0.067026 6 3.020860 -1.468331 0.723969 1 2.835381 -1.418081 1.793726 1 2.399345 -2.253206 0.285988 1 4.063793 -1.735435 0.540975 6 2.902649 0.086429 -1.366588	**Frequencies (cm^{-1}):** 17.2979, 22.8032, 35.3498, 43.503, 60.9597, 73.0904, 100.0733, 153.6927, 158.7598, 196.2318, 242.7639, 247.2562, 275.5636, 284.0457, 308.689, 326.5983, 348.028, 366.9551, 388.8633, 405.2265, 481.5998, 592.7604, 594.0371, 762.8467, 812.2487, 878.8721, 909.0483, 927.2355,

1 3.474324 1.010546 -1.479332 1 1.932100 0.285656 -1.826237 1 3.392019 -0.749553 -1.858712 1 -0.402135 0.904331 0.005496 6 -2.964966 1.033978 -0.974655 1 -4.037489 1.167304 -0.825370 1 -2.483183 2.002224 -0.829762 1 -2.803592 0.724679 -2.008282 6 -2.690132 0.454743 1.458337 1 -2.198744 1.407129 1.663042 1 -3.761760 0.588870 1.613408 1 -2.332046 -0.275338 2.185473 6 -3.057225 -1.385859 -0.239759 1 -4.138729 -1.332766 -0.105631 1 -2.853917 -1.731074 -1.253209 1 -2.663244 -2.135233 0.446392 8 2.207521 0.714618 0.814045 8 1.844274 1.920792 0.221456 8 -0.277516 -1.041507 -0.467843	929.6802, 950.91, 968.7064, 975.5163, 988.7815, 1056.1143, 1071.9655, 1088.6752, 1096.6944, 1228.0941, 1236.0747, 1294.6373, 1305.9418, 1387.4046, 1397.171, 1403.102, 1403.8518, 1422.9509, 1441.9525, 1452.9188, 1459.0625, 1470.889, 1476.7098, 1479.7185, 1486.6395, 1489.2461, 1499.6033, 1507.6607, 1520.0178, 1569.548, 1765.8735, 2917.0812, 3021.7958, 3024.2491, 3026.9097, 3033.5942, 3033.8071, 3076.4121, 3078.5359, 3086.4394, 3088.1301, 3088.8148, 3091.1404, 3095.2828, 3102.47, 3136.7388, 3139.921

Compound: $tBuCHCMe_2 + O_3$ TS_{AO} 2	**Energy (Hartree)** -539.326403788511
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.587253 0.071811 0.011905 6 -0.228285 -0.428369 -0.609920 6 1.341519 0.523091 -0.011397 6 1.553972 1.806890 -0.779421 1 1.688276 1.602184 -1.847609 1 0.703860 2.481492 -0.649815 1 2.451939 2.320270 -0.404824 6 1.297148 0.614307 1.496702 1 2.317909 0.844234 1.841062 1 0.984291 -0.323842 1.955195 1 0.639860 1.429082 1.813475 1 -0.148853 -0.105118 -1.671080 6 -2.649124 -0.608146 -0.890191 1 -3.656867 -0.286937 -0.590832 1 -2.509239 -0.340157 -1.947094 1 -2.588288 -1.700163 -0.804669 6 -1.769175 1.591626 -0.103129 1 -1.573122 1.945083 -1.125642 1 -2.807423 1.857682 0.139533 1 -1.124402 2.146165 0.589690 6 -1.806591 -0.403112 1.455771 1 -2.870364 -0.306711 1.714175 1 -1.520615 -1.455648 1.563937 1 -1.242786 0.188414 2.184583 8 2.189289 -0.422625 -0.504291 8 2.026645 -1.581648 0.106303 8 0.076885 -1.658804 -0.374762	-473.749, 71.1381, 88.826, 145.1644, 180.8624, 204.8006, 225.2504, 230.1856, 242.6057, 260.2243, 281.3929, 311.4431, 323.0625, 343.1809, 356.446, 388.8726, 392.508, 399.1523, 470.5705, 531.2167, 559.3571, 636.9642, 647.0485, 743.2231, 804.5353, 858.2963, 930.708, 945.5949, 947.8582, 961.2478, 979.4863, 993.5743, 1031.8814, 1033.7028, 1042.2973, 1150.4023, 1162.6698, 1211.1718, 1239.0388, 1247.7556, 1272.5574, 1281.5447, 1333.0739, 1379.2447, 1381.6098, 1386.7138, 1394.7887, 1401.9776, 1425.4645, 1452.8894, 1459.5414, 1462.2986, 1469.3594, 1473.1037, 1478.2628, 1483.6943, 1494.1374, 1498.1589, 1508.816, 2888.4072, 3023.5053, 3028.7236, 3033.835, 3041.6468, 3045.2088, 3088.5583, 3094.6876, 3105.8198, 3109.7537, 3117.2438, 3117.7991, 3128.0863, 3139.7508, 3164.5241, 3192.5219
IRC	



Compound: $tBuCHCMe_2 + O_3$ TS_{SYN}	**Energy (Hartree)** -539.321133713651
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.438273 0.245843 -0.061044 6 0.107187 -0.209754 -0.700605 1 0.028495 0.090043 -1.744129 8 -0.234201 -1.516831 -0.643497 8 -0.326074 -1.929025 0.609983 6 2.499238 -0.745953 -0.603273 1 3.485063 -0.434468 -0.256340 1 2.516111 -0.761074 -1.694288 1 2.317849 -1.757704 -0.246415 6 1.516401 0.241011 1.473868 1 0.774206 0.886615 1.933474 1 1.373175 -0.757495 1.873929 1 2.504116 0.599455 1.770676 6 1.790507 1.645586 -0.598777 1 1.150357 2.423779 -0.192009 1 2.816656 1.886883 -0.320285 1 1.729079 1.686433 -1.688252 6 -1.532930 0.338395 0.099715 6 -2.585056 0.049958 -0.979800 1 -2.632330 -1.014153 -1.195103 1 -2.398397 0.600598 -1.902919 1 -3.558876 0.359703 -0.595598 6 -1.382457 1.844354 0.374975 1 -0.662347 2.051009 1.158108 1 -2.357773 2.195773 0.716052 1 -1.125500 2.398958 -0.525252 8 -1.573082 -0.418018 1.143264	-474.0027, 73.0102, 103.0439, 163.8777, 184.0068, 193.272, 204.932, 235.8217, 248.8922, 264.6371, 265.9348, 286.8771, 307.9847, 343.4053, 368.4874, 400.7176, 415.1825, 423.4938, 461.5554, 502.4692, 558.0882, 586.722, 666.7763, 790.7271, 817.9262, 881.5021, 907.259, 932.4163, 943.6579, 974.1756, 982.3214, 989.7524, 1039.305, 1053.7853, 1064.0162, 1068.8144, 1128.4099, 1180.092, 1182.1331, 1215.1553, 1235.8341, 1263.8782, 1362.6203, 1392.7958, 1399.2851, 1405.1011, 1406.9841, 1410.373, 1443.6096, 1474.6778, 1481.1576, 1482.4375, 1491.0594, 1492.4354, 1497.5188, 1501.7278, 1506.5224, 1514.2586, 1525.1685, 3028.6247, 3030.4703, 3032.2384, 3040.2962, 3043.6867, 3084.6765, 3085.5197, 3091.144, 3101.5521, 3104.0364, 3118.4001, 3121.9951, 3131.6211, 3134.1343, 3152.5906, 3167.0636
IRC	



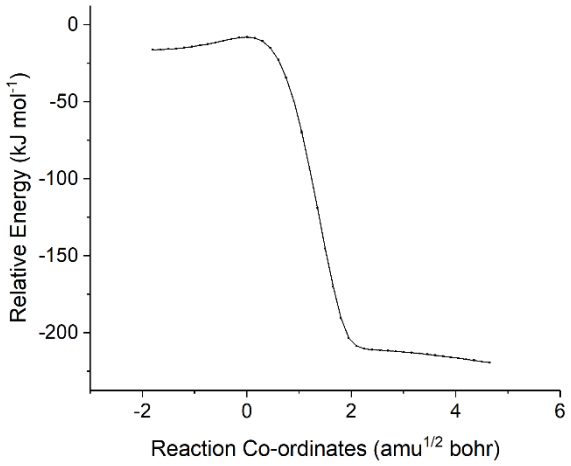
Compound: $tBuCHCMe_2 + O_3$ CPr_{SYN}	**Energy (Hartree)** -539.378570198983
Reaction Coordinates: 6 -1.942457 -0.487812 0.100242 6 -1.037153 0.097490 -0.936327 6 2.720780 -0.269734 0.028139 6 2.590147 1.115218 0.614385 1 1.563850 1.471436 0.576291 1 3.245567 1.815547 0.093346 1 2.926117 1.090529 1.654885 6 4.126505 -0.782489 -0.194435 1 4.105916 -1.828935 -0.486681 1 4.731748 -0.655173 0.704914 1 4.605758 -0.195881 -0.982021 1 -0.703091 -0.493177 -1.783466 6 -3.277000 0.295230 0.088581 1 -3.937660 -0.131889 0.844417 1 -3.774693 0.212321 -0.878687 1 -3.110296 1.345513 0.312187 6 -1.294135 -0.416352 1.500335 1 -0.352203 -0.962377 1.516730 1 -1.111085 0.614154 1.789372 1 -1.975286 -0.876366 2.218195 6 -2.190451 -1.956790 -0.280474 1 -1.259811 -2.525582 -0.285930 1 -2.862923 -2.416380 0.443490 1 -2.652549 -2.042971 -1.265866 8 -0.589453 1.270110 -0.999584 8 -0.866653 2.180982 0.001767 8 1.754009 -0.949759 -0.251413	**Frequencies (cm^{-1}):** 23.8496, 28.4593, 32.7835, 52.7825, 70.3128, 75.7995, 93.2174, 118.2773, 139.0582, 198.6539, 212.8402, 235.0021, 247.2438, 267.8687, 311.2885, 372.2292, 389.6111, 391.8509, 395.0511, 496.2453, 538.8213, 541.0535, 661.5679, 786.2641, 787.838, 855.2096, 863.3946, 888.3332, 898.8263, 925.0339, 940.014, 948.7482, 975.9066, 1047.9037, 1062.5769, 1086.8404, 1122.5259, 1215.1868, 1235.4501, 1239.9829, 1274.8997, 1386.0027, 1387.6143, 1392.2817, 1398.4277, 1401.5493, 1427.43, 1462.1511, 1466.0286, 1473.7763, 1474.7274, 1491.138, 1492.042, 1494.8275, 1500.3875, 1509.9896, 1529.5912, 1565.0894, 1764.5924, 3022.3243, 3024.6803, 3029.959, 3031.0956, 3036.3065, 3075.4265, 3083.9901, 3085.1599, 3088.8792, 3099.6017, 3104.1133, 3133.2902, 3136.038, 3137.0716, 3142.8817, 3152.8617

S10.12 Ozonolysis of Mesityl Oxide (Alkene 10)

Compound: Mes Oxy + O_3 PRC1.1	**Energy (Hartree)** -534.707074071554
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.966494 -2.493703 0.588069 6 1.395925 -1.123049 0.109650 6 0.651204 0.011125 0.705989 6 0.680758 1.306621 0.326879 6 -0.159651 2.314448 1.053846 1 -0.685289 1.884374 1.904288 1 -0.894950 2.755322 0.374448 1 0.461239 3.141332 1.408957 6 1.507790 1.857410 -0.793286 1 0.933615 2.597222 -1.354673 1 2.374045 2.382909 -0.378224 1 1.880348 1.084337 -1.454797 1 0.004118 -0.255276 1.534257 8 2.296727 -0.993578 -0.700493 1 -0.095766 -2.647066 0.388180 1 1.102066 -2.573677 1.669366 1 1.553592 -3.259734 0.089462 8 -2.773310 -0.908079 0.386682 8 -2.570487 -0.008900 -0.478998 8 -1.563949 -0.132799 -1.223209	17.7202, 27.6305, 32.2906, 37.4581, 50.1491, 62.0042, 71.3251, 121.4824, 155.1253, 193.9083, 203.5049, 217.9875, 343.1115, 375.1574, 440.461, 470.8107, 598.5393, 628.0504, 741.758, 822.1098, 855.8543, 912.3833, 963.3576, 972.1276, 996.7554, 1044.2347, 1092.9591, 1100.98, 1168.3065, 1188.3413, 1203.1426, 1239.451, 1382.9529, 1390.648, 1410.8358, 1414.9978, 1463.6882, 1468.0146, 1471.9552, 1475.4292, 1486.8516, 1492.4833, 1642.8037, 1741.2431, 3011.129, 3017.3469, 3027.8711, 3053.6877, 3060.8839, 3081.2563, 3109.0457, 3139.8213, 3141.9805, 3162.9066

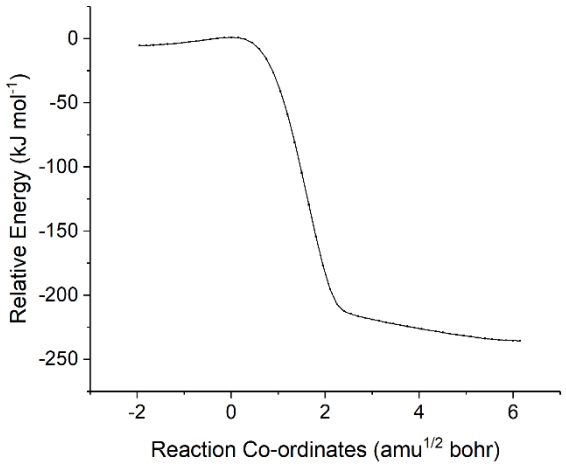
Compound: Mes Oxy + O_3 TS_{OZO} 1.1	**Energy (Hartree)** -534.698506360429
Reaction Coordinates: 6 -0.356106 -0.205421 0.687553 6 -1.673606 -0.382996 0.014841 8 -1.825572 -1.098076 -0.964783 6 -2.831720 0.374231 0.631521 1 -2.622464 1.453493 0.624232 1 -2.963737 0.075489 1.682738 1 -3.747576 0.165627 0.070342 6 0.844429 -0.823193 0.328464 6 1.971231 -0.816259 1.331322 1 1.907908 0.037468 2.017273 1 2.947562 -0.806521 0.833570 1 1.917902 -1.737585 1.934732 6 0.969130 -1.786601 -0.818304 1 2.025149 -1.947175 -1.066583 1 0.533343 -2.755734 -0.528710 1 0.421867 -1.442614 -1.698152 1 -0.389524 0.302867 1.651428 8 -0.140978 1.888903 -0.211357 8 1.148668 1.885866 -0.238028 8 1.621560 0.885321 -0.907489	**Frequencies (cm^{-1}):** -211.2311, 51.2459, 58.4127, 105.0959, 110.3152, 115.1166, 158.5968, 188.563, 194.8053, 217.9483, 224.6224, 342.4022, 369.3792, 442.3678, 455.5138, 481.5849, 598.9948, 625.6514, 743.3417, 815.4443, 862.849, 914.4808, 938.6592, 965.7756, 1008.7719, 1024.4916, 1059.9548, 1061.7307, 1087.9312, 1123.6406, 1184.6385, 1236.5047, 1363.2016, 1370.6699, 1391.0674, 1401.8472, 1439.95, 1445.5866, 1450.9085, 1451.9302, 1459.1158, 1475.2275, 1546.0802, 1738.6463, 3018.4462, 3031.4986, 3033.6036, 3092.356, 3096.6108, 3101.8261, 3133.6038, 3156.315, 3172.3647, 3179.2673
IRC:	



Compound: Mes Oxy + O_3 POZ1.1	**Energy (Hartree)** -534.792113773323
Reaction Coordinates: 6 0.232720 -0.355335 -0.559733 6 1.658427 -0.245774 -0.006791 8 2.037299 -0.911949 0.921775 6 2.547117 0.745606 -0.720267 1 2.022149 1.678499 -0.932702 1 3.435511 0.940256 -0.125901 1 2.845938 0.323490 -1.683388 6 -0.830400 0.612586 0.122171 6 -1.460493 1.533128 -0.916999 1 -2.221196 2.159163 -0.451947 1 -0.708395 2.185261 -1.364860 1 -1.924848 0.948756 -1.710033 6 -0.348919 1.363016 1.356690 1 -1.197885 1.846598 1.839016 1 0.116937 0.686620 2.069284 1 0.363453 2.141433 1.082550 8 -1.798210 -0.338550 0.610672 8 -1.693343 -1.429744 -0.307748 8 -0.266514 -1.654441 -0.316925 1 0.243775 -0.151972 -1.634635	**Frequencies (cm^{-1}):** 48.8583, 54.5844, 129.1908, 163.0119, 220.887, 230.9281, 260.6635, 277.3775, 321.9422, 350.8581, 373.9176, 393.6743, 494.1725, 569.4748, 581.4426, 629.9456, 698.5106, 761.6902, 776.7405, 858.2267, 929.0369, 934.5367, 941.4165, 950.6641, 963.3676, 1015.2591, 1040.2354, 1088.0874, 1176.7108, 1184.0756, 1205.151, 1236.8536, 1329.8222, 1374.5725, 1388.8704, 1405.7096, 1424.3902, 1463.0242, 1475.1827, 1481.9846, 1490.3103, 1498.083, 1510.9211, 1800.9056, 3014.6689, 3029.3552, 3033.7122, 3045.58, 3081.8287, 3096.3284, 3105.5248, 3116.2783, 3132.4802, 3141.9337

Compound: Mes Oxy + O_3 PRC1.2	**Energy (Hartree)** -534.704594960998
Reaction Coordinates: 6 0.592415 -0.482630 -0.769913 6 1.751345 0.274781 -0.233681 8 2.472283 0.843196 -1.035698 6 2.046253 0.389090 1.246537 1 1.144680 0.584256 1.825355 1 2.760637 1.196110 1.387669 1 2.495244 -0.534806 1.616422 6 -0.204199 -1.429999 -0.234418 6 -1.271759 -2.054763 -1.091568 1 -1.324592 -1.601500 -2.079119 1 -2.250046 -1.966688 -0.612531	**Frequencies (cm^{-1}):** 23.6592, 37.7428, 38.5841, 44.1712, 50.0253, 54.1445, 90.0346, 145.0702, 188.3823, 209.3195, 225.7722, 238.5944, 327.4102, 370.1096, 469.3341, 521.9023, 567.2346, 596.4632, 745.1888, 780.6778, 870.7128, 884.2999, 957.086, 1009.6045, 1010.1348, 1048.5655, 1090.4114, 1102.7155, 1174.9379, 1202.3441, 1215.9022, 1278.813, 1372.5299,

1 -1.083256 -3.125051 -1.214213 6 -0.125072 -2.017491 1.144171 1 -1.088409 -1.917202 1.649027 1 0.071055 -3.090650 1.067075 1 0.637453 -1.579692 1.774355 1 0.439405 -0.238623 -1.815219 8 -0.918742 2.189989 -0.410519 8 -1.971961 1.619555 -0.031528 8 -1.898588 0.872251 0.982047	1389.6694, 1409.362, 1419.3872, 1467.8418, 1471.1796, 1483.5714, 1484.0179, 1493.7021, 1500.8991, 1658.1629, 1717.1267, 3015.1422, 3025.3618, 3036.9242, 3056.6742, 3063.2853, 3100.4283, 3113.6883, 3135.7666, 3147.5157, 3183.3475

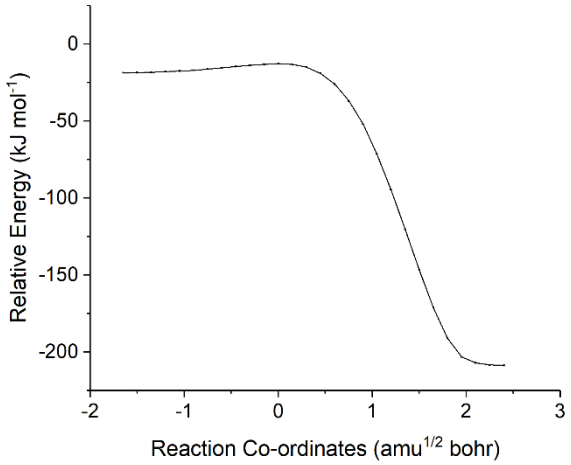
Compound: Mes Oxy + O_3 TS_{OZO} 1.2	**Energy (Hartree)** -534.695179931383
Reaction Coordinates: 6 0.351124 -0.266850 -0.743449 6 1.754256 -0.153625 -0.251700 8 2.641743 -0.168232 -1.082730 6 2.072313 0.016303 1.215321 1 1.272449 0.518359 1.754346 1 2.996285 0.584359 1.297493 1 2.244094 -0.962580 1.667933 6 -0.729944 -0.927984 -0.183905 6 -1.921484 -1.179204 -1.067638 1 -2.032473 -0.405584 -1.826100 1 -2.839863 -1.239969 -0.486634 1 -1.796552 -2.134332 -1.587460 6 -0.682452 -1.743079 1.075546 1 -1.659274 -1.752381 1.556452 1 -0.437331 -2.779041 0.822400 1 0.049998 -1.388979 1.790773 1 0.281399 -0.003788 -1.790919 8 -0.104847 1.918216 -0.255536 8 -1.358450 1.761751 -0.005828 8 -1.571147 0.874584 0.911177	**Frequencies (cm^{-1}):** -203.9293, 42.2512, 63.8996, 98.4315, 110.6976, 164.8593, 174.8074, 186.3833, 199.7198, 216.9075, 238.3345, 325.0365, 365.9207, 442.5551, 480.1867, 525.594, 563.4464, 609.922, 743.0238, 780.1646, 856.1936, 902.7492, 950.8256, 1007.4837, 1021.4108, 1043.6945, 1062.8886, 1073.1178, 1082.3066, 1121.8923, 1205.4466, 1267.419, 1361.3883, 1389.3699, 1406.9605, 1420.8978, 1466.976, 1468.7297, 1474.2813, 1484.4201, 1491.021, 1505.5514, 1550.462, 1731.2829, 3016.8014, 3025.6726, 3039.3612, 3081.9359, 3092.5138, 3106.4339, 3119.8271, 3140.8272, 3171.4166, 3172.7901
IRC:  	

Compound: Mes Oxy + O_3 POZ1.2	**Energy (Hartree)** -534.797488909827
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.228018 -0.195930 -0.698717 6 1.648138 0.194952 -0.281026 8 2.109227 1.220308 -0.727337 6 2.396686 -0.706818 0.659727 1 2.602662 -1.658416 0.165236 1 3.328728 -0.231438 0.952747 1 1.789285 -0.947559 1.532918 6 -0.922088 0.520997 0.126496 6 -1.991530 1.058920 -0.818123 1 -2.819405 1.474364 -0.244302 1 -1.575540 1.846043 -1.447565 1 -2.372040 0.266837 -1.460487 6 -0.469826 1.567199 1.132898 1 -1.333529 1.941576 1.680886 1 0.238164 1.155603 1.849928 1 0.001482 2.402002 0.617789 8 -1.427093 -0.584688 0.898988 8 -1.363804 -1.668272 -0.017766 8 0.017798 -1.584743 -0.481348 1 0.114781 0.054240 -1.754974	35.9509, 66.9584, 151.9999, 172.1197, 222.8066, 239.9914, 259.0011, 266.5828, 327.9963, 345.2904, 383.8728, 438.8488, 501.5514, 522.122, 591.1203, 621.042, 689.7289, 746.9947, 772.2767, 848.6953, 889.5146, 932.3283, 938.9608, 959.8788, 998.2174, 1020.8116, 1044.6947, 1056.424, 1178.6446, 1199.3972, 1232.2607, 1254.1917, 1302.32, 1341.7345, 1392.7723, 1405.2773, 1424.6052, 1457.6892, 1465.2794, 1481.1631, 1488.8698, 1498.7954, 1513.7212, 1778.6648, 3038.735, 3039.9281, 3050.3423, 3052.6879, 3091.9303, 3106.122, 3116.9338, 3120.4391, 3128.0958, 3144.1798

Compound: Mes Oxy + O_3 PRC 2.1	**Energy (Hartree)** -534.710263574005
Reaction Coordinates: 6 -0.160857 -0.782950 0.653593 6 -1.413577 -0.795694 -0.133820 8 -1.450943 -0.736696 -1.351368 6 -2.689168 -0.862838 0.680815 1 -2.760562 0.009924 1.333636 1 -2.686617 -1.744658 1.325020 1 -3.549297 -0.892350 0.017817 6 1.089714 -1.041238 0.214216 6 2.240212 -1.001522 1.176634 1 1.937778 -0.680472 2.171219 1 3.013577 -0.321198 0.812101 1 2.704872 -1.988415 1.253002 6 1.450814 -1.428160 -1.188196 1 2.060546 -0.642480 -1.641793 1 2.071627 -2.327689 -1.169453 1 0.582249 -1.586694 -1.816053 1 -0.288200 -0.579772 1.710348 8 -0.596128 2.239890 0.657177 8 0.030782 2.305911 -0.433165 8 1.242689 1.969423 -0.424557	**Frequencies (cm^{-1}):** 25.9802, 28.7382, 45.1804, 52.6124, 59.1388, 67.0696, 97.1328, 108.0249, 145.9557, 193.5056, 206.7742, 216.4951, 344.2889, 376.6945, 440.5134, 471.6263, 600.2664, 627.0059, 746.4433, 822.487, 853.4436, 912.877, 960.6881, 971.1167, 999.5386, 1044.0932, 1094.4783, 1104.5016, 1175.1535, 1189.3252, 1213.5919, 1242.5602, 1382.0962, 1389.2845, 1411.5415, 1415.0729, 1463.7146, 1466.6985, 1474.4187, 1475.508, 1486.1655, 1497.4367, 1640.7825, 1735.2755, 3016.2604, 3023.5835, 3028.4513, 3058.2883, 3063.6408, 3080.838, 3113.288, 3139.2433, 3148.7759, 3164.478

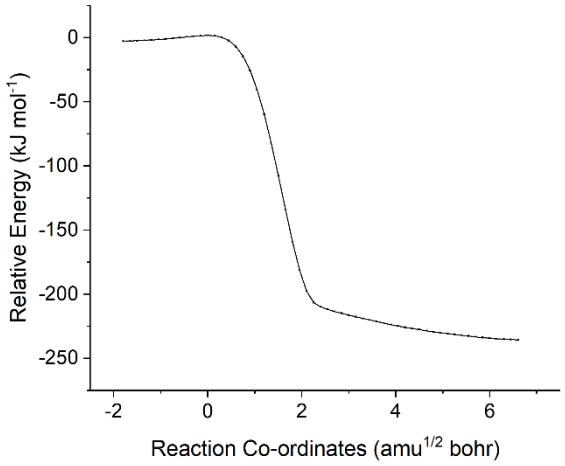
Compound: Mes Oxy + O_3 TS_{OZO} 2.1	**Energy (Hartree)** -534.699569322360
Reaction Coordinates: 6 -0.321957 -0.365462 0.682237 6 -1.598781 -0.431982 -0.070359 8 -1.654427 -0.731935 -1.248668 6 -2.842512 -0.108445 0.727034 1 -2.764908 0.891044 1.158021 1 -2.953608 -0.811242 1.556100 1 -3.715436 -0.165509 0.083047	**Frequencies (cm^{-1}):** -215.5984, 43.7579, 80.2933, 103.4714, 113.4622, 129.8935, 171.3373, 177.563, 198.9209, 217.8028, 232.9856, 339.9431, 374.9124, 456.4203, 468.9863, 479.0592, 612.3332, 627.2522, 746.658, 815.9238, 885.6802, 914.1677, 955.2251, 969.1381,

6 0.916280 -0.812568 0.235887 6 2.001163 -1.032392 1.249202 1 1.824592 -0.474143 2.165930 1 2.972863 -0.750962 0.845531 1 2.051295 -2.097477 1.496215 6 1.132340 -1.432029 -1.114300 1 2.196250 -1.535724 -1.318489 1 0.680736 -2.428367 -1.131554 1 0.654391 -0.867047 -1.907232 1 -0.407337 -0.124690 1.732364 8 -0.217081 1.873240 0.333414 8 0.620090 1.816853 -0.643086 8 1.719163 1.224515 -0.308927	1016.2315, 1041.9839, 1061.2929, 1073.1819, 1082.5874, 1124.3416, 1184.9313, 1236.109, 1376.3747, 1388.1064, 1409.538, 1420.8051, 1463.768, 1467.6979, 1472.172, 1474.6967, 1477.6041, 1494.5548, 1538.0649, 1736.5001, 3018.4427, 3026.688, 3031.3897, 3083.6266, 3086.5972, 3094.0378, 3124.381, 3142.592, 3153.676, 3180.5793
IRC:  	

Compound: Mes Oxy + O_3 POZ 2.1	**Energy (Hartree)** -534.792044532333
Reaction Coordinates: 6 0.245352 -0.212611 -0.692229 6 1.626468 -0.197985 -0.017902 8 1.972655 -1.071086 0.735192 6 2.522792 0.960365 -0.394345 1 1.979307 1.906587 -0.409822 1 3.360385 1.019970 0.295201 1 2.905137 0.797460 -1.405519 6 -0.873055 0.590442 0.090924 6 -1.306369 1.859953 -0.626350 1 -2.161654 2.303736 -0.117852 1 -0.499393 2.592520 -0.623275 1 -1.585299 1.646664 -1.657066 6 -0.544644 0.828615 1.561404 1 -1.404946 1.286463 2.048076 1 -0.309936 -0.106637 2.063565 1 0.305519 1.502338 1.674512 8 -1.974675 -0.329175 -0.024447 8 -1.342420 -1.589295 0.157176 8 -0.274068 -1.524204 -0.829469 1 0.335678 0.188313 -1.704452	**Frequencies (cm^{-1}):** 51.0298, 69.7701, 115.7249, 169.3575, 214.9059, 231.2789, 258.1257, 268.6933, 323.3572, 330.549, 371.7014, 409.714, 506.8461, 576.1476, 579.2623, 636.5966, 691.4151, 742.5116, 816.3254, 864.961, 893.071, 929.1058, 944.459, 951.0607, 965.8531, 1013.5964, 1040.7039, 1060.2442, 1173.0655, 1188.251, 1202.2852, 1238.061, 1304.1405, 1370.4463, 1386.1017, 1407.6351, 1424.896, 1463.0535, 1475.2677, 1481.08, 1489.4762, 1498.9758, 1510.2903, 1803.3439, 3027.5997, 3040.2202, 3041.6369, 3046.2436, 3081.3782, 3101.8036, 3109.1222, 3116.994, 3134.8567, 3140.4409

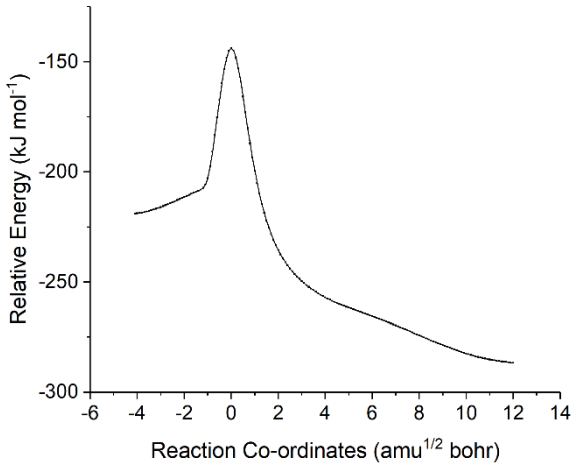
Compound: Mes Oxy + O_3 PRC 2.2	**Energy (Hartree)** -534.704122867276
Reaction Coordinates: 6 0.788178 -0.211594 0.000006 6 0.313680 1.188422 0.000007 8 -0.893862 1.377709 0.000010 6 1.238808 2.387510 0.000004 1 1.881206 2.388588 0.881297 1 0.629316 3.287146 0.000009 1 1.881196 2.388592 -0.881298 6 2.014495 -0.763651 -0.000001 6 2.133767 -2.264167 0.000001 1 1.162370 -2.753106 0.000011 1 2.693863 -2.603585 0.875688 1 2.693845 -2.603588 -0.875698 6 3.343772 -0.066406 -0.000011 1 3.288809 1.013838 -0.000018 1 3.921942 -0.379361 0.873738 1 3.921935 -0.379372 -0.873761 1 -0.058716 -0.887886 0.000012 8 -2.913485 -0.644329 -1.075333 8 -3.405674 -0.225514 0.000002 8 -2.913474 -0.644361 1.075320	**Frequencies (cm^{-1}):** 12.4087, 19.5325, 22.9232, 32.8742, 56.397, 62.9345, 80.6485, 142.98, 144.8051, 213.7758, 232.2177, 242.8921, 322.0617, 374.1857, 473.4836, 525.8892, 584.7314, 586.201, 749.4671, 782.3707, 877.5935, 889.3302, 956.4738, 1007.6729, 1015.8919, 1050.601, 1093.1779, 1104.8973, 1193.6333, 1204.6019, 1241.9039, 1288.9911, 1379.5975, 1391.3639, 1410.5514, 1420.1125, 1467.1998, 1470.9165, 1483.3021, 1483.8396, 1495.3879, 1501.5063, 1682.416, 1703.2213, 3013.0954, 3022.2276, 3037.8419, 3051.7413, 3056.7095, 3097.2822, 3117.6208, 3135.5978, 3153.4351, 3184.1817

Compound: Mes Oxy + O_3 TS_{OZO} 2.2	**Energy (Hartree)** -534.695849937139
Reaction Coordinates: 6 0.322965 -0.419851 -0.717441 6 1.721020 -0.290713 -0.217985 8 2.618639 -0.432035 -1.026683 6 2.036809 0.009749 1.229762 1 1.348234 0.733493 1.663668 1 3.053742 0.389999 1.282725 1 1.981422 -0.905758 1.821491 6 -0.805113 -0.918223 -0.089505 6 -1.948605 -1.369079 -0.952087 1 -1.910634 -0.919852 -1.941595 1 -2.905474 -1.127407 -0.490886 1 -1.910433 -2.457080 -1.067052 6 -0.861108 -1.374851 1.342563 1 -0.417932 -2.371798 1.428543 1 -0.330205 -0.717399 2.023002 1 -1.894014 -1.447846 1.676440 1 0.291085 -0.354977 -1.796184 8 -0.042906 1.833301 -0.678262 8 -0.765047 1.875484 0.383772 8 -1.823387 1.142804 0.299673	**Frequencies (cm^{-1}):** -186.9738, 42.8294, 76.3793, 110.6847, 129.4643, 154.841, 170.2827, 192.9062, 203.4787, 217.6898, 247.006, 323.3496, 372.5964, 451.9266, 471.0942, 527.3511, 574.1249, 606.0575, 742.909, 780.0591, 861.0281, 907.4923, 959.5767, 1005.7347, 1021.1014, 1044.8461, 1069.2749, 1079.1834, 1087.8139, 1124.5456, 1204.5939, 1270.6468, 1364.5027, 1393.826, 1408.4514, 1420.2996, 1463.1585, 1471.2756, 1472.7095, 1483.6868, 1488.9416, 1508.612, 1549.6958, 1727.147, 3016.2138, 3021.8339, 3040.8502, 3082.2535, 3098.1436, 3102.4889, 3127.6516, 3137.4874, 3149.4437, 3184.0356
IRC:	

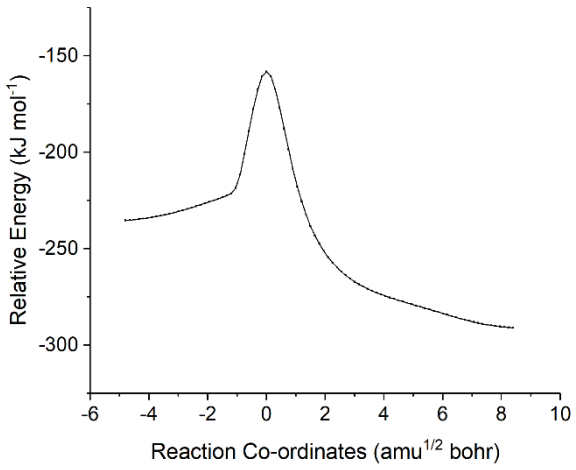


Compound: Mes Oxy + O_3 POZ 2.2	**Energy (Hartree)** -534.797714881535
Reaction Coordinates: 6 -0.234839 0.080930 -0.742274 6 -1.581980 -0.410372 -0.203275 8 -1.865547 -1.577340 -0.354005 6 -2.499507 0.584878 0.450439 1 -2.844321 1.304244 -0.295410 1 -3.350070 0.064779 0.882172 1 -1.971807 1.163775 1.208917 6 1.022186 -0.405318 0.086956 6 1.880214 -1.394797 -0.685313 1 2.792329 -1.616066 -0.131758 1 1.330188 -2.324437 -0.825845 1 2.151291 -0.992825 -1.660365 6 0.695563 -0.899940 1.492323 1 1.625468 -1.123955 2.013397 1 0.160628 -0.141931 2.061961 1 0.092060 -1.804988 1.457874 8 1.777584 0.823368 0.158652 8 0.766959 1.806824 0.322955 8 -0.119475 1.498731 -0.794323 1 -0.151760 -0.273550 -1.770301	**Frequencies (cm^{-1}):** 38.8592, 63.7719, 145.3558, 174.2169, 226.7094, 233.3381, 250.3973, 274.9418, 315.6352, 336.4519, 406.039, 445.9726, 508.7695, 525.2494, 587.9163, 624.5293, 688.7089, 740.3333, 791.1881, 843.1909, 887.346, 933.3965, 944.2567, 959.9606, 1000.8196, 1015.7992, 1038.3557, 1046.1565, 1182.8305, 1197.0859, 1228.5177, 1246.1747, 1297.856, 1335.5448, 1391.3942, 1406.0038, 1422.6586, 1458.1648, 1467.2145, 1484.9996, 1489.2996, 1504.0195, 1511.9606, 1775.4871, 3039.1633, 3042.701, 3050.027, 3068.1365, 3093.2995, 3110.849, 3116.3622, 3118.8149, 3126.2189, 3145.0632

Compound: Mes Oxy + O_3 TS_{ANTI} 1	**Energy (Hartree)** -534.758759688438
Reaction Coordinates: 6 0.307354 0.474926 -0.494682 6 1.675085 0.186170 0.069766 8 2.008803 0.622869 1.145480 6 2.581397 -0.650739 -0.797864 1 2.889535 -0.063348 -1.666860 1 3.461995 -0.941811 -0.232189 1 2.068247 -1.533936 -1.179691 6 -1.091420 -0.683485 0.130948 6 -0.908593 -1.929350 -0.746837	**Frequencies (cm^{-1}):** -486.4642, 45.5532, 83.3248, 99.3583, 148.9841, 183.3597, 205.4112, 226.6078, 247.1195, 279.102, 307.4185, 371.6308, 423.7204, 437.2622, 478.7305, 560.9162, 591.8926, 615.2779, 627.983, 777.5695, 916.3132, 925.5042, 960.8785, 979.924, 1010.6716, 1034.7561, 1062.4514, 1116.1454, 1135.8682, 1182.992,

1 0.053359 -2.413409 -0.584873 1 -1.030449 -1.682457 -1.799507 1 -1.687734 -2.643857 -0.477903 6 -0.834140 -0.884121 1.621060 1 -0.802089 0.072655 2.137041 1 0.090081 -1.424715 1.819516 1 -1.664285 -1.462872 2.030033 1 0.151129 0.326001 -1.557831 8 -0.224357 1.617351 -0.027883 8 -1.403029 1.806432 -0.588604 8 -2.119904 0.039265 -0.176754	1194.9168, 1232.4895, 1355.9078, 1381.9894, 1394.4578, 1400.8688, 1411.346, 1464.2128, 1469.397, 1475.7154, 1485.7221, 1491.2044, 1504.7369, 1773.7117, 3031.2801, 3036.8738, 3041.0962, 3087.7763, 3097.7763, 3102.662, 3124.7053, 3131.7965, 3135.1955, 3144.967
IRC:  	

Compound: Mes Oxy + O_3 C_{ANTI} 1	**Energy (Hartree)** -534.806025516833
Reaction Coordinates: 6 2.015139 -1.978640 -0.627637 6 2.029624 -0.708258 0.177696 6 1.366504 0.455653 -0.486008 1 0.932497 0.418571 -1.476744 8 1.306888 1.543149 0.143938 8 0.677772 2.589573 -0.440287 8 2.522625 -0.603796 1.277522 1 2.543517 -2.758984 -0.087924 1 0.981378 -2.278671 -0.810124 1 2.484331 -1.819389 -1.601504 6 -2.199338 -0.327217 0.002243 6 -2.360041 1.142815 0.290958 1 -3.278537 1.526001 -0.156475 1 -1.500551 1.713369 -0.055357 1 -2.459343 1.276906 1.371974 6 -3.427717 -1.192744 0.156522 1 -3.166792 -2.243839 0.069255 1 -4.151007 -0.932996 -0.620291 1 -3.913952 -1.003348 1.114957 8 -1.134356 -0.809836 -0.334974	**Frequencies (cm^{-1}):** 26.0742, 30.0187, 57.5506, 68.762, 74.6665, 81.6325, 106.6702, 131.6677, 147.406, 188.1096, 194.8649, 228.9937, 374.9457, 393.9947, 462.2004, 497.2747, 544.1782, 565.0713, 617.3798, 791.5103, 888.09, 892.8297, 908.2755, 912.6079, 932.612, 1032.3061, 1048.5668, 1090.4772, 1122.7511, 1199.4668, 1245.9589, 1363.8349, 1389.0051, 1390.9899, 1399.1185, 1461.8245, 1463.4678, 1466.4785, 1473.1354, 1475.8169, 1493.8168, 1505.5236, 1753.6192, 1763.0578, 3020.6804, 3029.7557, 3032.2759, 3077.5571, 3085.7906, 3086.0933, 3122.681, 3139.6836, 3147.3204, 3189.3751

Compound: Mes Oxy + O_3 TS_{ANTI} 2	**Energy (Hartree)** -534.764679805393
Reaction Coordinates: 6 0.291126 0.364665 -0.620373 6 1.639607 -0.202418 -0.283078 8 1.982729 -1.223240 -0.839049 6 2.496939 0.516970 0.723535 1 3.394669 -0.066141 0.908016 1 2.769224 1.502251 0.339437 1 1.953801 0.682710 1.653876 6 -1.155893 -0.544763 0.217021 6 -1.308131 -1.769418 -0.692541 1 -0.374764 -2.320245 -0.793734 1 -1.665490 -1.466612 -1.674408 1 -2.055063 -2.428092 -0.246517 6 -0.707262 -0.849318 1.646547 1 -0.496469 0.071843 2.186463 1 0.160078 -1.508483 1.680282 1 -1.528929 -1.351736 2.159599 1 -0.038205 0.228243 -1.643959 8 0.051384 1.585025 -0.109595 8 -1.159766 1.979274 -0.466944 8 -2.081493 0.354185 0.101123	**Frequencies (cm^{-1}):** -490.0647, 61.7722, 86.9588, 110.0727, 144.9355, 198.8362, 217.9317, 236.7446, 250.3079, 292.1201, 307.0353, 390.5085, 425.3732, 473.3876, 484.485, 539.1787, 573.0902, 610.4145, 619.6787, 773.0316, 843.5264, 917.7925, 981.8813, 1007.4702, 1014.2731, 1041.5659, 1067.8061, 1115.61, 1139.4584, 1189.152, 1222.533, 1251.804, 1348.5371, 1361.7125, 1392.768, 1395.2136, 1407.4258, 1461.6891, 1470.3874, 1480.2014, 1486.6685, 1496.8677, 1503.6097, 1759.4355, 3034.1803, 3039.0026, 3040.9695, 3094.068, 3098.2812, 3104.7718, 3120.4132, 3131.1522, 3147.4591, 3151.0265
IRC:  	

Compound: Mes Oxy + O_3 C_{ANTI} 2	**Energy (Hartree)** -534.809649087298
Reaction Coordinates: 6 2.391909 -1.027762 1.192280 6 2.046755 -0.710723 -0.234146 6 1.327980 0.554056 -0.528402 1 0.939043 0.763382 -1.516997 8 1.210547 1.417504 0.379347 8 0.547705 2.570205 0.101639 8 2.307917 -1.428212 -1.177187 1 3.005653 -1.923397 1.220973 1 2.912574 -0.194555 1.664890 1 1.470564 -1.192981 1.754056 6 -2.186800 -0.391089 -0.006413	**Frequencies (cm^{-1}):** 25.409, 34.8438, 40.4654, 59.4227, 78.0114, 87.9757, 105.9357, 108.8285, 139.8925, 166.5056, 193.5539, 246.2413, 391.7459, 395.1423, 494.9224, 495.7167, 544.2258, 558.989, 569.8111, 790.1655, 833.6049, 889.9159, 908.067, 919.8319, 979.2988, 1024.8148, 1050.7451, 1091.2863, 1122.9055, 1244.8312, 1245.4119, 1341.1692, 1388.5361, 1396.3568, 1399.0772, 1462.1583,

6 -2.536636 1.056956 -0.239885 1 -2.982327 1.153368 -1.234209 1 -1.651504 1.687629 -0.180042 1 -3.290199 1.393488 0.473860 6 -3.333448 -1.339506 0.255430 1 -2.982588 -2.367795 0.258391 1 -4.118518 -1.211035 -0.491736 1 -3.780136 -1.105511 1.224905 8 -1.038811 -0.791270 -0.029709	1464.1392, 1464.7127, 1470.8219, 1475.8703, 1493.0306, 1510.513, 1748.8812, 1757.3464, 3018.6245, 3031.3335, 3041.8106, 3077.0785, 3084.9171, 3099.1432, 3119.7206, 3139.8553, 3148.141, 3192.3128

Compound: Mes Oxy + O_3 TS_{AO} 1.1	**Energy (Hartree)** -534.766832706485
Reaction Coordinates: 6 0.382137 -0.443930 0.750952 6 1.659912 -0.213869 -0.071683 8 1.782719 -0.656753 -1.184598 6 2.748631 0.565164 0.633002 1 3.126566 -0.022931 1.473042 1 3.561490 0.774706 -0.056816 1 2.361268 1.496211 1.051509 6 -0.957766 0.654717 -0.074835 6 -0.419856 1.871967 -0.776075 1 -1.247903 2.501323 -1.109271 1 0.185107 2.465299 -0.092261 1 0.179661 1.593471 -1.639210 6 -1.913181 0.885944 1.071052 1 -2.856265 1.256271 0.659954 1 -2.111176 -0.026051 1.622936 1 -1.510996 1.643632 1.740628 1 0.375785 0.064947 1.727684 8 -0.126237 -1.618778 0.715600 8 -1.735628 -1.390999 -0.377930 8 -1.303705 -0.291825 -0.974657	**Frequencies (cm^{-1}):** -423.199, 58.1878, 75.3686, 112.4049, 147.1989, 185.0204, 214.8614, 238.1603, 246.9126, 289.1586, 334.0638, 351.6465, 371.6548, 399.697, 524.1063, 543.7577, 625.3093, 646.4945, 673.2083, 790.4517, 832.4498, 945.6563, 956.3447, 989.534, 1006.1283, 1016.5101, 1032.8363, 1114.1777, 1144.73, 1175.0422, 1281.9692, 1294.8162, 1330.9133, 1380.671, 1404.0493, 1413.8666, 1419.9495, 1462.4207, 1470.8338, 1471.6616, 1484.8058, 1495.472, 1505.7601, 1794.5339, 2931.3097, 3028.6794, 3031.2055, 3039.0142, 3079.81, 3099.0411, 3107.0033, 3138.2118, 3140.5717, 3162.9852

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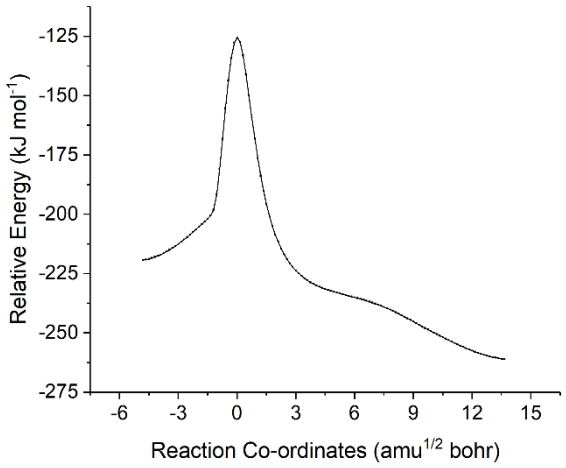
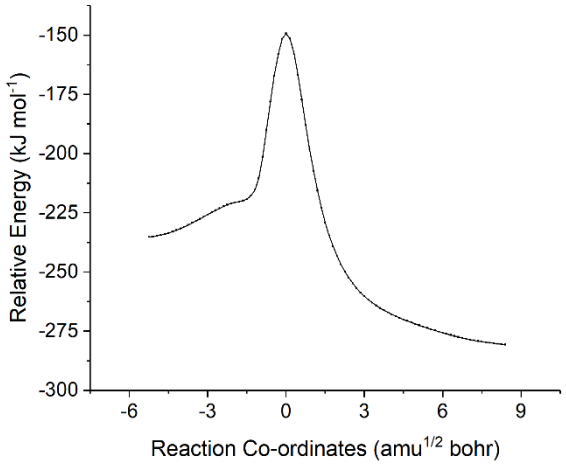


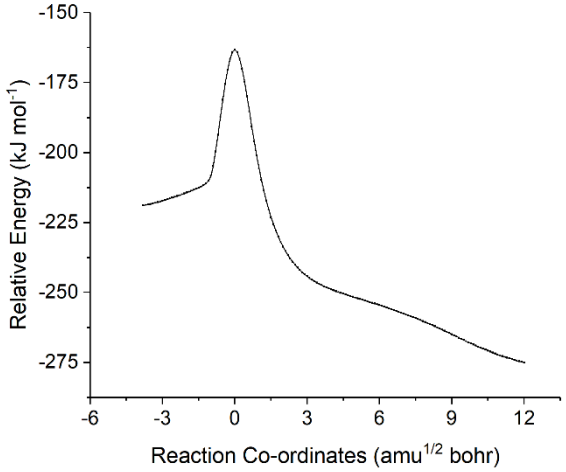
Compound: Mes Oxy + O_3 CPr_{AO} 1.1	**Energy (Hartree)** -534.815354982453
Reaction Coordinates: 6 2.442611 1.409196 0.015735 6 1.595120 0.267945 -0.478472 6 1.767799 -1.067195 0.276889 1 2.328831 -1.005160 1.226341 8 1.352224 -2.109283 -0.152429 8 0.869250 0.333087 -1.445268 1 3.497048 1.180161 -0.166244 1 2.183997 2.326047 -0.506978 1 2.316973 1.539135 1.090232 6 -1.861276 0.079257 0.085087 6 -2.788474 -0.870504 -0.576735 1 -3.823084 -0.598092 -0.357043 1 -2.656840 -0.794836 -1.658769 1 -2.593140 -1.891193 -0.260469 6 -1.896824 1.537543 -0.131214 1 -1.865644 2.041762 0.836284 1 -0.990280 1.835411 -0.661197 1 -2.773611 1.825336 -0.704896 8 -1.030274 -0.443805 0.877188 8 -0.088448 0.395500 1.472384	**Frequencies (cm^{-1}):** 33.324, 54.8279, 71.7283, 92.7006, 98.0452, 127.6262, 132.0077, 151.8264, 161.643, 205.0216, 276.4828, 310.0763, 315.2038, 372.2681, 402.9845, 481.0672, 487.7678, 592.7621, 643.9583, 811.7403, 825.0493, 891.4262, 912.0428, 929.1655, 976.5939, 988.1836, 1058.8944, 1076.6211, 1100.8795, 1187.3553, 1306.5343, 1384.0861, 1387.4657, 1403.1761, 1404.8894, 1448.2479, 1456.3786, 1461.1197, 1468.5441, 1473.5069, 1481.7586, 1578.8017, 1762.2916, 1800.6774, 2927.2434, 3024.061, 3029.6445, 3039.6222, 3078.6609, 3091.3265, 3091.9224, 3140.3127, 3141.1911, 3146.268

Compound: Mes Oxy + O_3 TS_{AO} 1.2	**Energy (Hartree)** -534.777037370371
Reaction Coordinates: 6 -0.342941 -0.225277 -0.887784 6 -1.667639 0.184987 -0.241120 8 -2.167247 1.248774 -0.562697 6 -2.295182 -0.777458 0.731622 1 -1.574704 -1.058092 1.512193 1 -3.193730 -0.330831 1.168017 1 -2.547198 -1.707643 0.202594 6 1.018377 0.543753 0.156498 6 0.611357 1.834643 0.818868 1 1.503850 2.360151 1.186673 1 0.102795 2.480046 0.093810 1 -0.068326 1.654380 1.658674 6 2.183018 0.606023 -0.808737 1 3.105957 0.729078 -0.222147 1 2.268033 -0.301871 -1.409384 1 2.065970 1.478949 -1.461097 1 -0.125827 0.377413 -1.791219 8 -0.045410 -1.480907 -0.922724 8 1.351845 -1.625638 0.478897 8 1.038467 -0.477430 1.062249	**Frequencies (cm^{-1}):** -414.7799, 67.8122, 95.123, 119.4608, 152.9746, 199.2026, 207.4744, 245.6865, 257.4259, 276.9652, 331.1384, 371.2906, 395.0585, 436.46, 518.7693, 538.3302, 594.8471, 643.8782, 665.9342, 775.9286, 818.6798, 953.35, 973.5207, 988.5287, 994.1375, 1007.9702, 1026.0946, 1113.6375, 1144.1686, 1235.435, 1269.3768, 1278.0736, 1294.1246, 1369.3055, 1390.301, 1393.5927, 1406.7836, 1433.3335, 1441.0118, 1450.8911, 1456.8379, 1471.0281, 1483.4895, 1762.878, 2964.9345, 3040.6314, 3044.2257, 3046.1238, 3107.3246, 3120.0513, 3122.5491, 3146.8091, 3161.0402, 3175.8067
IRC:	

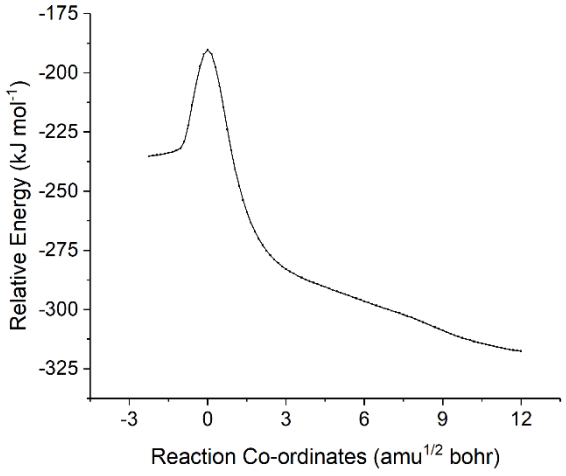


Compound: Mes Oxy + O_3 CPr_{AO} 1.2	**Energy (Hartree)** -534.819148971057
Reaction Coordinates: 6 1.877572 1.658149 -0.395539 6 1.373668 0.576861 0.509975 6 2.021231 -0.802848 0.377948 1 1.501443 -1.589108 0.953037 8 3.041412 -0.999308 -0.227513 8 0.535269 0.738014 1.375468 1 1.700092 1.366349 -1.431040 1 1.379699 2.597581 -0.171469 1 2.957453 1.761915 -0.278701 6 -2.000084 -0.121331 -0.120688 6 -3.043319 0.921817 0.040489 1 -4.034186 0.479403 -0.084835 1 -2.996084 1.322888 1.055466 1 -2.906011 1.727650 -0.675305 6 -1.936339 -1.341925 0.700508 1 -1.778954 -2.203018 0.048553 1 -1.054300 -1.279232 1.342662 1 -2.829792 -1.453203 1.308866 8 -1.156499 0.090595 -1.037430 8 -0.132149 -0.838746 -1.203448	**Frequencies (cm^{-1}):** 39.4941, 51.369, 72.8599, 82.9, 91.1104, 97.365, 135.5356, 162.3678, 173.1807, 198.0153, 256.5841, 307.963, 312.7899, 370.0074, 468.6213, 482.9884, 491.7759, 584.4694, 591.5706, 786.0934, 812.1789, 907.4165, 917.5145, 928.9838, 987.5831, 1013.742, 1064.8698, 1073.7737, 1098.723, 1250.4509, 1306.3545, 1366.908, 1385.6182, 1388.2229, 1405.5694, 1445.3441, 1456.6532, 1457.7634, 1466.9281, 1469.5568, 1482.1726, 1569.4418, 1750.0017, 1789.7738, 2939.7544, 3028.4894, 3033.7141, 3043.6484, 3077.8838, 3082.955, 3101.6395, 3140.0222, 3141.97, 3143.2545

Compound: Mes Oxy + O_3 TS_{AO} 2.1	**Energy (Hartree)** -534.766584568438
Reaction Coordinates: 6 0.357100 -0.518082 -0.701274 6 1.665042 -0.269723 0.096919 8 1.866119 -0.749428 1.179034 6 2.695952 0.546791 -0.650479 1 2.254787 1.430717 -1.111694 1 3.499118 0.828697 0.024900 1 3.105884 -0.060726 -1.461043	**Frequencies (cm^{-1}):** -415.4877, 62.9614, 92.5795, 126.0664, 166.2667, 172.9802, 190.637, 241.2498, 256.1407, 287.3618, 333.6769, 361.8137, 371.8115, 390.6598, 532.578, 538.8522, 607.0818, 641.2281, 652.9859, 788.2777, 827.8611, 948.3359, 961.133, 983.4487,

6 -0.890346 0.669712 0.124729 6 -0.701293 2.088016 -0.339709 1 -1.443585 2.734620 0.132945 1 0.281303 2.453402 -0.048232 1 -0.809074 2.168091 -1.419751 6 -0.844503 0.397505 1.604254 1 -1.832017 0.631716 2.010637 1 -0.616980 -0.638463 1.827230 1 -0.106602 1.035358 2.083432 1 0.396623 -0.082021 -1.712495 8 -0.181593 -1.665483 -0.571427 8 -2.073398 -1.174371 -0.192914 8 -1.913774 0.090944 -0.556264	999.2857, 1023.0105, 1044.3651, 1125.0069, 1135.3224, 1168.8388, 1273.4584, 1287.3457, 1363.0214, 1381.2592, 1403.9143, 1411.1983, 1422.1879, 1464.4898, 1466.9975, 1470.4454, 1478.9342, 1492.1068, 1496.1282, 1801.1189, 2925.6171, 3034.0219, 3034.4714, 3039.1016, 3090.0016, 3100.604, 3119.0698, 3130.2733, 3142.1014, 3168.0626
IRC:  	

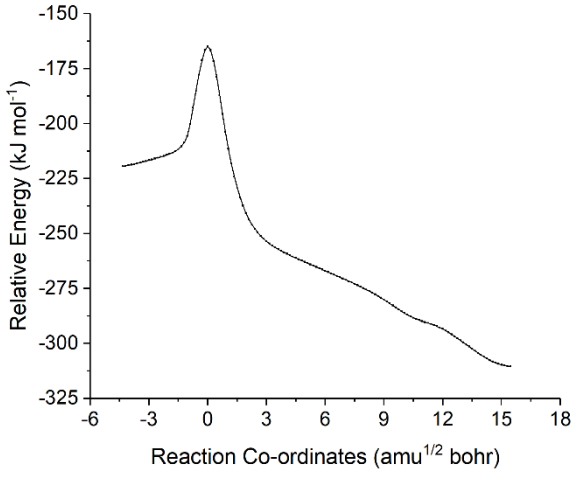
Compound: Mes Oxy + O_3 CPr_{AO} 2.1	**Energy (Hartree)** -534.815991219137
Reaction Coordinates: 6 1.892839 0.850304 0.209507 6 1.489821 -0.477774 -0.461408 8 0.719705 -0.480679 -1.396314 6 2.160484 -1.712267 0.076491 1 1.977013 -1.795422 1.147665 1 1.790640 -2.594822 -0.438256 1 3.242102 -1.635797 -0.067656 6 -1.844394 0.016633 0.090456 6 -2.913015 -0.749857 -0.597268 1 -3.884297 -0.291748 -0.398504 1 -2.746679 -0.697632 -1.675623 1 -2.920023 -1.788825 -0.279807 6 -1.608681 1.451198 -0.136683 1 -1.426337 1.941400 0.820771 1 -0.689709 1.570807 -0.717126 1 -2.440721 1.900816 -0.672219 1 2.390227 0.750476 1.190673 8 1.733523 1.919318 -0.318544 8 -0.096648 0.006704 1.554299 8 -1.150898 -0.648928 0.910998	**Frequencies (cm^{-1}):** 55.2014, 58.9985, 85.6964, 87.0779, 109.4312, 113.6025, 139.6153, 165.1225, 185.6452, 209.8405, 276.9853, 312.7902, 317.8043, 374.2839, 400.2894, 483.3275, 494.8155, 590.387, 646.0556, 811.9878, 829.2425, 897.067, 905.6429, 924.4675, 981.1784, 988.4061, 1061.9845, 1075.3485, 1099.2239, 1189.7704, 1306.9756, 1381.0137, 1383.0929, 1400.9374, 1404.3508, 1446.7048, 1457.7563, 1461.3306, 1469.5896, 1475.7308, 1484.7034, 1571.5732, 1759.6992, 1793.3069, 2927.6127, 3025.8224, 3027.7778, 3033.0489, 3080.6817, 3083.3703, 3091.6944, 3139.0643, 3141.2045, 3143.487

Compound: Mes Oxy + O_3 TS_{AO} 2.2	**Energy (Hartree)** -534.773958861196
Reaction Coordinates: 6 0.340222 -0.347517 -0.839418 6 1.658856 0.147793 -0.210856 8 2.084147 1.232958 -0.528948 6 2.401329 -0.806590 0.682335 1 2.940717 -1.507796 0.040356 1 3.118515 -0.261020 1.290170 1 1.726679 -1.402868 1.290767 6 -0.968934 0.568084 0.177703 6 -1.105954 1.976062 -0.323899 1 -1.723041 2.563035 0.358904 1 -0.121862 2.439372 -0.380414 1 -1.558136 1.990729 -1.313552 6 -0.635731 0.380313 1.635931 1 -1.506864 0.689794 2.219410 1 -0.417468 -0.654258 1.873117 1 0.200081 1.016884 1.917505 1 0.167160 0.141075 -1.808958 8 0.051811 -1.588242 -0.719435 8 -1.794838 -1.488970 0.034070 8 -1.961685 -0.221223 -0.312947	**Frequencies (cm^{-1}):** -416.8877, 75.8852, 97.5141, 120.5624, 167.026, 194.7282, 219.8246, 235.3631, 266.1258, 271.6497, 332.9154, 372.7159, 393.7847, 449.5794, 526.4177, 538.9167, 577.664, 629.4933, 642.7996, 772.3633, 805.8098, 956.234, 984.7878, 992.5555, 1005.0136, 1022.3623, 1039.3268, 1127.7345, 1156.8232, 1195.065, 1278.1147, 1285.6328, 1332.9809, 1383.2269, 1401.4295, 1403.8934, 1421.3189, 1460.3512, 1462.564, 1476.2653, 1481.992, 1495.6464, 1504.8607, 1769.5191, 2963.1101, 3033.6092, 3038.428, 3040.6494, 3102.4461, 3107.6683, 3110.7951, 3128.2779, 3154.5482, 3169.4089
IRC:  	

Compound: Mes Oxy + O_3 CPr_{AO} 2.2	**Energy (Hartree)** -534.818525930480
Reaction Coordinates: 6 -1.919020 -0.959574 0.280125 6 -1.400974 0.450901 0.570323 8 -0.549689 0.590814 1.427175 6 -2.066037 1.581354 -0.157660 1 -3.135864 1.571388 0.057800 1 -1.633310 2.530865 0.146770 1 -1.960973 1.437735 -1.232908 6 2.017805 -0.110141 -0.115496 6 3.011888 -0.627706 0.856267	**Frequencies (cm^{-1}):** 36.6001, 54.7023, 63.415, 82.5663, 94.5904, 108.6572, 138.1355, 149.9398, 162.3128, 204.9669, 258.5808, 309.3476, 314.3382, 370.6683, 464.5625, 483.0074, 490.5077, 585.972, 594.72, 784.0162, 812.2534, 914.3613, 922.3675, 927.8266, 987.777, 1012.3435, 1063.811, 1074.3558, 1097.8847, 1248.8111, 1306.751,

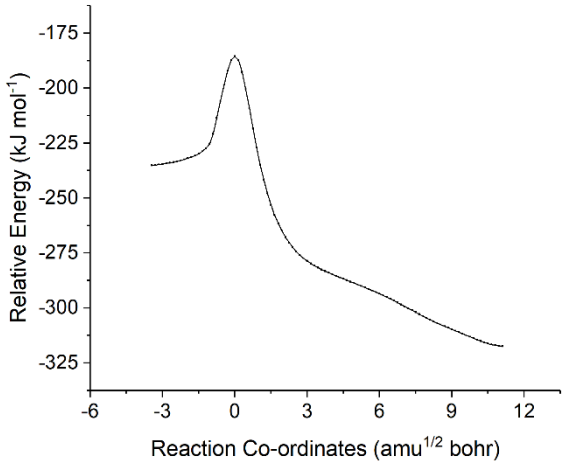
1 4.020577 -0.525475 0.450003 1 2.967908 -0.024689 1.766328 1 2.814640 -1.667474 1.101880 6 2.050460 1.256403 -0.667204 1 1.978893 1.200222 -1.755590 1 1.160829 1.794329 -0.336461 1 2.945990 1.785484 -0.353380 1 -1.269987 -1.759236 0.675812 8 -2.979225 -1.171720 -0.248181 8 0.143589 -0.473723 -1.344512 8 1.128646 -0.931691 -0.474281	1367.8396, 1387.0755, 1388.9487, 1405.5525, 1446.5177, 1457.2004, 1458.1362, 1466.7473, 1469.0909, 1480.0455, 1573.2151, 1748.0797, 1786.387, 2951.1199, 3029.286, 3039.1847, 3043.0613, 3077.8234, 3091.3687, 3101.9214, 3138.9607, 3142.2627, 3143.6408

Compound: Mes Oxy + O_3 TS_{SYN} 1	**Energy (Hartree)** -534.750836106521
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.309641 -0.239607 0.785086 6 1.592586 0.028284 0.021253 8 2.000735 -0.693349 -0.850369 6 2.376612 1.222177 0.524408 1 1.730194 2.035003 0.852211 1 3.051012 1.565889 -0.255289 1 2.972965 0.907869 1.384984 6 -1.212399 0.489005 -0.214384 6 -0.658570 1.684803 -0.996458 1 -0.221323 2.445329 -0.351044 1 0.065893 1.359119 -1.739204 1 -1.495538 2.143125 -1.525869 6 -2.164748 0.850300 0.930598 1 -1.753251 1.613229 1.592009 1 -3.085831 1.242911 0.495589 1 -2.419659 -0.036246 1.507711 1 0.295087 0.188091 1.783369 8 -0.157310 -1.496385 0.861355 8 -0.369825 -1.994973 -0.335552 8 -1.548384 -0.524556 -0.931369	-464.5031, 39.7641, 65.4695, 100.4754, 154.7862, 203.2515, 223.4725, 247.8715, 252.2338, 278.8153, 287.6317, 351.952, 409.8556, 442.8117, 478.5336, 548.153, 561.1297, 618.1822, 694.5184, 801.9295, 880.3942, 909.729, 958.274, 991.3133, 994.3453, 1031.2095, 1061.4952, 1072.0162, 1123.2957, 1162.3909, 1187.5601, 1195.951, 1369.0131, 1385.5481, 1388.9193, 1403.3874, 1429.734, 1465.8359, 1475.4142, 1478.9255, 1488.0494, 1495.7885, 1507.0638, 1786.7108, 3029.8372, 3033.3644, 3038.8842, 3088.3017, 3094.3861, 3099.0109, 3121.0407, 3131.3353, 3132.7259, 3144.0328
IRC	



Compound: Mes Oxy + O_3 CPr_{SYN} 1	**Energy (Hartree)** -534.799290258670
Reaction Coordinates: 6 -1.559092 -0.093942 -0.887184 6 -1.610145 0.761615 0.332125 8 -1.654514 0.313010 1.453835 6 -1.628502 2.240313 0.022247 1 -0.720617 2.514116 -0.517760 1 -1.690304 2.799960 0.950990 1 -2.481077 2.491876 -0.612860 6 2.103605 0.076950 -0.072309 6 1.850463 -1.131336 0.791457 1 2.041288 -0.865464 1.834819 1 0.826328 -1.484256 0.697463 1 2.550242 -1.930805 0.540596 6 3.536854 0.543088 -0.189302 1 3.989005 0.647914 0.798416 1 4.119845 -0.210539 -0.724058 1 3.587340 1.486201 -0.726549 1 -1.594148 0.359613 -1.869446 8 -1.501938 -1.357900 -0.964798 8 -1.401135 -2.142174 0.118938 8 1.209212 0.663471 -0.652202	**Frequencies (cm^{-1}):** 25.756, 32.466, 59.6795, 68.9403, 74.3434, 76.5639, 82.5302, 96.1902, 119.1334, 133.2616, 213.6681, 315.1372, 343.2935, 393.8668, 467.8377, 497.8666, 543.9537, 595.6251, 691.5942, 791.3941, 820.1253, 863.3732, 889.4761, 902.7117, 970.9562, 995.0567, 1042.5735, 1090.5236, 1123.6725, 1183.9596, 1245.0277, 1385.702, 1388.2064, 1388.6345, 1401.152, 1461.8246, 1464.0065, 1465.6522, 1474.9298, 1476.5967, 1489.2045, 1498.3617, 1753.8295, 1758.4496, 3022.472, 3030.7998, 3032.7043, 3076.4512, 3086.1686, 3088.6814, 3131.0123, 3138.5276, 3145.5435, 3184.5613

Compound: Mes Oxy + O_3 TS_{SYN} 2	**Energy (Hartree)** -534.761576102987
Reaction Coordinates: 6 0.235237 0.128753 -0.876663 6 1.525533 -0.410075 -0.286315 8 1.919402 -1.455627 -0.756029 6 2.258804 0.332526 0.790390 1 3.186877 -0.192158 1.001412 1 2.462271 1.358363 0.481554 1 1.639695 0.405388 1.684318 6 -1.209307 -0.355636 0.274581 6 -2.410721 -0.349245 -0.673904 1 -2.546355 0.635305 -1.116134 1 -2.318239 -1.095650 -1.462750 1 -3.303753 -0.580620 -0.090681 6 -0.825000 -1.746674 0.799407 1 -0.554332 -2.431005 -0.001767 1 -0.008977 -1.684777 1.514471 1 -1.697723 -2.147133 1.317303 1 0.035487 -0.300547 -1.852806 8 -0.043428 1.445356 -0.904818 8 -0.001699 1.968334 0.308731 8 -1.167053 0.596304 1.147129	**Frequencies (cm^{-1}):** -473.9806, 64.3865, 80.3371, 149.8119, 207.4112, 208.8863, 234.3095, 243.6465, 260.406, 282.2636, 303.2425, 353.1323, 408.7603, 466.2164, 491.2692, 547.1306, 561.5524, 607.6317, 690.6367, 802.5275, 826.8206, 916.0209, 971.5595, 996.9674, 1024.3189, 1040.1003, 1058.6034, 1065.1741, 1128.1852, 1183.1503, 1191.2676, 1239.4622, 1354.7154, 1389.29, 1397.3085, 1398.8233, 1411.8265, 1454.9541, 1464.198, 1475.5414, 1485.0414, 1494.2323, 1503.292, 1750.8556, 3034.5701, 3043.8728, 3046.3842, 3094.9725, 3103.7546, 3109.8154, 3125.5191, 3140.3013, 3143.7237, 3153.7004
IRC	

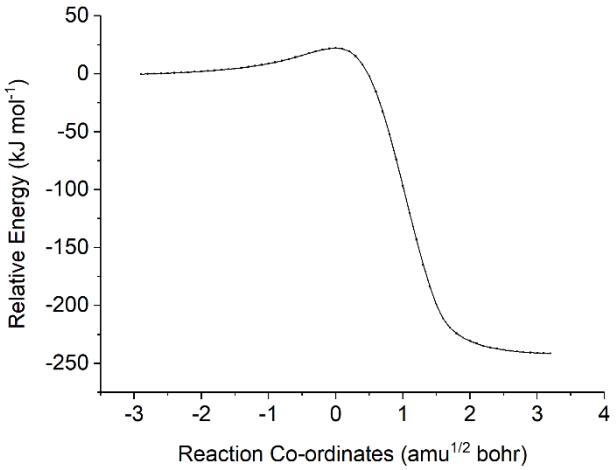


Compound: Mes Oxy + O_3 CPr_{SYN} 2	**Energy (Hartree)** -534.806174822771
Reaction Coordinates: 6 1.857919 -0.465199 1.511062 6 1.916930 -0.777898 0.051499 6 1.482819 0.205575 -0.989070 1 1.478603 -0.144055 -2.014165 8 1.171926 1.422453 -0.878352 8 1.104754 2.031304 0.333187 8 2.332920 -1.826500 -0.400871 1 2.175896 -1.341995 2.069688 1 2.492736 0.393396 1.732850 1 0.847798 -0.165359 1.785750 6 -2.195995 -0.245545 -0.018333 6 -3.479765 -1.042178 -0.061004 1 -3.293334 -2.039476 -0.449737 1 -3.894578 -1.117196 0.947091 1 -4.228155 -0.534002 -0.671796 6 -2.309012 1.213760 0.347726 1 -2.926861 1.338290 1.239070 1 -1.326214 1.653521 0.501686 1 -2.818322 1.745840 -0.460396 8 -1.127719 -0.767264 -0.270380	**Frequencies (cm^{-1}):** 24.2836, 35.5953, 43.8971, 60.4944, 66.0332, 74.8258, 91.9163, 95.5158, 148.8765, 184.1353, 242.686, 323.1557, 352.3544, 389.5705, 496.1505, 498.5493, 541.2358, 583.8794, 667.1188, 789.2391, 817.1219, 863.4568, 888.5761, 901.1413, 904.0688, 1040.6037, 1050.8463, 1090.6546, 1123.6791, 1243.4168, 1259.3988, 1360.9666, 1388.8475, 1396.3479, 1398.3708, 1441.1237, 1455.758, 1461.2233, 1466.3962, 1473.9967, 1493.8767, 1510.1376, 1735.9384, 1760.7047, 3021.7191, 3031.7938, 3047.234, 3075.6494, 3084.5583, 3107.7516, 3128.1691, 3139.7368, 3144.563, 3189.0573

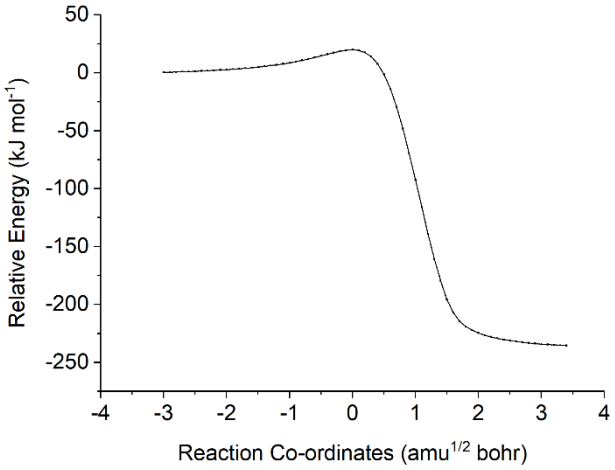
S10.13 Ozonolysis of HFO-1234yf (Alkene 11)

Compound: CF_3CFCH_2 + O_3 PRC1	**Energy (Hartree)** -739.704017975154
Reaction Coordinates: 6 2.366534 0.192348 0.000014 6 0.923971 -0.246650 -0.000202 6 -0.132815 0.538171 -0.001543 1 -0.008047 1.608388 -0.002625 1 -1.128809 0.121555 -0.001567 9 0.831934 -1.587107 0.001197 9 3.016742 -0.273685 -1.082685	**Frequencies (cm^{-1}):** 2.8018, 9.7622, 13.5268, 16.7997, 36.1499, 59.3702, 71.5957, 235.0321, 239.2738, 366.5013, 415.5494, 494.267, 570.7015, 611.3137, 680.5606, 748.0155, 762.6568, 786.9689, 945.1032, 956.0301, 1139.1849, 1151.2571, 1177.1701,

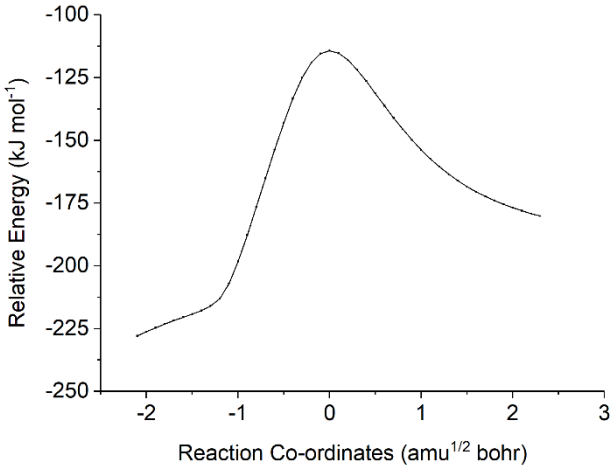
9 2.468925 1.530510 -0.001349 9 3.015716 -0.271400 1.084312 8 -4.650726 -0.099369 0.000307 8 -4.369788 1.122942 0.001566 8 -3.705628 -0.925825 -0.001709	1189.6372, 1249.9106, 1352.2013, 1426.4206, 1747.0728, 3178.2036, 3275.138

Compound: $CF_3CFCH_2 + O_3$ TS_{OZO} 1	**Energy (Hartree)** -739.686579729444
Reaction Coordinates: 6 -1.301722 -0.168739 0.139210 6 -0.069540 0.670016 -0.137723 6 0.716401 1.242251 0.813683 1 0.568747 0.983442 1.847529 1 1.293952 2.119082 0.569552 9 -2.391949 0.630610 0.158584 9 -1.511202 -1.098758 -0.793832 9 -1.208691 -0.763671 1.334270 9 -0.036038 1.134116 -1.388193 8 2.318546 -0.502838 -0.419425 8 2.518359 0.080807 0.715867 8 1.212769 -1.163515 -0.434638	**Frequencies (cm^{-1}):** -284.5197, 59.9672, 81.6435, 126.8502, 181.0213, 216.8594, 242.4476, 291.8462, 359.0811, 417.05, 477.8938, 504.9689, 573.9183, 609.601, 660.6419, 751.9521, 788.7854, 825.8995, 954.5578, 968.1963, 1067.5536, 1098.2635, 1125.741, 1168.7243, 1202.602, 1352.8469, 1412.0436, 1577.7424, 3190.092, 3293.9674
IRC:  	

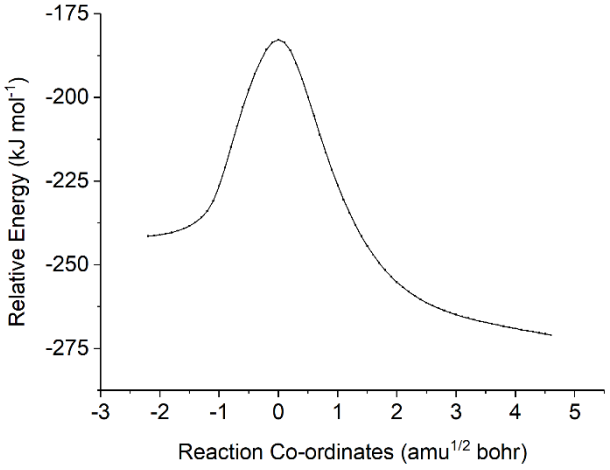
Compound: $CF_3CFCH_2 + O_3$ POZ1	**Energy (Hartree)** -739.797128378695
Reaction Coordinates: 6 -1.215887 0.208797 -0.082906 6 0.184908 -0.408426 0.129831 6 1.109475 0.363563 1.108437 1 1.506422 -0.350926 1.829824 1 0.630982 1.206286 1.599374 8 2.117299 0.878910 0.256960 8 2.252487 -0.170115 -0.691708 8 0.850401 -0.395257 -1.078096 9 -0.010116 -1.687709 0.596196 9 -1.107461 1.489756 -0.456922 9 -1.905318 -0.452814 -1.013462 9 -1.907090 0.167738 1.067673	**Frequencies (cm^{-1}):** 63.8141, 102.5079, 182.3465, 227.1793, 312.4554, 332.8409, 368.5427, 399.5693, 461.5239, 536.5317, 571.1624, 599.0191, 675.8711, 737.0759, 745.3646, 813.8926, 933.0012, 941.2868, 1022.1221, 1095.7224, 1116.7061, 1137.5328, 1185.3372, 1207.3091, 1233.585, 1346.0986, 1353.9955, 1489.0164, 3066.8896, 3150.1913

Compound: $CF_3CFCH_2 + O_3$ TS_{OZO} 2	**Energy (Hartree)** -739.688008555115
Reaction Coordinates: 6 1.242497 -0.239984 -0.128900 6 0.109980 0.759838 0.013940 6 -0.714783 1.137281 -0.997235 1 -0.668214 0.629372 -1.945531 1 -1.233867 2.079277 -0.934307 9 0.234426 1.514799 1.100668 9 1.539689 -0.846241 1.020200 9 0.937827 -1.167825 -1.048997 9 2.360425 0.396151 -0.545689 8 -2.088697 -0.921790 0.030786 8 -2.584580 0.173438 -0.433429 8 -1.273645 -0.717075 1.004812	**Frequencies (cm^{-1}):** -260.716, 60.9396, 84.7628, 121.9684, 186.6972, 210.3566, 254.1304, 288.8069, 361.1063, 423.453, 473.2666, 497.0548, 573.9981, 610.2223, 649.4718, 748.4911, 785.8867, 813.4827, 953.2475, 969.0414, 1075.8996, 1103.8236, 1123.6842, 1167.4126, 1202.5834, 1357.1061, 1411.8363, 1584.3306, 3190.0946, 3291.253
IRC:  	

Compound: $CF_3CFCH_2 + O_3$ POZ 2	**Energy (Hartree)** -739.794322813255
Reaction Coordinates: 6 1.246372 -0.168078 0.099672 6 -0.191001 0.316956 -0.195205 6 -1.091184 0.461244 1.044530 1 -1.072476 1.470358 1.444145 1 -0.852362 -0.287911 1.799581 9 1.217957 -1.364820 0.701651 9 1.966941 -0.268658 -1.016693 9 1.858619 0.698366 0.926048 9 -0.074108 1.524332 -0.844404 8 -2.114253 -0.916744 -0.309054 8 -2.365350 0.234524 0.468494 8 -0.843518 -0.586051 -1.014082	**Frequencies (cm^{-1}):** 62.5132, 89.2922, 177.374, 225.3333, 306.5514, 327.7609, 370.1787, 383.4959, 464.4149, 484.5684, 569.2694, 578.7513, 689.2232, 735.1249, 745.9715, 833.2725, 937.4981, 947.591, 1017.9447, 1056.6006, 1137.732, 1156.8917, 1178.7283, 1214.4183, 1256.9172, 1313.7162, 1367.0753, 1480.8355, 3068.2629, 3161.6058

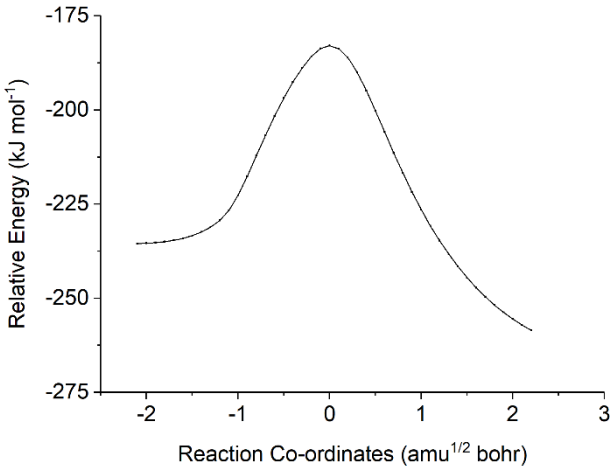
Compound: $CF_3CFCH_2 + O_3$ TS_{ANTI}	**Energy (Hartree)** -739.744889303011
Reaction Coordinates: 6 -1.323211 0.055491 -0.108681 6 0.151087 -0.199734 0.226234 6 1.308963 1.373380 -0.100397 1 0.941219 1.851850 0.820259 1 0.886258 1.748740 -1.042349 9 -1.478730 0.247354 -1.418125 9 -2.082051 -0.980191 0.269919 9 -1.743647 1.144465 0.544898 9 0.355723 -0.424299 1.511677 8 2.020397 -1.221720 -0.283984 8 2.449244 0.844360 -0.089699 8 0.766589 -0.980312 -0.633337	**Frequencies (cm^{-1}):** -424.4518, 50.0441, 116.1709, 141.132, 193.3669, 239.6595, 281.1479, 296.9608, 366.0627, 412.4421, 441.5573, 519.6081, 539.6682, 575.7821, 629.0636, 735.7756, 810.945, 840.983, 1080.5561, 1101.4987, 1155.0155, 1180.401, 1206.7092, 1226.2239, 1330.9602, 1346.3726, 1420.7761, 1557.0537, 2927.3856, 3005.0632
IRC:  	

Compound: $CF_3CFCH_2 + O_3$ C_{ANTI}	**Energy (Hartree)** -739.776841541082
Reaction Coordinates: 6 1.373556 -0.259006 -0.115945 6 0.138511 0.563762 0.231956 9 -0.185019 0.625415 1.477947 8 -0.451523 1.207739 -0.646878 8 -1.552393 1.965126 -0.283631 9 1.470007 -0.428445 -1.428662 9 2.468239 0.389625 0.320747 9 1.324429 -1.443151 0.489424 6 -2.930388 -1.078249 -0.123109 1 -3.244913 -0.024337 -0.090866 1 -3.712585 -1.838846 -0.293104 8 -1.775018 -1.396223 0.016940	**Frequencies (cm^{-1}):** 23.739, 47.6668, 51.7628, 81.1309, 98.966, 128.1685, 131.7745, 173.6461, 189.4533, 296.5251, 347.524, 369.5338, 406.7679, 514.3385, 576.5233, 664.3793, 728.5641, 857.9193, 881.2041, 1137.7419, 1178.2712, 1216.7635, 1232.8472, 1273.0752, 1403.8184, 1527.2196, 1623.8384, 1786.6602, 2911.3223, 3007.0573

Compound: $CF_3CFCH_2 + O_3$ TS_{FO} 1	**Energy (Hartree)** -739.771495440171
Reaction Coordinates: 6 -1.216967 -0.270321 -0.078312 6 0.074082 0.598053 -0.115209 6 1.217915 -0.219836 1.107939 1 1.610849 0.712920 1.495511 1 0.712108 -0.895826 1.784744 9 -1.719544 -0.359412 1.164229 9 -2.153379 0.262938 -0.866089 9 -0.944412 -1.505786 -0.508257 9 -0.200364 1.781515 0.560040 8 2.576216 -0.042854 -0.576251 8 2.010908 -0.873164 0.259414 8 0.711145 0.656297 -1.172673	**Frequencies (cm^{-1}):** -384.5764, 64.7709, 100.7807, 170.0438, 226.311, 288.4162, 306.4745, 333.9714, 370.0746, 450.9903, 483.2011, 539.9964, 582.2279, 600.527, 653.3495, 685.0321, 782.1583, 918.4408, 1020.1608, 1062.9688, 1105.8913, 1171.6779, 1193.3069, 1222.7526, 1246.8546, 1258.9605, 1484.2703, 1511.4265, 3112.1632, 3236.1854
IRC:  	

Compound: $CF_3CFCH_2 + O_3$ CPr_{FO} 1	**Energy (Hartree)** -739.812611750193
Reaction Coordinates: 6 1.276276 -0.317441 0.042768 6 0.199237 0.765686 0.278781 9 0.332320 1.754487 -0.609756 8 -0.466774 0.863601 1.257424 9 1.452943 -0.610239 -1.240654 9 2.442962 0.159259 0.528183 9 0.975427 -1.429876 0.713343 6 -2.711550 -0.451865 0.655072 1 -2.030034 -1.117147 1.167434 1 -3.638928 -0.080588 1.070988 8 -2.468023 -0.081048 -0.512669 8 -1.283662 -0.487955 -1.072029	**Frequencies (cm^{-1}):** 42.1251, 63.9575, 88.0625, 113.404, 161.9039, 192.8444, 220.1104, 240.5009, 279.5027, 379.8265, 428.5047, 513.3363, 528.5897, 586.6354, 680.5969, 693.1995, 716.2171, 802.101, 885.1881, 1024.7157, 1084.4537, 1147.2233, 1223.5333, 1243.7926, 1311.4472, 1417.8105, 1571.3513, 1851.8505, 3127.1564, 3272.4481

Compound: $CF_3CFCH_2 + O_3$ TS_{FO} 2	**Energy (Hartree)** -739.771113693420
Reaction Coordinates:	**Frequencies (cm^{-1}):**

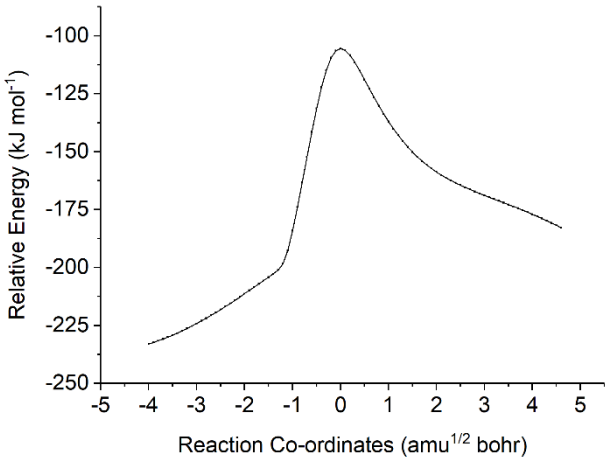
6 -1.298987 -0.198865 -0.033111 6 0.107368 0.452863 -0.197846 6 1.144499 -0.545739 0.973930 1 0.897596 -1.545399 0.634602 1 0.934082 -0.257871 1.995443 9 -1.285531 -1.449663 -0.505100 9 -1.674536 -0.244058 1.256359 9 -2.207933 0.505557 -0.707130 9 0.059625 1.695737 0.417969 8 2.550828 -0.405976 -0.680190 8 2.322631 -0.077164 0.562263 8 0.679844 0.356336 -1.287918	-378.0235, 64.8244, 111.6296, 175.0858, 229.2574, 273.908, 292.0458, 320.4111, 371.2873, 436.9077, 489.869, 537.3613, 580.4607, 591.9972, 651.465, 713.9643, 792.452, 906.042, 1012.2988, 1073.6458, 1110.1415, 1172.2038, 1190.0287, 1227.6708, 1240.8853, 1266.5903, 1481.885, 1515.8434, 3109.1164, 3237.8153
IRC  	

Compound: $CF_3CFCH_2 + O_3$ $CPr_{FO}2$	**Energy (Hartree)** -739.813259682201
Reaction Coordinates: 6 1.260836 -0.292596 -0.100143 6 0.149504 0.780864 -0.149444 9 0.297955 1.652770 0.857863 8 -0.528324 1.011186 -1.101148 9 0.919770 -1.358554 -0.820669 9 2.367461 0.250369 -0.655394 9 1.568501 -0.670948 1.136250 6 -2.843813 0.077420 -0.381769 1 -2.757537 1.070839 0.035688 1 -3.523078 -0.196672 -1.178448 8 -2.165570 -0.862809 0.084248 8 -1.243822 -0.539755 1.050455	**Frequencies (cm^{-1}):** 47.5136, 65.2631, 85.3942, 118.6927, 174.3963, 200.9237, 245.3677, 260.8967, 295.8934, 379.0472, 431.0075, 513.1768, 531.8408, 586.9013, 683.8108, 689.5254, 708.551, 800.1059, 888.7153, 1029.3867, 1075.4919, 1142.7536, 1227.7508, 1241.4539, 1305.2938, 1418.1905, 1572.9376, 1830.5607, 3129.4158, 3274.4357

Compound: $CF_3CFCH_2 + O_3$ TS_{SYN}	**Energy (Hartree)** -739.741532989524
Reaction Coordinates: 6 -1.060471 -0.333333 -0.070663 6 0.091876 0.684665 0.125441 6 1.482220 0.198652 -1.254549 1 1.873204 1.221182 -1.359152	**Frequencies (cm^{-1}):** -375.3467, 39.9264, 123.0034, 166.8233, 201.7191, 225.6332, 259.4709, 308.2617, 366.9875, 434.446, 474.8721, 485.108,

1 0.725701 -0.102745 -1.996675 9 -0.649258 -1.568473 -0.293643 9 -1.827339 -0.320315 1.030200 9 -1.804937 0.069271 -1.108354 9 -0.322645 1.926767 -0.065492 8 1.414098 -0.600232 1.332427 8 2.158210 -0.681905 -0.678618 8 0.897312 0.609188 1.157449	534.9566, 581.6948, 615.5931, 663.9282, 779.1994, 812.9961, 1093.5939, 1103.6017, 1154.7925, 1177.0012, 1215.7391, 1232.0429, 1316.4748, 1328.6756, 1437.0707, 1572.1713, 2918.396, 2990.8998

IRC



Compound: $CF_3CFCH_2 + O_3$ CPr_{SYN}	**Energy (Hartree)** -739.762725474063
Reaction Coordinates: 6 1.111331 -0.309681 0.025383 6 -0.152560 0.583121 -0.030935 6 -1.146402 0.408203 1.121136 1 -1.615137 1.379800 1.293864 1 -0.683400 0.030882 2.031464 9 1.874009 -0.126592 -1.053416 9 1.838891 -0.010053 1.116237 9 0.766359 -1.600393 0.095233 9 0.282139 1.868780 -0.116658 8 -1.934787 -0.617224 -0.797867 8 -2.068196 -0.555599 0.671125 8 -0.925549 0.337047 -1.172182	**Frequencies (cm^{-1}):** 15.633, 16.7936, 37.3743, 39.162, 59.8455, 67.599, 72.3947, 183.6602, 221.2273, 270.1777, 293.4127, 363.8324, 483.1669, 493.255, 581.7978, 630.3575, 657.9854, 778.8575, 924.4956, 1154.9874, 1197.3309, 1202.6062, 1204.5994, 1265.2001, 1396.8657, 1531.6116, 1582.1827, 1810.1959, 2892.081, 2950.9964

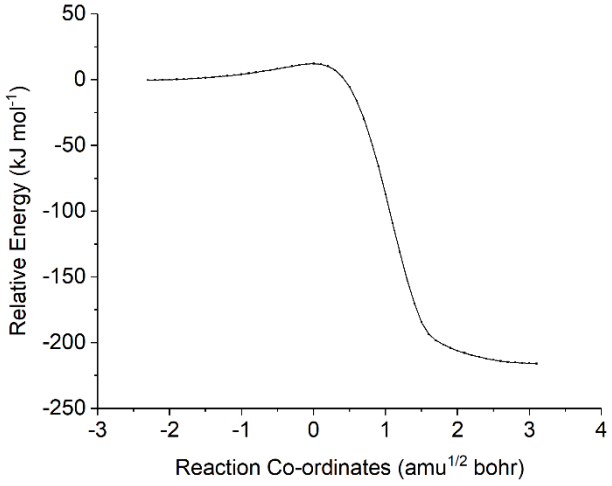
Compound: $CF_3CFCH_2 + O_3$ TS_{POZ} 1	**Energy (Hartree)** -739.781901277090
Reaction Coordinates: 6 1.111331 -0.309681 0.025383 6 -0.152560 0.583121 -0.030935 6 -1.146402 0.408203 1.121136 1 -1.615137 1.379800 1.293864 1 -0.683400 0.030882 2.031464 9 1.874009 -0.126592 -1.053416 9 1.838891 -0.010053 1.116237 9 0.766359 -1.600393 0.095233 9 0.282139 1.868780 -0.116658	**Frequencies (cm^{-1}):** -217.8941, 59.6792, 100.7244, 192.2746, 214.1565, 313.9204, 327.2066, 371.7674, 450.4214, 527.938, 571.46, 589.2847, 695.92, 711.685, 780.3448, 811.3369, 928.2147, 969.3171, 1062.8998, 1108.0534, 1115.6848, 1174.7636, 1195.1615, 1210.9755, 1223.6617,

8 -1.934787 -0.617224 -0.797867 8 -2.068196 -0.555599 0.671125 8 -0.925549 0.337047 -1.172182	1337.0756, 1371.2487, 1507.5895, 3038.0034, 3114.2192
IRC TS energy too close to POZ to perform IRC	

S10.14 Ozonolysis of HFO-1345fz (Alkene 12)

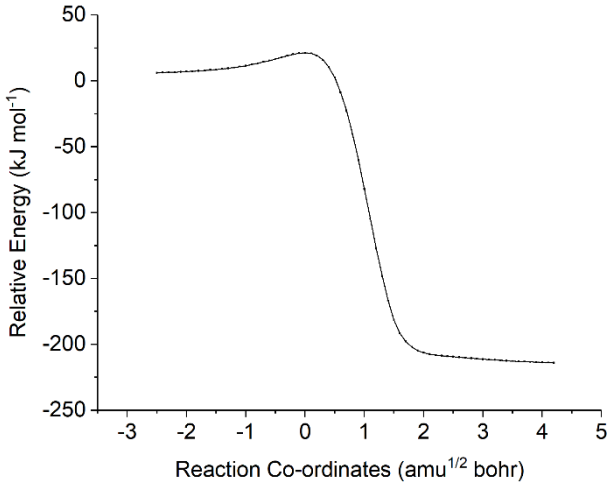
Compound: $CF_3CF_2CHCH_2$ + O_3 PRC1.1	**Energy (Hartree)** -878.141781427975
Reaction Coordinates: 6 -1.236517 0.531170 0.437861 6 0.202710 0.727240 0.080330 6 0.658224 1.800873 -0.544424 1 1.711003 1.898340 -0.767660 1 0.003235 2.606036 -0.845739 1 0.856328 -0.081124 0.379248 6 -1.919744 -0.637050 -0.328049 9 -1.243216 -1.779050 -0.126061 9 -1.938175 -0.385778 -1.643467 9 -3.177157 -0.813609 0.085559 9 -1.982329 1.642636 0.201584 9 -1.350227 0.237035 1.769143 8 4.321719 0.562966 -0.489544 8 4.492690 -0.549671 0.065234 8 3.488258 -1.146765 0.521689	**Frequencies (cm^{-1}):** 9.8792, 11.2729, 14.8647, 33.4046, 37.649, 62.9296, 70.5328, 82.022, 203.2553, 220.9725, 277.2121, 316.6621, 354.7651, 378.8707, 460.3974, 523.1339, 566.9711, 580.3836, 646.9792, 731.0786, 747.3116, 768.7346, 1008.8436, 1024.0496, 1029.8492, 1037.5318, 1125.1706, 1181.8648, 1189.7479, 1191.9055, 1245.9206, 1250.1604, 1312.9506, 1327.9285, 1454.5802, 1713.1957, 3155.2576, 3188.6359, 3242.7309

Compound: $CF_3CF_2CHCH_2$+ O_3 TS_{OZO} 1.1	**Energy (Hartree)** -878.131328640169
Reaction Coordinates: 6 -1.215445 1.487943 -0.230475 6 -0.592664 0.355700 -0.670308 6 0.437703 -0.357712 0.159101 6 1.884717 0.166613 -0.094155 1 -1.748700 2.121105 -0.921460 1 -1.005703 1.889757 0.748310 1 -0.612028 0.068625 -1.710977 9 0.460313 -1.684160 -0.131280 9 0.197680 -0.215237 1.486418 9 1.984001 1.456663 0.256261 9 2.773610 -0.532483 0.611367 9 2.191326 0.058631 -1.396079 8 -3.088362 0.690958 0.506913 8 -3.205106 -0.288126 -0.326652 8 -2.229257 -1.121016 -0.247890	**Frequencies (cm^{-1}):** -251.8685, 46.5152, 60.8627, 84.0151, 107.6669, 170.0386, 219.795, 241.4667, 259.808, 289.5022, 354.2552, 387.4531, 420.641, 469.5385, 487.4296, 530.0538, 581.2424, 610.3762, 664.4918, 736.683, 761.5447, 771.5974, 969.6046, 993.9601, 1025.0917, 1043.3897, 1076.9138, 1119.2093, 1156.7359, 1183.8756, 1195.8595, 1240.1666, 1292.5511, 1298.9294, 1449.086, 1580.0551, 3174.0227, 3207.193, 3268.0812
IRC:	



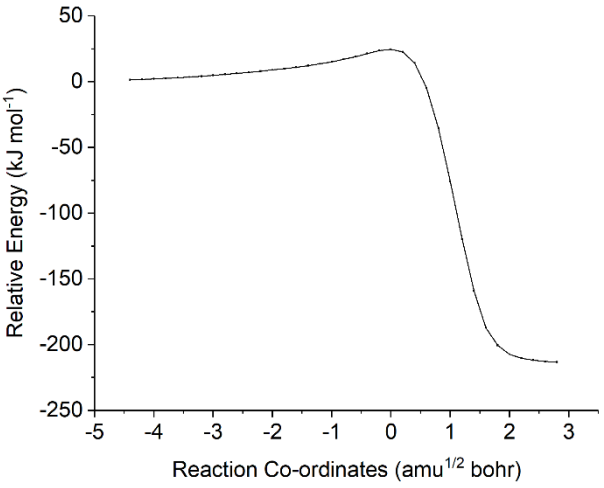
Compound: $CF_3CF_2CHCH_2$+ O_3 POZ1.1	**Energy (Hartree)** -878.225644669177
Reaction Coordinates: 6 -1.481142 -1.258772 0.092572 6 -0.813024 0.055616 0.589835 6 0.414269 0.508220 -0.211423 6 1.706948 -0.287090 0.128412 1 -1.710763 -1.906849 0.938344 1 -0.908212 -1.790948 -0.660352 1 -0.539142 -0.016498 1.643623 9 0.680623 1.810549 0.057554 9 0.201061 0.391283 -1.543453 9 1.531422 -1.598446 -0.114146 9 2.731416 0.143987 -0.602293 9 2.011509 -0.143554 1.425892 8 -2.665692 -0.799630 -0.537350 8 -3.043034 0.274244 0.323027 8 -1.817332 1.046898 0.398075	**Frequencies (cm^{-1}):** 45.3202, 62.661, 76.497, 139.4397, 217.0306, 235.8331, 262.1586, 299.416, 340.963, 369.662, 398.6802, 450.879, 525.4452, 575.0189, 603.5812, 689.4584, 720.7625, 747.7636, 769.9985, 783.6651, 928.9611, 948.9021, 1005.6814, 1017.245, 1042.937, 1071.5994, 1151.6993, 1173.7314, 1197.4637, 1234.0993, 1255.292, 1299.8876, 1324.2562, 1363.7984, 1404.4211, 1501.4561, 3055.1724, 3067.1804, 3152.2089

Compound: $CF_3CF_2CHCH_2$ + O_3 PRC1.2	**Energy (Hartree)** -878.139007095758
Reaction Coordinates: 6 1.026704 -0.582157 -0.000016 6 -0.308571 0.090153 -0.000049 6 -0.548452 1.391691 -0.000051 1 -1.568249 1.749543 -0.000077 1 0.232632 2.137417 -0.000029 1 -1.121418 -0.626289 -0.000072 6 2.295996 0.310947 0.000018 9 2.327172 1.095912 1.087324 9 2.327223 1.095921 -1.087281 9 3.395923 -0.445893 0.000040 9 1.127188 -1.395616 -1.095594 9 1.127133 -1.395619 1.095565 8 -4.387692 1.051769 -0.000005 8 -4.798327 -0.134183 0.000049 8 -3.948828 -1.057189 -0.000010	**Frequencies (cm^{-1}):** 11.5615, 14, 15.0554, 32.165, 36.956, 63.6659, 78.7207, 97.8705, 177.8762, 218.1651, 288.791, 316.0225, 347.0276, 417.7337, 426.8409, 498.3885, 573.8987, 587.3896, 651.5009, 714.8363, 747.3627, 760.936, 982.578, 1004.3847, 1030.9237, 1088.8833, 1132.288, 1182.0928, 1182.1315, 1190.001, 1197.9348, 1250.1782, 1317.758, 1376.3304, 1472.2865, 1717.7914, 3159.1586, 3169.1975, 3243.7808

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 1.2	**Energy (Hartree)** -878.127589524666
Reaction Coordinates: 6 -1.207443 -0.095965 1.565864 6 -0.633273 0.860812 0.777927 6 0.723366 0.766955 0.131258 6 1.305936 -0.642863 -0.174476 1 -2.023955 0.169511 2.218308 1 -0.740789 -1.051840 1.737809 1 -0.988212 1.881658 0.807867 9 1.626286 1.380164 0.961616 9 0.735223 1.461421 -1.033988 9 0.494998 -1.342867 -0.967933 9 1.486422 -1.334397 0.965189 9 2.491463 -0.520400 -0.775486 8 -2.602987 -1.007411 0.190110 8 -2.893329 0.053987 -0.486595 8 -1.864694 0.562394 -1.067515	**Frequencies (cm^{-1}):** -263.9454, 35.5308, 65.3488, 85.1656, 128.665, 174.9015, 218.794, 234.5999, 283.2629, 292.5673, 350.9422, 384.1623, 428.5588, 458.7717, 507.2156, 515.5332, 587.8166, 594.341, 648.2225, 733.7161, 759.2155, 770.3966, 962.6699, 981.9849, 1018.1307, 1073.5411, 1083.3322, 1115.134, 1142.1393, 1178.1561, 1184.22, 1210.6587, 1289.3436, 1359.9333, 1460.7652, 1583.6638, 3179.8362, 3190.2156, 3271.9818
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ POZ1.2	**Energy (Hartree)** -878.224904510059
Reaction Coordinates: 6 -1.675355 0.258240 1.164365 6 -0.897747 0.918648 -0.005243 6 0.628553 0.775343 0.019747 6 1.259161 -0.647392 -0.034735 1 -2.436017 0.943672 1.537411 1 -1.047100 -0.100261 1.973722 1 -1.083474 1.995728 -0.027619 9 1.066763 1.361383 1.171008 9 1.151077 1.472718 -1.020439 9 0.996262 -1.256011 -1.187670 9 2.586085 -0.546389 0.100446 9 0.794296 -1.405487 0.971202 8 -2.269915 -0.872448 0.549965 8 -2.650671 -0.329787 -0.711883	**Frequencies (cm^{-1}):** 26.4184, 66.3457, 91.8999, 160.5666, 195.1393, 223.7344, 272.0259, 322.562, 355.1185, 365.7783, 402.6798, 482.9657, 508.3151, 575.7327, 590.4381, 635.2202, 718.037, 740.6714, 761.8933, 773.9347, 930.0483, 956.3489, 996.6716, 1024.6946, 1053.4317, 1109.6471, 1140.6767, 1176.715, 1191.3975, 1215.8685, 1241.7288, 1293.7557, 1318.6713, 1361.7077, 1420.7409, 1502.8601, 3038.5984, 3064.8928, 3153.0076

8 -1.413343 0.289224 -1.170487	

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (Hartree)** -878.128995844190
Reaction Coordinates: 6 1.713899 1.434917 0.492549 6 0.646173 0.633062 0.769726 6 -0.589737 0.693833 -0.088715 6 -1.575408 -0.502993 0.045653 1 2.461077 1.629378 1.245130 1 1.721460 2.062809 -0.385028 1 0.524902 0.172874 1.738139 9 -0.285844 0.840267 -1.399610 9 -1.310264 1.802431 0.283000 9 -1.842192 -0.722884 1.345064 9 -1.072823 -1.620161 -0.478035 9 -2.722502 -0.224051 -0.578787 8 3.094709 0.067249 -0.474847 8 2.768086 -0.999907 0.171619 8 1.540409 -1.329640 -0.004049	**Frequencies (cm^{-1}):** -237.1764, 22.8776, 67.1404, 82.2527, 114.1043, 172.085, 217.9739, 233.1311, 275.5604, 298.005, 343.4735, 375.1809, 401.3593, 447.7179, 497.2209, 524.5576, 583.3496, 595.9025, 697.0222, 733.321, 758.2642, 774.5082, 970.0289, 1008.4917, 1026.4475, 1048.5436, 1081.1016, 1081.8754, 1133.2057, 1175.6821, 1206.2228, 1240.9817, 1299.8893, 1322.7218, 1450.303, 1581.572, 3172.0816, 3213.9879, 3265.9439
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ POZ1.3	**Energy (Hartree)** -878.226966377122
Reaction Coordinates: 6 2.068577 0.956273 0.424907 6 0.830250 0.038793 0.635869 6 -0.419734 0.566420 -0.075509 6 -1.679276 -0.338480 0.024652 1 2.573939 1.130579 1.374537 1 1.840008 1.895323 -0.072026 1 0.601343 -0.069467 1.697103 9 -0.181922 0.802326 -1.384024 9 -0.742677 1.755322 0.513216 9 -1.938033 -0.610743 1.314334 9 -2.737815 0.286561 -0.496450	**Frequencies (cm^{-1}):** 44.2044, 64.7431, 77.5873, 131.1057, 216.0336, 233.5827, 262.9289, 299.1599, 341.9378, 372.3824, 402.0765, 444.6021, 524.669, 577.8985, 615.9997, 669.3166, 727.9152, 739.3241, 769.659, 783.0207, 928.344, 937.8548, 1001.7575, 1036.7278, 1050.0949, 1078.9292, 1124.0817, 1186.0785, 1205.7748, 1229.4852, 1255.8886, 1294.9825, 1329.8955,

9 -1.498474 -1.487922 -0.624951 8 2.880817 0.200138 -0.457263 8 2.665696 -1.123562 0.026564 8 1.212999 -1.202123 0.060917	1359.9716, 1400.7825, 1501.3593, 3057.0616, 3068.8621, 3140.3132

Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.1	**Energy (Hartree)** -878.143298472086
Reaction Coordinates: 6 -0.932594 1.582928 -0.620343 6 -0.276634 0.434742 -0.692503 6 0.709504 -0.015349 0.339389 6 2.169642 -0.109118 -0.187234 1 -1.646993 1.858606 -1.381981 1 -0.779070 2.275501 0.195008 1 -0.419017 -0.258931 -1.510064 9 0.377873 -1.266019 0.784273 9 0.733396 0.807454 1.420355 9 2.608689 1.099555 -0.560559 9 2.223289 -0.925636 -1.251327 9 2.989423 -0.585559 0.752404 8 -3.902428 0.685743 0.363717 8 -3.710008 -0.554485 0.321410 8 -3.333620 -1.056577 -0.765770	**Frequencies (cm^{-1}):** 10.6521, 15.0289, 16.4412, 37.9615, 50.9073, 66.3684, 88.0201, 125.0772, 202.1667, 220.2032, 277.0756, 315.1452, 354.5689, 378.6379, 459.194, 522.9282, 565.7729, 580.2998, 646.2519, 729.5036, 746.9122, 768.7139, 1009.0499, 1019.8311, 1023.9611, 1037.6217, 1123.4635, 1182.9974, 1187.5537, 1193.1183, 1243.088, 1246.301, 1312.7889, 1325.6119, 1456.6463, 1707.3894, 3158.5205, 3187.7715, 3246.4749

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.1	**Energy (Hartree)** -878.131034335178
Reaction Coordinates: 6 1.190001 1.519627 0.276042 6 0.573981 0.403234 0.766992 6 -0.407965 -0.389329 -0.047815 6 -1.857677 0.183660 0.011077 1 1.671205 2.209364 0.949683 1 1.016742 1.853253 -0.735412 1 0.556887 0.195474 1.825899 9 -0.491412 -1.668799 0.396252 9 -0.051533 -0.415465 -1.360783 9 -1.896602 1.418739 -0.508256 9 -2.273020 0.248110 1.284941 9 -2.701627 -0.588439 -0.673609 8 3.155990 0.777111 -0.221302 8 2.850818 -0.461094 -0.424204 8 2.304799 -1.004587 0.604898	**Frequencies (cm^{-1}):** -262.9292, 45.7288, 60.2135, 84.718, 105.674, 172.9141, 217.8631, 228.6404, 263.5263, 291.2651, 353.8901, 388.8815, 420.9498, 476.7102, 494.8223, 533.874, 580.3525, 613.8902, 662.1593, 745.9821, 754.3414, 771.9327, 974.8388, 985.1461, 1028.2646, 1042.8705, 1074.8484, 1118.3319, 1159.8399, 1184.8255, 1195.3548, 1233.094, 1289.5409, 1296.3925, 1443.9672, 1576.2241, 3175.3436, 3211.3284, 3270.31
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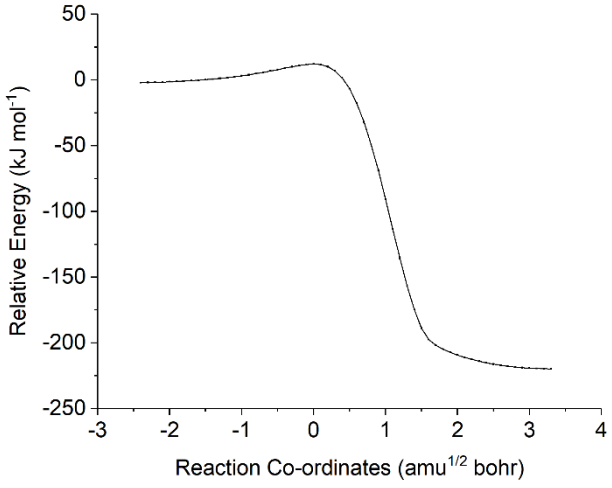
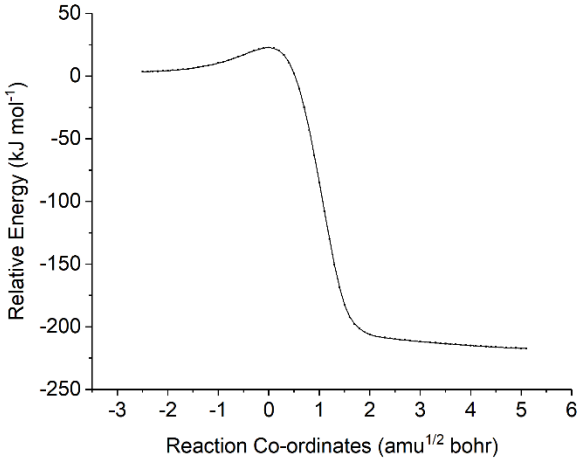


Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.1	**Energy (Hartree)** -878.226983332881
Reaction Coordinates: 6 1.442878 1.258271 0.004513 6 0.815219 -0.016401 0.635149 6 -0.418509 -0.561476 -0.102512 6 -1.684920 0.326398 0.045814 1 1.317565 2.145026 0.619956 1 1.072681 1.428004 -1.004726 1 0.549928 0.124433 1.682234 9 -0.735713 -1.778585 0.404737 9 -0.175417 -0.712927 -1.426737 9 -1.461515 1.551013 -0.463407 9 -2.723299 -0.211492 -0.587946 9 -1.997125 0.468975 1.342970 8 2.828251 0.949663 -0.010380 8 2.800007 -0.428163 -0.373580 8 1.867923 -0.970384 0.606232	**Frequencies (cm^{-1}):** 44.5308, 73.425, 86.788, 139.2935, 214.8697, 232.1562, 267.8255, 298.4755, 340.417, 367.7882, 413.0171, 458.0614, 527.6602, 571.7052, 607.1067, 672.1154, 716.83, 732.2008, 755.3072, 801.1359, 925.7964, 941.4223, 998.7884, 1005.8708, 1057.7656, 1078.5876, 1156.0363, 1172.5531, 1191.4808, 1236.9797, 1251.9412, 1294.8535, 1323.589, 1360.9366, 1397.9815, 1499.9499, 3077.0529, 3089.9436, 3144.4833

Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.2	**Energy (Hartree)** -878.143726505406
Reaction Coordinates: 6 -0.929864 0.742644 0.098633 6 0.228025 0.637060 1.039694 6 0.676909 -0.457605 1.635306 1 1.529898 -0.403150 2.295838 1 0.229543 -1.430783 1.497574 1 0.699445 1.598494 1.204854 6 -1.733109 -0.546646 -0.219955 9 -2.262288 -1.066880 0.896801 9 -0.941649 -1.472717 -0.782822 9 -2.727442 -0.275928 -1.067864 9 -0.495419 1.233600 -1.102796 9 -1.829220 1.649448 0.585606 8 3.429338 -1.168130 -0.004697 8 3.444299 -0.139455 -0.724516	**Frequencies (cm^{-1}):** 9.6204, 15.4637, 17.084, 39.1426, 48.6847, 81.7188, 94.1674, 120.5956, 176.2415, 218.0713, 288.2365, 312.2791, 347.0333, 416.5943, 426.5513, 498.0488, 573.5807, 587.0454, 651.3666, 711.0839, 747.0108, 760.9173, 981.2825, 1003.6475, 1022.1198, 1090.1209, 1132.2266, 1181.1905, 1181.5656, 1188.0612, 1199.5517, 1244.4236, 1315.5223, 1375.9186, 1473.6869, 1712.4531, 3161.4402, 3169.43, 3246.7236

8 3.425551 0.979461 -0.155871	

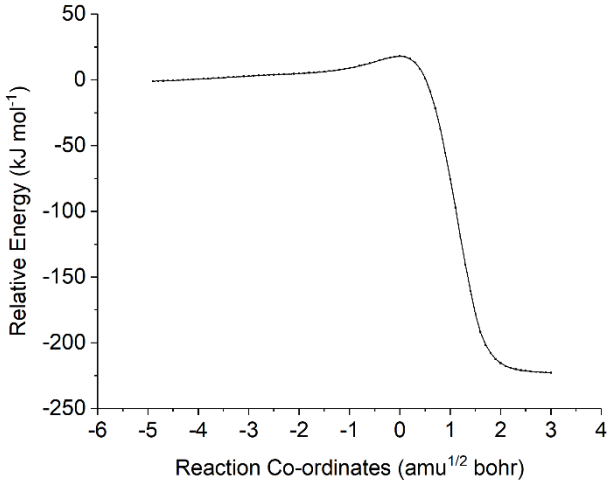
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (Hartree)** -878.128280531763
Reaction Coordinates: 6 -1.239465 0.391379 1.531729 6 -0.612711 1.089450 0.534709 6 0.744869 0.779476 -0.038223 6 1.240564 -0.693990 -0.008422 1 -2.006132 0.876879 2.112421 1 -0.841804 -0.530619 1.924335 1 -0.904376 2.109091 0.326670 9 1.672032 1.506501 0.665503 9 0.824073 1.199890 -1.325225 9 0.370853 -1.502122 -0.625510 9 1.384553 -1.120446 1.257471 9 2.421313 -0.793948 -0.618137 8 -2.853832 -0.561701 0.487473 8 -2.318223 -0.637420 -0.686826 8 -1.965776 0.516355 -1.134284	**Frequencies (cm^{-1}):** -285.7393, 36.5395, 73.0945, 81.7421, 127.9564, 176.7332, 219.3405, 230.0436, 278.0444, 296.7981, 352.9024, 382.7606, 437.3771, 470.0553, 505.9447, 528.7509, 590.0696, 592.2243, 648.3149, 747.2529, 759.8374, 764.0507, 970.0373, 977.428, 1021.7369, 1071.0593, 1080.4107, 1111.436, 1143.0665, 1177.0123, 1185.0736, 1207.1537, 1287.3031, 1359.5582, 1454.0313, 1576.4673, 3182.0756, 3193.3038, 3273.4742
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.2	**Energy (Hartree)** -878.228055342350
Reaction Coordinates: 6 -1.753991 0.622009 0.966387 6 -0.912193 0.887997 -0.314087 6 0.610684 0.771106 -0.133699 6 1.245930 -0.622362 0.145544 1 -2.296559 1.503284 1.298331 1 -1.150431 0.216446 1.775079 1 -1.072631 1.893045 -0.705907 9 0.961260 1.588028 0.902481 9 1.212799 1.247254 -1.253329 9 1.041703 -1.457757 -0.870925 9 2.563962 -0.479374 0.321006 9 0.735032 -1.165963 1.261269 8 -2.726450 -0.316842 0.521322 8 -1.993310 -1.068752 -0.447439	**Frequencies (cm^{-1}):** 47.9223, 70.352, 92.1224, 167.7802, 197.2627, 223.1259, 275.2895, 321.7806, 352.356, 362.1329, 403.2616, 497.256, 518.8909, 571.3127, 593.0343, 649.075, 699.6232, 731.5869, 761.9929, 782.781, 922.4345, 945.9983, 1000.4315, 1042.0624, 1049.2011, 1104.4041, 1143.1138, 1173.4643, 1191.6124, 1214.3423, 1234.035, 1286.8625, 1299.3839, 1359.9943, 1414.8875, 1513.0213, 3077.9226, 3084.3567, 3141.7154

8 -1.437208 -0.008778 -1.273494	

Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.3	**Energy (Hartree)** -878.140337910834
Reaction Coordinates: 6 0.795004 2.075660 0.108036 6 -0.040931 1.257416 0.728737 6 -1.261503 0.682219 0.081013 6 -1.208668 -0.862164 -0.092577 1 1.657037 2.476491 0.620558 1 0.643944 2.370312 -0.920690 1 0.103575 0.959425 1.758476 9 -1.484364 1.207540 -1.151944 9 -2.363713 0.946406 0.845648 9 -2.339578 -1.326949 -0.626094 9 -1.023752 -1.454740 1.096548 9 -0.189596 -1.204499 -0.895707 8 3.367671 0.318026 -0.828464 8 3.065269 -0.722233 -0.193697 8 2.879692 -0.625148 1.043955	**Frequencies (cm^{-1}):** 13.9294, 17.4663, 21.143, 36.2041, 47.8907, 67.9227, 90.8125, 122.6484, 200.0749, 220.2201, 278.3247, 314.4285, 354.3369, 378.6923, 458.762, 522.8694, 566.1051, 580.0621, 647.0074, 729.5473, 747.2036, 768.623, 1009.6519, 1020.0518, 1024.0725, 1036.5779, 1126.4821, 1179.1538, 1186.1086, 1193.9366, 1243.7111, 1246.7655, 1313.2581, 1325.3967, 1456.6071, 1707.6325, 3158.9084, 3186.796, 3246.8065

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.3	**Energy (Hartree)** -878.126204877084
Reaction Coordinates: 6 1.725996 1.406097 0.608681 6 0.625259 0.628467 0.826305 6 -0.502386 0.622687 -0.171026 6 -1.629617 -0.413389 0.099380 1 2.396558 1.631522 1.421347 1 1.825206 1.992884 -0.292200 1 0.408208 0.234515 1.806443 9 -0.044261 0.428631 -1.435438 9 -1.118405 1.848215 -0.160925 9 -2.637246 -0.232219 -0.757251 9 -2.097729 -0.247820 1.349036 9 -1.189988 -1.665712 -0.022331 8 3.205691 -0.014517 -0.087376 8 2.410578 -0.931317 -0.526751 8 1.614127 -1.366910 0.379946	**Frequencies (cm^{-1}):** -253.9467, 27.6194, 64.3472, 80.5302, 113.2473, 173.37, 213.4668, 220.4703, 280.9776, 289.7567, 346.3492, 374.4681, 411.7751, 455.2236, 502.1917, 530.3331, 582.8332, 594.3762, 701.1745, 738.0915, 752.4013, 770.3841, 967.9284, 1002.9547, 1020.8741, 1053.7359, 1078.6464, 1084.8731, 1131.3627, 1176.2823, 1204.3163, 1234.519, 1297.3635, 1324.4983, 1447.4626, 1578.5854, 3171.7828, 3218.6068, 3267.756
IRC:	

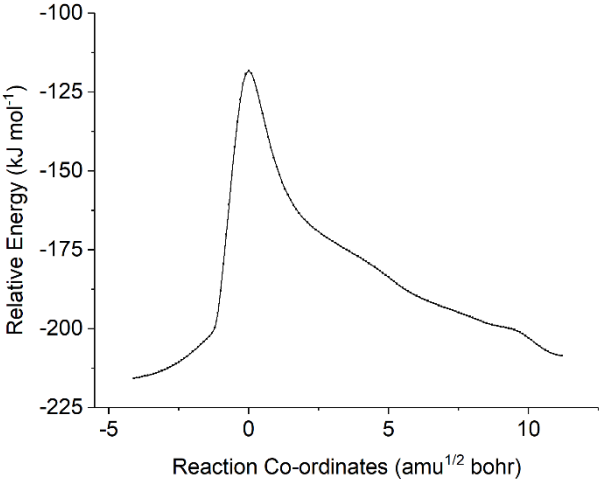


Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.3	**Energy (Hartree)** -878.225983904001
Reaction Coordinates: 6 2.056416 0.986667 0.368416 6 0.824289 0.076107 0.641117 6 -0.398124 0.514901 -0.176605 6 -1.698059 -0.290814 0.095034 1 2.340342 1.586491 1.228686 1 1.900558 1.613565 -0.508659 1 0.548207 0.061794 1.694332 9 -0.151821 0.461339 -1.504464 9 -0.665231 1.814676 0.150593 9 -1.981543 -0.262259 1.408580 9 -2.723271 0.247131 -0.569630 9 -1.563316 -1.562480 -0.281660 8 3.098750 0.048031 0.150622 8 2.413600 -0.979693 -0.561864 8 1.271449 -1.226923 0.309629	**Frequencies (cm^{-1}):** 40.2086, 64.8579, 92.6896, 130.8291, 215.699, 233.8287, 263.8061, 298.2783, 338.1326, 366.5094, 416.226, 449.4973, 527.6184, 576.3057, 621.4072, 673.0262, 711.5844, 729.5339, 761.9613, 791.1097, 920.7236, 935.2848, 1000.7288, 1023.8434, 1042.6045, 1102.1431, 1120.645, 1184.4084, 1204.4831, 1235.6017, 1246.8055, 1286.151, 1330.6358, 1356.0678, 1395.4919, 1503.4997, 3069.5139, 3095.9757, 3141.8284

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 1	**Energy (Hartree)** -878.185149537149
Reaction Coordinates: 6 1.612496 1.405798 0.314271 6 0.837940 -0.264420 -0.380427 6 -0.528258 -0.644643 0.157072 6 -1.633877 0.409704 -0.138454 1 1.015795 2.046698 -0.350830 1 1.267541 1.351895 1.354912 1 0.902242 -0.009853 -1.430866 9 -0.926553 -1.805578 -0.434267 9 -0.489535 -0.849859 1.490720 9 -1.639719 0.707904 -1.446555 9 -2.826838 -0.068308 0.200560 9 -1.410288 1.534514 0.551429 8 2.838403 1.251797 0.055367 8 2.956864 -0.761507 -0.457306	**Frequencies (cm^{-1}):** -410.7211, 35.4565, 64.4701, 115.9392, 125.4556, 173.8612, 218.8248, 245.5775, 253.8434, 315.9323, 358.4816, 372.6244, 430.4355, 473.984, 513.1193, 535.4215, 549.7502, 596.4287, 636.982, 737.5812, 828.4935, 880.1703, 973.5688, 1016.4138, 1104.2432, 1134.2492, 1154.4767, 1186.1443, 1200.9677, 1222.2792, 1233.9885, 1271.9367, 1322.1525, 1401.7932, 1409.8475, 1552.8677, 2934.544, 3011.2965, 3171.3174

8 1.794858 -1.052218 0.083816	

IRC:

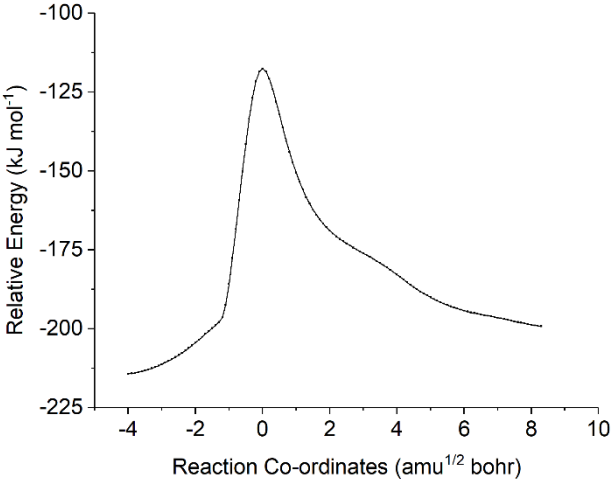


Compound: $CF_3CF_2CHCH_2 + O_3$ C_{ANTI} 1	**Energy (Hartree)** -878.217442305939
Reaction Coordinates: 6 3.048840 1.215818 0.049682 6 0.661739 -0.731100 -0.475519 6 -0.808800 -0.758565 -0.128847 6 -1.434687 0.651626 0.103462 1 3.348346 1.146331 1.105979 1 3.841941 1.042215 -0.692375 1 1.011076 -0.371252 -1.432560 9 -1.459947 -1.321298 -1.183655 9 -1.035188 -1.503236 0.967504 9 -1.217617 1.424994 -0.963443 9 -2.751119 0.528514 0.286276 9 -0.900279 1.220540 1.181478 8 1.926148 1.543153 -0.275686 8 2.778940 -1.223478 0.057381 8 1.454092 -1.223375 0.359910	**Frequencies (cm^{-1}):** 21.7524, 60.3706, 63.2349, 75.8706, 95.2498, 154.9196, 184.6019, 220.5153, 241.4755, 261.6599, 286.006, 330.7034, 356.1271, 379.0355, 406.0506, 425.2923, 482.7281, 531.3688, 590.3276, 624.549, 730.5959, 831.2543, 886.1366, 958.6118, 1056.2563, 1132.043, 1175.7641, 1198.7188, 1216.4605, 1237.2984, 1258.4791, 1297.208, 1348.1177, 1524.3012, 1551.6116, 1743.374, 2940.2776, 3007.3874, 3218.2102

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -878.187251466993
Reaction Coordinates: 6 1.966336 -1.004623 -0.793336 6 0.877978 -0.227355 0.626175 6 -0.607672 -0.519929 0.538832 6 -1.458151 0.363697 -0.422064 1 1.922495 -2.016733 -0.365983 1 1.318987 -0.831328 -1.661459 1 1.384914 -0.717993 1.449605 9 -1.150771 -0.397179 1.779967 9 -0.761142 -1.813031 0.156231 9 -0.953889 0.324898 -1.661447 9 -2.707778 -0.101050 -0.456291	**Frequencies (cm^{-1}):** -418.4449, 42.1802, 67.3174, 96.8445, 140.51, 157.2943, 218.5922, 244.9642, 265.3093, 338.641, 354.149, 383.3285, 415.4344, 484.7322, 516.8936, 525.7433, 550.6504, 599.7717, 643.4242, 710.69, 790.3154, 857.6712, 987.1169, 1100.2156, 1105.816, 1121.6389, 1153.3489, 1183.3814, 1199.6355, 1213.1668, 1223.1965, 1270.6172, 1328.4843,

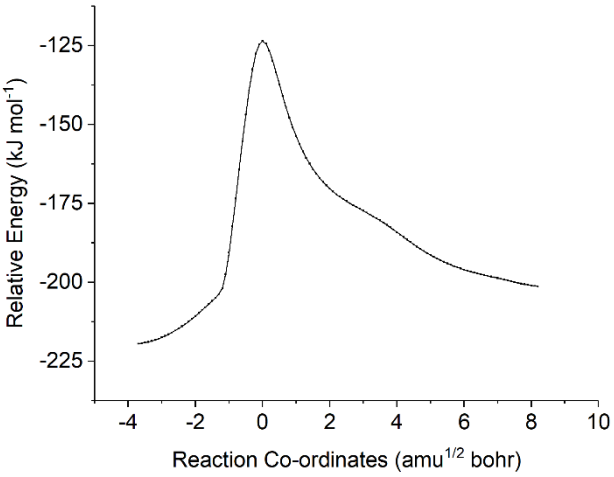
9 -1.482514 1.628950 -0.002941 8 3.042357 -0.349928 -0.681955 8 2.512040 1.207831 0.594122 8 1.221540 1.031100 0.405397	1399.8279, 1411.3928, 1555.0234, 2939.2028, 3020.7832, 3153.4617

IRC:



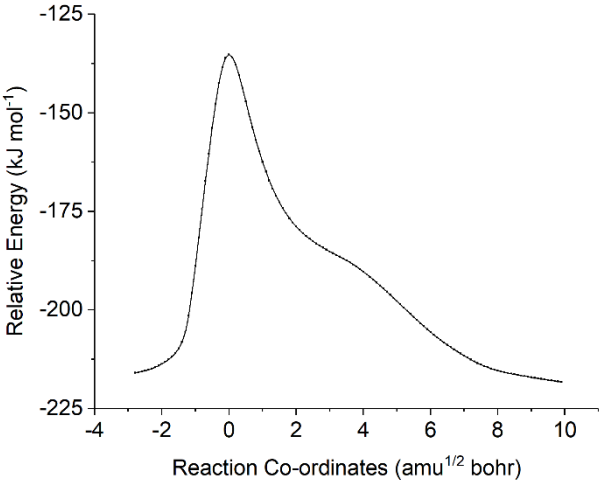
Compound: $CF_3CF_2CHCH_2 + O_3$ C_{ANTI} 2	**Energy (Hartree)** -878.217388987709
Reaction Coordinates: 6 4.394194 -0.177693 -0.000004 6 0.672116 0.052462 0.000003 6 -0.649639 -0.666423 0.000002 6 -1.934170 0.211555 -0.000002 1 4.049553 0.868288 -0.000004 1 5.482420 -0.360222 -0.000009 1 1.612244 -0.503398 0.000004 9 -0.694170 -1.469284 1.095482 9 -0.694167 -1.469289 -1.095474 9 -1.971869 0.984001 -1.088518 9 -3.007717 -0.580834 -0.000003 9 -1.971873 0.984004 1.088510 8 3.610859 -1.095812 0.000000 8 1.847087 1.969757 0.000003 8 0.669423 1.305873 0.000002	**Frequencies (cm^{-1}):** 16.9931, 55.0188, 55.4791, 72.1958, 100.2692, 107.152, 130.0457, 158.8648, 178.3775, 213.4398, 233.9815, 259.0309, 337.4695, 368.9536, 379.8365, 393.6261, 481.6903, 529.9689, 591.7952, 643.7123, 693.9922, 788.9396, 961.106, 973.3076, 1112.7973, 1113.4334, 1183.9023, 1207.3913, 1212.1435, 1222.0298, 1276.1492, 1339.8434, 1379.57, 1524.0824, 1554.2167, 1784.9011, 2914.7637, 3003.6302, 3062.3179

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 3	**Energy (Hartree)** -878.184687501881
Reaction Coordinates: 6 -2.345072 1.105757 0.145356 6 -0.815259 -0.086648 0.334580 6 0.468832 0.548060 -0.156328 6 1.746941 -0.296727 0.132539 1 -2.082227 1.699453 1.033050 1 -2.107105 1.570289 -0.820617 1 -0.906889 -0.255542 1.400399 9 0.621035 1.734336 0.487215	**Frequencies (cm^{-1}):** -412.4762, 41.8326, 58.7804, 90.3238, 128.5461, 185.4369, 192.8816, 226.1049, 275.034, 345.0588, 361.8574, 383.1289, 414.4096, 463.164, 507.0612, 531.4281, 550.6522, 592.2678, 639.2766, 736.1057, 826.1605, 873.4859, 983.9466, 1028.1781, 1104.0411, 1145.7766, 1167.3253,

9 0.420827 0.778813 -1.485030 9 1.683176 -1.464660 -0.510783 9 2.836379 0.358316 -0.263067 9 1.839245 -0.535555 1.448681 8 -3.315588 0.300361 0.224814 8 -2.385323 -1.563523 0.043574 8 -1.279388 -1.046600 -0.448745	1193.4624, 1204.8899, 1220.4882, 1237.2047, 1268.1015, 1300.6037, 1400.8299, 1406.6919, 1555.1306, 2932.9204, 3006.928, 3169.3833
IRC:  	

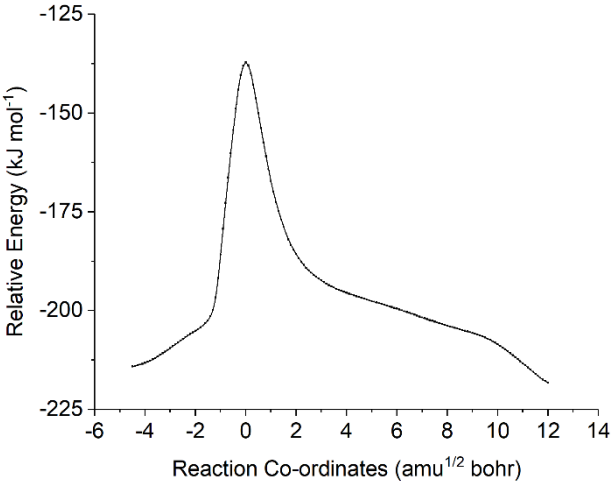
Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 3	**Energy (Hartree)** -878.213470266616
Reaction Coordinates: 6 -3.660603 -0.402862 -0.146371 6 -0.660991 0.224629 -0.324135 6 0.552941 -0.483533 0.232565 6 1.888943 0.208297 -0.183610 1 -4.060109 -0.146242 0.845585 1 -4.171068 0.050592 -1.008480 1 -0.981266 0.078276 -1.345589 9 0.574684 -1.740085 -0.265991 9 0.515122 -0.536276 1.576324 9 1.940055 1.444020 0.320478 9 2.931416 -0.487519 0.260144 9 1.953980 0.286935 -1.520578 8 -2.760262 -1.207459 -0.283687 8 -2.350940 1.660708 -0.051902 8 -1.232124 1.051066 0.423637	**Frequencies (cm^{-1}):** 24.6187, 52.1716, 58.6166, 67.0842, 89.6055, 144.1909, 188.1244, 220.5349, 254.9541, 263.2544, 292.0326, 345.4654, 356.6234, 391.333, 411.4932, 417.8418, 479.632, 533.8024, 588.296, 632.7926, 724.4713, 815.479, 893.2168, 963.0413, 1051.1914, 1161.8621, 1172.1598, 1193.9585, 1205.8268, 1238.8724, 1257.4394, 1293.2058, 1347.1651, 1522.9163, 1551.0644, 1734.9883, 2942.7355, 3010.641, 3218.3356

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.1	**Energy (Hartree)** -878.191870642997
Reaction Coordinates: 6 -1.666865 -1.289336 0.341985 6 -0.725088 0.370932 0.804177 6 0.435314 0.536746 -0.220010	**Frequencies (cm^{-1}):** -393.1971, 31.1371, 62.7836, 100.741, 150.7392, 184.3902, 217.74, 260.0773, 288.8735, 313.8745, 352.3384, 380.4285,

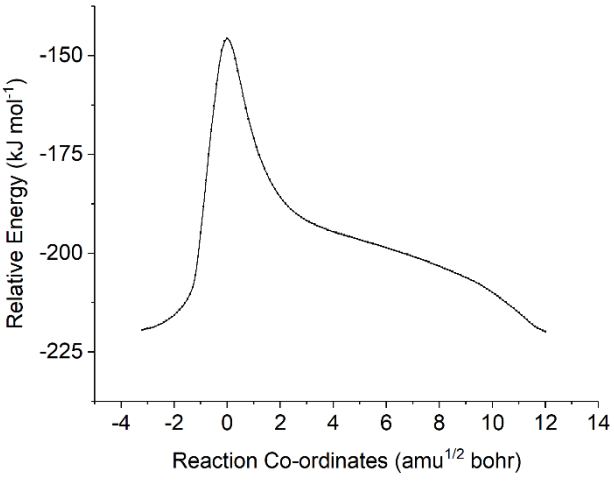
6 1.690657 -0.317508 0.099447 1 -2.123190 -1.414883 1.314952 1 -0.992406 -2.038994 -0.047244 1 -0.393642 -0.005060 1.782973 9 0.044080 0.239665 -1.483050 9 0.837415 1.830946 -0.208199 9 1.384855 -1.631341 0.082254 9 2.152205 -0.020608 1.322503 9 2.659491 -0.104727 -0.787252 8 -2.434965 -0.765991 -0.593506 8 -3.235791 0.153951 -0.106023 8 -1.653905 1.215606 0.756957	442.412, 492.131, 525.0755, 570.4812, 580.6364, 589.256, 643.7908, 735.0275, 783.2452, 894.111, 938.5579, 1007.4483, 1059.3028, 1118.3931, 1152.071, 1161.248, 1179.2866, 1221.0667, 1238.6421, 1275.1796, 1322.0673, 1365.0007, 1483.7941, 1491.8188, 2959.746, 3125.0961, 3254.9611
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (Hartree)** -878.221138678696
Reaction Coordinates: 6 -1.127851 0.398599 0.511237 6 -0.321163 1.497445 -0.235536 1 0.761698 1.297807 -0.305131 8 -0.863444 2.473644 -0.663389 6 -1.343320 -0.883951 -0.331068 9 -0.156999 -1.383201 -0.713432 9 -2.055717 -0.601205 -1.426859 9 -1.989036 -1.818183 0.371020 9 -0.423100 0.046817 1.623969 9 -2.333109 0.857322 0.892356 6 4.420411 -0.678201 0.171644 1 5.164636 -0.104241 -0.367507 1 4.610808 -1.595150 0.711612 8 3.234814 -0.279768 0.193807 8 2.918136 0.866660 -0.462933	**Frequencies (cm^{-1}):** 9.9051, 12.4069, 18.7233, 31.9423, 44.5688, 63.7407, 84.3027, 93.5374, 203.5268, 212.684, 260.1576, 310.3685, 357.3105, 378.0548, 446.7042, 530.4741, 535.3708, 576.4928, 599.5383, 676.9456, 721.7579, 788.3761, 899.9906, 936.3491, 979.9024, 1087.8306, 1136.1265, 1183.1457, 1192.8531, 1228.1979, 1241.8796, 1317.3742, 1408.8512, 1433.6968, 1555.5953, 1822.9888, 2964.0595, 3115.8508, 3265.9796

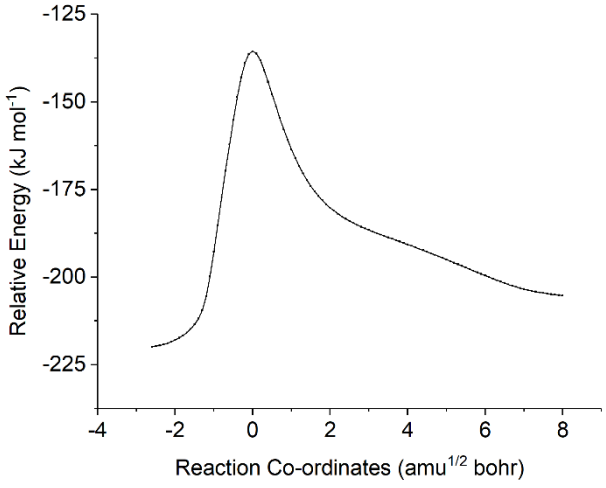
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.2	**Energy (Hartree)** -878.196099775528
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.094798 0.846546 -0.674941 6 0.761663 0.841902 0.715865 6 -0.646809 0.767107 0.069133 6 -1.274914 -0.642008 -0.106711 1 2.869109 1.319642 -0.084878 1 1.727584 1.323564 -1.573077 1 0.967892 1.888075 0.999725 9 -1.481216 1.482063 0.872790 9 -0.658715 1.380310 -1.149786 9 -1.466579 -1.232198 1.070607 9 -0.486798 -1.413664 -0.863510 9 -2.461421 -0.526940 -0.720049 8 2.194662 -0.466016 -0.804158 8 2.624129 -1.026037 0.303730 8 1.158653 -0.085285 1.468887	-396.6204, 26.3368, 70.6211, 94.7554, 158.1296, 191.2392, 221.2302, 266.7036, 294.3232, 308.1402, 351.6752, 395.1605, 456.6452, 500.3507, 515.6803, 570.5036, 585.725, 596.2072, 638.9174, 687.5652, 761.9465, 893.7987, 942.6459, 1060.1255, 1090.7246, 1105.47, 1141.5147, 1160.4382, 1192.1456, 1212.507, 1234.6097, 1273.4461, 1292.0787, 1363.3247, 1484.599, 1495.7038, 2922.8539, 3121.0855, 3249.1406
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (Hartree)** -878.220855101528
Reaction Coordinates: 6 -4.464489 -0.674308 0.169090 6 0.302588 1.484384 -0.232614 6 1.129161 0.400057 0.513572 6 1.373472 -0.875042 -0.332094 1 -5.180345 -0.132666 -0.437669 1 -4.684375 -1.555110 0.755998 1 -0.776307 1.264761 -0.303658 9 2.323374 0.882420 0.900374 9 0.427911 0.030446 1.622686 9 2.087756 -0.575269 -1.422030 9 0.198785 -1.393801 -0.724002 9 2.031359 -1.800253 0.370620 8 -3.278646 -0.279146 0.219613 8 -2.926252 0.822947 -0.492361 8 0.826644 2.471273 -0.658655	**Frequencies (cm^{-1}):** 10.0669, 15.4785, 23.4823, 30.9468, 46.1634, 64.8526, 84.1569, 93.8584, 204.104, 213.1544, 260.1363, 310.4732, 357.4415, 378.2179, 447.023, 530.8074, 535.4789, 576.5496, 599.6859, 676.978, 721.7174, 788.3689, 900.2447, 936.4886, 979.7705, 1088.1542, 1135.9008, 1183.2657, 1193.3651, 1228.4107, 1241.8521, 1317.5969, 1408.674, 1434.5642, 1555.3283, 1823.2457, 2964.8668, 3116.4954, 3266.5907

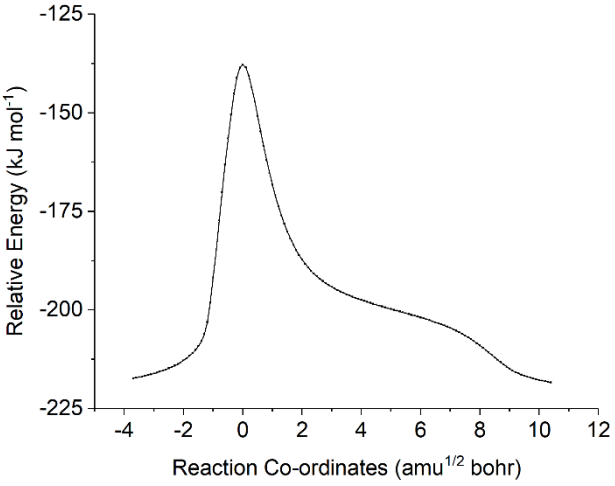
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.3	**Energy (Hartree)** -878.192619327385
Reaction Coordinates: 6 2.245427 0.876409 0.628119 6 0.684157 -0.268750 0.775865 6 -0.386278 0.443243 -0.082249 6 -1.780395 -0.238774 -0.002071 1 2.720228 0.526629 1.535419 1 1.963406 1.915704 0.525608 1 0.543607 -0.070562 1.849480 9 -0.550064 1.721333 0.374541 9 -0.027498 0.501447 -1.380634 9 -2.169157 -0.317951 1.282191 9 -1.738315 -1.468742 -0.510966 9 -2.689406 0.473600 -0.674380 8 2.705230 0.362347 -0.498633 8 3.017779 -0.905128 -0.358939 8 1.122649 -1.386185 0.401916	**Frequencies (cm^{-1}):** -387.224, 40.8521, 60.8481, 102.0519, 125.633, 205.2782, 221.084, 243.5904, 287.5039, 295.9966, 354.0148, 396.8541, 442.87, 501.4165, 521.9906, 572.1916, 586.5832, 597.2737, 646.4937, 725.0205, 777.0694, 893.3888, 950.9197, 1013.5516, 1063.7946, 1116.749, 1148.5615, 1178.8286, 1204.3342, 1221.6653, 1234.3162, 1272.5252, 1306.4089, 1341.2321, 1483.7214, 1493.8895, 2952.7844, 3120.4829, 3247.478
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.3	**Energy (Hartree)** -878.221083896414
Reaction Coordinates: 6 4.818140 -0.713634 -0.000040 6 0.002613 1.242162 -0.000030 6 -0.622367 -0.173889 0.000059 6 -2.168191 -0.250615 -0.000021 1 5.585452 0.051365 0.000374 1 4.999893 -1.779274 -0.000352 1 1.107161 1.209102 0.000026 9 -0.165549 -0.832889 -1.098182 9 -0.165671 -0.832701 1.098461 9 -2.665880 0.340964 -1.088860 9 -2.666002 0.341147 1.088663 9 -2.561854 -1.532495 0.000065 8 3.613734 -0.375618 -0.000184 8 3.305790 0.947831 0.000184 8 -0.650658 2.245092 -0.000146	**Frequencies (cm^{-1}):** 8.1377, 9.3044, 20.1166, 33.9614, 46.0446, 77.4805, 89.4291, 107.201, 156.0501, 213.7851, 274.0906, 313.6535, 345.7037, 417.0359, 426.8573, 511.0041, 530.4766, 582.0183, 586.7174, 676.9538, 686.0654, 766.2192, 899.5497, 980.1265, 1004.8218, 1096.4291, 1139.3452, 1169.4056, 1201.4159, 1207.1122, 1241.8379, 1318.4059, 1409.1012, 1449.7151, 1555.6054, 1823.6133, 2948.414, 3115.8774, 3265.981

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.1	**Energy (Hartree)** -878.192105449945
Reaction Coordinates: 6 1.559851 -1.210906 -0.131505 6 0.768319 0.401727 0.688087 6 -0.535512 0.640661 -0.123841 6 -1.648189 -0.423435 0.068139 1 1.197574 -2.114130 0.339566 1 1.270897 -0.969169 -1.145767 1 0.586566 -0.015092 1.687784 9 -1.065397 1.820991 0.288692 9 -0.281316 0.741784 -1.450002 9 -1.246344 -1.619571 -0.406319 9 -1.926557 -0.570775 1.371575 9 -2.762172 -0.076883 -0.571436 8 2.805804 -0.938795 0.198755 8 3.216005 0.182329 -0.354400 8 1.679970 1.255240 0.533212	**Frequencies (cm^{-1}):** -401.2565, 36.8365, 72.6064, 95.2189, 142.1401, 199.2199, 220.0017, 278.125, 284.5553, 313.1287, 349.9672, 388.187, 438.3785, 472.703, 525.2997, 561.361, 589.528, 601.9336, 607.2616, 732.9412, 800.9593, 891.0291, 940.4118, 1013.355, 1061.0385, 1109.6247, 1143.8764, 1165.1707, 1175.4003, 1218.8912, 1241.8796, 1277.953, 1323.3761, 1367.9756, 1477.5558, 1488.5312, 2979.7272, 3123.4258, 3253.5784
IRC:  	

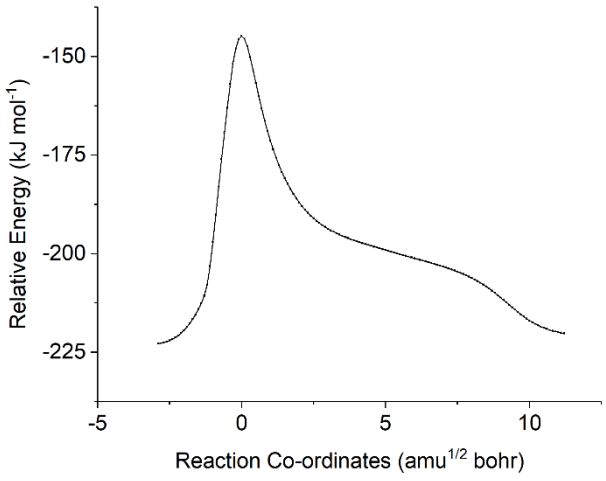
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.1	**Energy (Hartree)** -878.219669309907
Reaction Coordinates: 6 -3.956913 0.587962 0.726644 6 -0.335898 0.448274 -0.199479 6 1.190537 0.520499 -0.453858 6 1.980699 -0.567731 0.322353 1 -3.179069 1.240779 1.100199 1 -5.005860 0.628525 0.995080 1 -0.853032 -0.362041 -0.738463 9 1.395031 0.311367 -1.781136 9 1.674332 1.728212 -0.116751 9 1.833382 -0.386876 1.636183 9 1.500242 -1.779805 0.002799 9 3.275433 -0.524009 0.017009 8 -3.566597 -0.285081 -0.086142 8 -4.461933 -1.156933 -0.611095	**Frequencies (cm^{-1}):** 5.951, 26.3097, 35.9769, 41.4905, 66.8022, 84.5972, 92.6116, 121.1413, 201.9541, 211.8061, 268.7564, 308.9315, 357.0317, 382.4642, 450.5368, 530.4239, 537.3527, 577.227, 598.6507, 697.2893, 724.1617, 792.4988, 908.2894, 927.0687, 982.6487, 1079.1366, 1144.2595, 1187.5628, 1203.0546, 1237.1323, 1248.7182, 1314.3492, 1395.561, 1398.7189, 1536.9809, 1822.9769, 2983.3175, 3111.8514, 3263.0469

8 -0.888766 1.244354 0.503022	

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.2	**Energy (Hartree)** -878.192918747499
Reaction Coordinates: 6 -1.877602 0.656085 -0.883716 6 -0.775433 0.656732 0.720181 6 0.673246 0.738934 0.179340 6 1.371336 -0.600619 -0.182707 1 -1.253273 0.000541 -1.474788 1 -2.067428 1.666195 -1.220418 1 -1.080160 1.644797 1.099699 9 0.729549 1.545783 -0.921751 9 1.424186 1.336973 1.140673 9 2.577906 -0.350413 -0.706212 9 0.650960 -1.266506 -1.102127 9 1.526521 -1.371968 0.887317 8 -2.941209 0.101973 -0.331651 8 -2.672450 -1.105864 0.114773 8 -1.152654 -0.379002 1.331354	**Frequencies (cm^{-1}):** -404.7679, 52.4352, 69.6298, 86.2313, 164.8344, 178.1855, 220.0956, 273.4951, 300.5241, 310.6259, 352.2768, 394.094, 462.5867, 483.6803, 513.296, 547.7329, 590.2925, 596.7691, 636.4384, 674.401, 767.3964, 893.1762, 957.956, 1060.4836, 1085.0359, 1101.403, 1140.7811, 1152.2147, 1185.7532, 1214.7865, 1235.5117, 1274.3196, 1301.7635, 1371.3658, 1482.6163, 1494.3566, 2946.8638, 3128.8965, 3253.5307
IRC:  	

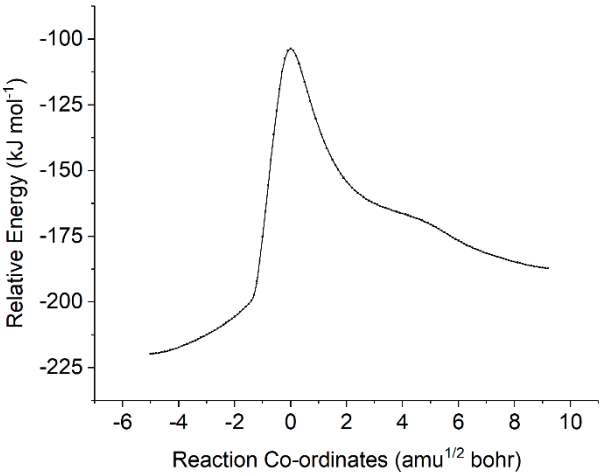
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.2	**Energy (Hartree)** -878.221532816887
Reaction Coordinates: 6 -0.688421 0.358814 0.639415 6 -0.108828 1.653597 0.016278 1 0.589393 2.170566 0.691742 8 -0.449135 2.064190 -1.052393 6 -1.350142 -0.639479 -0.343206 9 -1.750600 -1.733706 0.320799 9 -0.462850 -1.022178 -1.275018 9 -2.407295 -0.101001 -0.943556 9 0.289018 -0.306073 1.308977 9 -1.624074 0.735126 1.552939 6 2.974235 -1.293367 -0.138181	**Frequencies (cm^{-1}):** 24.8851, 29.2079, 47.5469, 59.3746, 63.7761, 80.287, 109.3165, 140.38, 165.112, 214.5639, 274.9771, 322.8784, 347.1834, 410.0588, 437.9375, 511.9743, 525.583, 581.7893, 586.5209, 677.597, 684.7822, 765.6862, 893.9743, 949.9735, 988.5189, 1093.7273, 1128.1754, 1162.8397, 1193.117, 1213.1953, 1243.7259, 1311.9298, 1410.9521,

1 3.575685 -2.047910 0.349617 1 2.199101 -1.490973 -0.868579 8 3.223969 -0.113744 0.194079 8 2.509789 0.892231 -0.378673	1419.1031, 1557.7245, 1831.4776, 2992.5806, 3117.9217, 3266.2286

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.3	**Energy (Hartree)** -878.195879308203
Reaction Coordinates: 6 2.158658 1.013020 -0.205478 6 0.716879 -0.241519 -0.589277 6 -0.449267 0.438904 0.163132 6 -1.817840 -0.253680 -0.086841 1 2.177110 1.816480 -0.929235 1 1.875872 1.212358 0.820308 1 0.658676 -0.076407 -1.674515 9 -0.235195 0.460586 1.496295 9 -0.576501 1.729447 -0.268255 9 -2.799941 0.424062 0.514533 9 -1.809735 -1.501259 0.378973 9 -2.070985 -0.287748 -1.405364 8 3.146926 0.156142 -0.378230 8 3.077463 -0.835582 0.483332 8 1.159233 -1.335382 -0.149029	**Frequencies (cm^{-1}):** -395.2815, 51.339, 61.1772, 89.5926, 125.2833, 210.8998, 218.8086, 252.3359, 293.2252, 300.2598, 354.7231, 395.296, 448.318, 482.756, 524.7101, 562.0803, 590.0082, 598.2503, 639.6327, 714.7967, 785.4388, 896.3058, 959.4529, 1015.0878, 1064.3098, 1119.0588, 1143.6651, 1180.3723, 1201.9183, 1216.6423, 1236.9696, 1271.4747, 1308.5925, 1355.8902, 1481.1959, 1489.7891, 2971.4078, 3119.0066, 3246.9931
IRC:  	

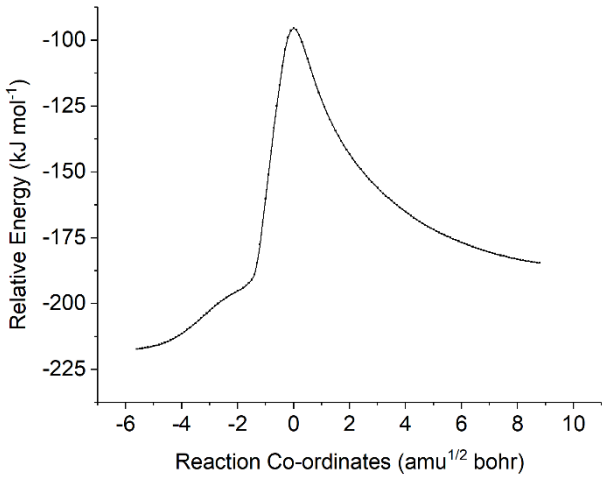
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (Hartree)** -878.222926627158
Reaction Coordinates: 6 -3.265638 -1.116654 0.497317 6 -0.031599 1.413095 -0.344367 6 0.351418 -0.040440 0.044893 6 1.875420 -0.310286 -0.072264 1 -3.833526 -2.024945 0.349665 1 -2.661106 -0.894765 1.368378 1 -0.403797 1.517538 -1.373373 9 -0.022910 -0.315016 1.315644	**Frequencies (cm^{-1}):** 17.3195, 37.0939, 51.8558, 56.7679, 64.4067, 73.9557, 108.1933, 122.6172, 215.2052, 228.5097, 252.6861, 322.591, 357.5067, 387.6918, 452.6098, 524.1586, 533.7999, 578.3556, 610.4902, 677.3269, 701.7983, 777.084, 886.7439, 905.8324, 993.9249, 1070.5734, 1142.3353,

9 -0.274732 -0.916869 -0.784863 9 2.147679 -1.597657 0.163182 9 2.557612 0.436751 0.795193 9 2.286088 -0.008880 -1.315472 8 -3.337374 -0.285209 -0.433609 8 -2.651781 0.886047 -0.319114 8 0.123805 2.317028 0.420060	1176.748, 1201.2961, 1219.5467, 1244.5254, 1301.8579, 1396.0704, 1412.6124, 1559.6935, 1829.0401, 3002.4913, 3117.6933, 3265.8612

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 1	**Energy (Hartree)** -878.181094934155
Reaction Coordinates: 6 1.797687 1.498506 0.241899 6 0.722848 -0.070484 0.839767 6 -0.297987 -0.358454 -0.271755 6 -1.699415 0.202713 0.115024 1 2.115655 1.835324 1.238634 1 0.930136 2.023650 -0.182623 1 0.297137 0.150725 1.811141 9 0.017406 0.148970 -1.475352 9 -0.430444 -1.701679 -0.401443 9 -1.625936 1.531047 0.304279 9 -2.584029 -0.046239 -0.843503 9 -2.126845 -0.357068 1.255865 8 2.635373 0.981501 -0.539035 8 2.378417 -1.093300 -0.174758 8 1.769572 -0.865535 0.966873	**Frequencies (cm^{-1}):** -404.1259, 45.6791, 59.839, 127.1398, 144.2152, 201.8457, 213.6418, 225.984, 270.7525, 308.7399, 362.624, 368.9365, 433.3007, 470.2606, 517.3366, 543.0944, 576.491, 600.5164, 616.2938, 751.1182, 822.5543, 878.1264, 916.6022, 1001.2136, 1079.6858, 1135.9659, 1153.5907, 1175.7646, 1195.7349, 1217.7335, 1227.9447, 1261.9339, 1318.296, 1414.7836, 1452.0161, 1559.0014, 2933.9114, 2999.7079, 3173.543
IRC  	

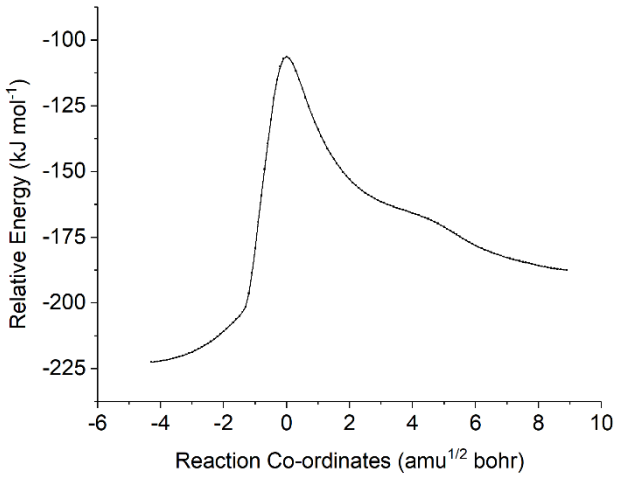
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 1	**Energy (Hartree)** -878.211755328963
Reaction Coordinates: 6 3.135416 -1.099536 0.421642 6 0.439861 0.540113 -0.960801 6 -0.443957 0.385466 0.262270 6 -1.758863 -0.360454 -0.106780	**Frequencies (cm^{-1}):** 28.3497, 48.9568, 61.6998, 78.6241, 97.9848, 105.1398, 141.1293, 159.1722, 201.0592, 213.3859, 224.3797, 262.0911,

1 4.115153 -0.684297 0.132724 1 2.880263 -1.048373 1.492513 1 0.114345 0.214990 -1.938491 9 0.150545 -0.299207 1.255777 9 -0.788143 1.612196 0.724547 9 -1.479035 -1.583905 -0.568898 9 -2.549050 -0.465208 0.956183 9 -2.408921 0.315485 -1.067985 8 2.390782 -1.593561 -0.388446 8 2.097986 1.534593 0.206214 8 1.552099 1.122705 -0.952935	299.2154, 361.2793, 404.0391, 468.624, 535.6438, 555.9826, 595.5279, 599.7374, 751.5107, 795.6352, 871.0264, 938.4116, 1028.5517, 1139.4955, 1185.864, 1192.4755, 1194.5388, 1237.7107, 1263.2013, 1326.5309, 1383.3995, 1530.3836, 1551.9963, 1785.8155, 2919.7671, 2984.6482, 3215.6869

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 2	**Energy (Hartree)** -878.181994650982
Reaction Coordinates: 6 -2.005620 0.116757 1.240885 6 -0.930295 1.089730 -0.165924 6 0.552583 0.789781 0.065060 6 1.172051 -0.643679 0.015629 1 -2.782908 0.887986 1.337417 1 -1.201829 0.153156 1.989624 1 -1.112831 2.152755 -0.044443 9 1.225665 1.522262 -0.868704 9 0.855639 1.312375 1.282079 9 1.133711 -1.149888 -1.212178 9 2.458863 -0.534447 0.380528 9 0.566134 -1.466048 0.867340 8 -2.280497 -0.975598 0.687967 8 -1.570242 -0.695841 -1.293338 8 -1.623618 0.612974 -1.176889	**Frequencies (cm^{-1}):** -401.3096, 34.4455, 83.3088, 125.4053, 149.1583, 176.5452, 210.2508, 223.1739, 271.5724, 319.8813, 356.2181, 377.3091, 434.0127, 467.7121, 503.5742, 535.0893, 576.1544, 594.5496, 624.271, 750.0336, 787.0845, 834.482, 912.9544, 1054.9176, 1088.4526, 1118.131, 1134.6094, 1154.8704, 1189.6926, 1222.0719, 1230.8719, 1273.8772, 1319.3351, 1420.4009, 1451.9934, 1567.2684, 2934.1054, 3002.0453, 3155.0511
IRC  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 2	**Energy (Hartree)** -878.210817367452
Reaction Coordinates: 6 -4.870455 -0.256001 -0.391966 6 -0.717972 0.410241 0.230416	**Frequencies (cm^{-1}):** 11.5958, 14.2006, 21.6377, 40.9262, 46.7572, 78.2062, 92.801, 108.9059,

6 0.533714 -0.364712 0.579447 6 1.712802 -0.311091 -0.465699 1 -5.051321 0.787731 -0.701845 1 -5.747817 -0.924900 -0.375844 1 -1.674412 -0.095381 0.161421 9 1.006876 0.002545 1.791149 9 0.133953 -1.661466 0.665018 9 2.588605 0.641768 -0.195783 9 2.358419 -1.483891 -0.460522 9 1.203846 -0.120188 -1.693924 8 -3.774478 -0.647490 -0.086810 8 0.387385 2.366803 0.085204 8 -0.750442 1.649814 0.032811	154.5018, 202.5036, 241.153, 272.951, 333.6686, 355.876, 413.9532, 479.2006, 507.4484, 558.1199, 584.09, 652.8856, 749.0842, 803.0369, 857.0297, 936.5627, 1077.8155, 1132.3484, 1169.017, 1201.3243, 1207.3993, 1220.9303, 1265.0306, 1282.0354, 1380.0753, 1531.445, 1551.808, 1804.8891, 2908.2906, 2976.1534, 3175.4144

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 3	**Energy (Hartree)** -878.177394077252
Reaction Coordinates: 6 2.456567 0.903285 0.342526 6 0.762685 -0.003337 0.894245 6 -0.291294 0.578495 -0.046482 6 -1.630169 -0.228685 -0.019825 1 2.940177 0.885672 1.329379 1 1.954793 1.845288 0.075588 1 0.563728 0.216914 1.936412 9 -0.578551 1.822490 0.433323 9 0.089472 0.701428 -1.323771 9 -2.070651 -0.329250 1.244731 9 -2.554848 0.398364 -0.744436 9 -1.452661 -1.455851 -0.507744 8 2.888532 0.161566 -0.575318 8 1.605480 -1.519988 -0.469479 8 1.238453 -1.226706 0.759411	**Frequencies (cm^{-1}):** -400.299, 45.1944, 62.7737, 118.9086, 131.0253, 200.681, 212.6134, 219.9965, 271.6798, 313.8946, 351.2265, 370.8021, 432.3038, 457.9481, 512.5468, 518.9986, 581.0936, 581.847, 665.371, 751.2784, 815.2217, 866.1749, 919.023, 1016.6171, 1075.3657, 1114.8106, 1157.0195, 1187.733, 1210.4942, 1218.8302, 1240.2853, 1261.1394, 1293.3918, 1410.7845, 1442.8013, 1562.312, 2928.4341, 2994.5322, 3173.8819
IRC  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 3	**Energy (Hartree)** -878.209591261981
Reaction Coordinates:	**Frequencies (cm^{-1}):**

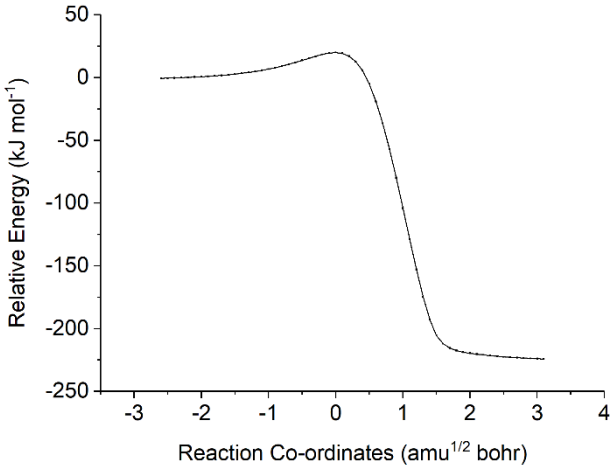
6 -3.558334 -0.531686 -0.596428 6 -0.515222 0.449472 1.025459 6 0.255459 -0.459777 0.090087 6 1.753656 -0.056604 -0.107968 1 -4.658335 -0.588164 -0.668946 1 -3.014319 -0.244833 -1.510502 1 -0.700424 0.115114 2.035909 9 0.269058 -1.681743 0.687101 9 -0.318950 -0.588251 -1.119612 9 2.331570 0.068568 1.099567 9 2.387426 -1.015487 -0.785781 9 1.878515 1.090379 -0.762254 8 -2.985219 -0.771435 0.435439 8 -0.822581 2.114577 -0.485019 8 -0.963306 1.587891 0.750261	16.3641, 31.6549, 45.8556, 56.5894, 63.1381, 98.9647, 113.51, 120.5207, 168.4692, 197.1066, 214.4432, 278.6076, 312.0045, 354.8284, 426.7119, 462.6521, 489.5737, 558.6296, 582.2516, 649.8693, 749.3077, 786.8985, 831.316, 916.018, 1057.9379, 1133.3465, 1180.8173, 1207.2246, 1217.0806, 1226.8656, 1267.1246, 1286.047, 1372.9276, 1530.5975, 1550.5376, 1796.5979, 2913.5603, 2989.0976, 3218.3092

S10.15 Ozonolysis of HFO-1233zd(E) (Alkene 13)

Compound: *E*-$CF_3CHCHCl$ + O_3 PRC1	**Energy (Hartree)** -1099.697139477880
Reaction Coordinates: 6 -1.863849 -0.209081 -0.033137 6 -0.652192 0.546740 -0.477226 6 0.092994 1.239108 0.367874 1 -0.103462 1.300789 1.426488 17 1.486868 2.136911 -0.131944 1 -0.442201 0.499406 -1.535919 9 -2.976032 0.272045 -0.634674 9 -1.776962 -1.512552 -0.366433 9 -2.069073 -0.143878 1.295820 8 2.532664 -1.303180 -0.003452 8 1.900555 -1.637289 -1.035601 8 1.967506 -1.450634 1.108425	**Frequencies (cm^{-1}):** 12.7356, 19.492, 22.3207, 32.3352, 47.1761, 89.0705, 108.3222, 160.5259, 168.2442, 298.9084, 393.3984, 401.3337, 547.7035, 563.1713, 660.3183, 745.7689, 831.5793, 850.4282, 872.1853, 966.3596, 1117.6021, 1130.4312, 1185.1453, 1240.7191, 1260.6004, 1283.1824, 1321.6576, 1691.0746, 3205.319

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{OZO} 1	**Energy (Hartree)** -1099.684080713040
Reaction Coordinates: 6 -1.607718 -0.285980 0.003325 6 -0.184938 -0.394378 -0.477443 6 0.816781 -0.726041 0.393684 1 0.663592 -0.887361 1.446933 17 2.335520 -1.260177 -0.217291 9 -2.338579 0.518575 -0.778938 9 -2.189738 -1.510670 -0.037396 9 -1.696918 0.154589 1.265821 1 -0.073473 -0.567087 -1.536772 8 1.290940 1.806390 -0.208083 8 1.275670 1.373949 1.008528 8 0.131941 1.676335 -0.772820	**Frequencies (cm^{-1}):** -297.3646, 47.3597, 86.2763, 120.7455, 145.9362, 175.9493, 234.4353, 289.8255, 334.1032, 398.7629, 461.8145, 514.9512, 555.8573, 571.8834, 669.6838, 753.5779, 839.4216, 854.8088, 885.254, 931.2785, 1053.8401, 1097.7758, 1111.1226, 1157.7569, 1260.4159, 1275.7591, 1277.9832, 1536.378, 3217.1266, 3242.5287

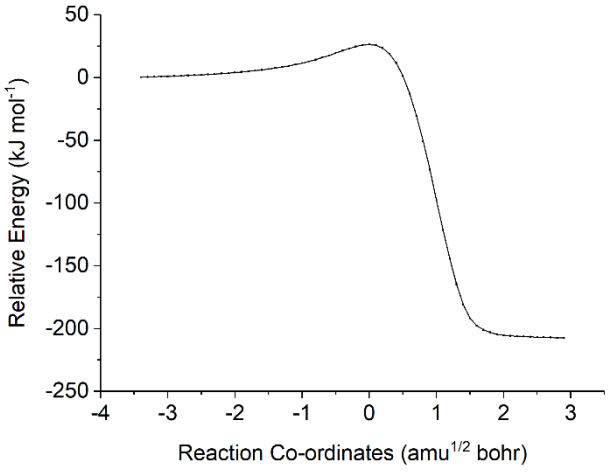
IRC:



Compound: *E*-$CF_3CHCHCl$ + O_3 POZ1	**Energy (Hartree)** -1099.783475506850
Reaction Coordinates: 6 -1.560379 -0.284706 0.009022 6 -0.179828 0.140370 -0.491240 6 0.965680 -0.183558 0.513436 17 2.214200 -1.245278 -0.262073 1 0.650068 -0.690549 1.418657 9 -1.829990 0.196215 1.230197 9 -2.521344 0.130543 -0.825857 9 -1.612006 -1.629126 0.072200 1 0.006546 -0.333497 -1.454164 8 1.210686 1.868158 -0.296682 8 1.451192 1.061521 0.881175 8 -0.159477 1.555628 -0.582670	**Frequencies (cm^{-1}):** 53.5193, 58.7984, 146.4808, 197.743, 242.6995, 293.9954, 343.8689, 391.9754, 449.4155, 525.0808, 554.4552, 648.7714, 694.4097, 745.4883, 761.0446, 801.3107, 892.1098, 936.5363, 994.8701, 1030.4386, 1062.3442, 1149.5034, 1175.3986, 1248.7726, 1270.4621, 1298.0152, 1316.0913, 1398.5159, 3090.6429, 3147.8929

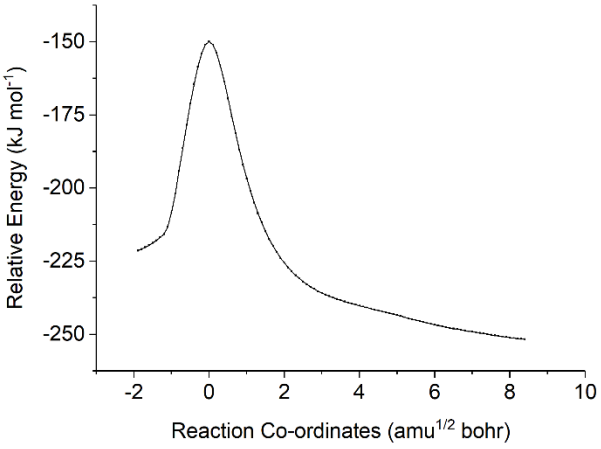
Compound: *E*-$CF_3CHCHCl$ + O_3 PRC 2	**Energy (Hartree)** -1099.697151869550
Reaction Coordinates: 6 -1.748565 -0.112589 -0.036399 6 -0.566987 0.690590 -0.474869 6 0.221613 1.315996 0.384093 1 0.084708 1.302253 1.453821 17 1.586352 2.247547 -0.118475 1 -0.400179 0.725426 -1.541557 9 -2.882852 0.325162 -0.622971 9 -1.611876 -1.413327 -0.388526 9 -1.946018 -0.080801 1.294737 8 1.709162 -2.124423 0.040362 8 1.904368 -1.437789 1.074172 8 1.871199 -1.572698 -1.075071	**Frequencies (cm^{-1}):** 14.5947, 23.3402, 27.7962, 31.9741, 49.5163, 92.9431, 103.0491, 159.8478, 167.4873, 299.4901, 394.3785, 401.3599, 547.4544, 564.032, 660.9847, 745.1349, 835.7105, 848.9702, 873.8801, 966.781, 1112.4101, 1127.2687, 1186.2971, 1242.2777, 1261.2837, 1282.7331, 1320.192, 1689.2485, 3206.0904, 3221.5627

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{OZO} 2	**Energy (Hartree)** -1099.683067598280
Reaction Coordinates: 6 1.539643 -0.404169 0.016015 6 0.126567 -0.452425 -0.497235 6 -0.915656 -0.626404 0.372668 1 -0.786841 -0.662154 1.441922 17 -2.441874 -1.183125 -0.185608 9 1.991445 -1.658650 0.259283 9 2.379170 0.145938 -0.869817 9 1.634728 0.280578 1.171011 1 0.021586 -0.704577 -1.540721 8 -0.422586 2.059598 0.191443 8 -1.495664 1.508194 0.649940 8 -0.116038 1.615589 -0.983739	**Frequencies (cm^{-1}):** -284.5431, 50.0707, 85.7975, 123.4802, 143.1393, 167.6327, 245.0318, 289.7436, 327.87, 397.4713, 428.4715, 509.6353, 552.0916, 575.0795, 669.2979, 748.9252, 845.3186, 858.1306, 883.6247, 936.0313, 1057.7236, 1102.3502, 1110.3566, 1155.3844, 1250.1135, 1278.9477, 1288.0714, 1533.2182, 3220.1951, 3229.9288
IRC:	



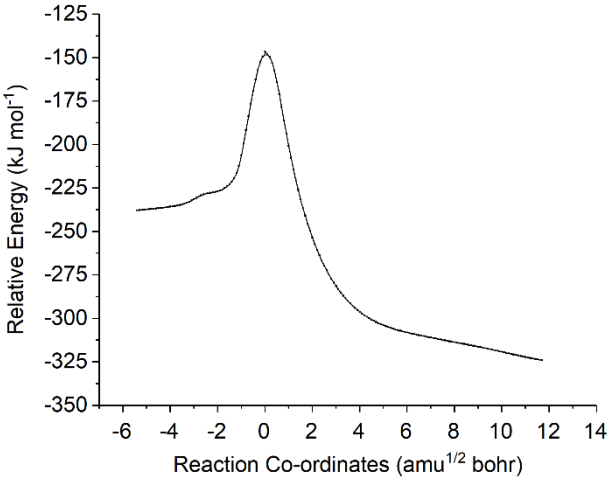
Compound: *E*-$CF_3CHCHCl$ + O_3 POZ 2	**Energy (Hartree)** -1099.781041505120
Reaction Coordinates: 6 1.484125 -0.394957 -0.037682 6 0.159554 0.061082 0.585019 6 -1.041350 -0.064217 -0.398648 17 -2.332923 -1.147328 0.176342 1 -0.742379 -0.414109 -1.382991 9 1.801139 0.288468 -1.145688 9 2.489058 -0.257794 0.837105 9 1.394416 -1.701056 -0.368183 1 0.000061 -0.513360 1.494885 8 -0.404144 2.055769 -0.231222 8 -1.569495 1.248798 -0.447126 8 0.176953 1.427186 0.939480	**Frequencies (cm^{-1}):** 50.8946, 53.1878, 155.6462, 184.3678, 235.3709, 296.1415, 370.4406, 374.7677, 413.6619, 521.8744, 559.8255, 646.2795, 699.8993, 732.8479, 743.1348, 864.0995, 885.9077, 928.2605, 985.5578, 1031.6728, 1049.7556, 1139.8366, 1167.4606, 1264.4395, 1274.98, 1302.3205, 1318.2613, 1393.687, 3109.9909, 3116.4402

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{ANTI} 1	**Energy (Hartree)** -1099.751193570360
Reaction Coordinates: 6 1.538842 -0.342961 0.019241 6 0.260604 0.351844 -0.418168 6 -1.265844 -0.042003 0.637764 17 -2.090925 -1.385640 -0.321628 1 -0.784228 -0.502246 1.504133 9 1.915760 0.040738 1.245419 9 2.543116 -0.069440 -0.830584 9 1.348122 -1.667684 0.026715 1 -0.154763 0.026884 -1.364517 8 -0.834313 2.220907 -0.549892 8 -1.845180 1.049668 0.750843 8 0.307008 1.666604 -0.210815	**Frequencies (cm^{-1}):** -448.8569, 37.3453, 73.39, 130.0882, 184.7786, 211.4026, 271.04, 378.9562, 391.5565, 418.7483, 469.8872, 510.0042, 571.535, 582.6383, 596.4865, 678.6213, 714.891, 892.2412, 950.9424, 1090.3448, 1118.9694, 1156.2221, 1187.9595, 1234.784, 1246.8758, 1266.7048, 1409.3547, 1445.3992, 3038.4737, 3163.5184
IRC:	



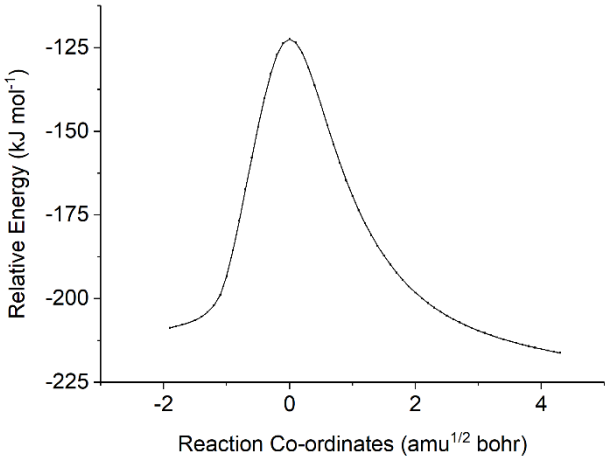
Compound: *E*-$CF_3CHCHCl$ + O_3 C_{ANTI} 1	**Energy (Hartree)** -1099.789970143740
Reaction Coordinates: 6 -2.190343 -0.244864 0.106547 6 -0.825583 0.326960 0.412350 1 -0.206915 -0.084867 1.199054 8 -0.453628 1.321976 -0.247091 8 0.763520 1.856247 0.016554 9 -2.745602 0.310266 -0.967092 9 -3.001262 -0.042391 1.163810 9 -2.092367 -1.567255 -0.083839 6 2.253467 -0.241237 -0.750965 1 2.490800 0.543998 -1.469179 17 3.510709 -0.312795 0.517560 8 1.335344 -0.989767 -0.788451	**Frequencies (cm^{-1}):** 21.3535, 24.1484, 46.7831, 51.4304, 121.0836, 144.0041, 194.2213, 216.1558, 238.8818, 387.6089, 404.8863, 417.3378, 451.5101, 552.5758, 562.0901, 700.5596, 718.3626, 887.2558, 900.3009, 920.9395, 966.4096, 1137.8093, 1181.2451, 1269.9661, 1327.8637, 1359.3784, 1561.4702, 1800.6882, 3096.8505, 3200.5397

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{SYN} 1	**Energy (Hartree)** -1099.746713532770
Reaction Coordinates: 6 -1.538839 -0.270084 0.044095 6 -0.406497 0.428232 -0.735674 6 1.187315 -0.051829 0.324106 1 0.702937 -0.061053 1.293043 17 1.961101 -1.519044 -0.145473 9 -1.673092 0.213123 1.287663 9 -2.706132 -0.100026 -0.596255 9 -1.319913 -1.599255 0.136218 1 -0.127099 -0.112793 -1.648897 8 1.236020 2.119666 0.395210 8 1.891956 1.033285 0.024875 8 -0.387251 1.688937 -0.721947	**Frequencies (cm^{-1}):** -422.0769, 42.0386, 71.0916, 135.1528, 194.1276, 238.99, 305.5824, 334.4469, 358.3122, 424.6465, 463.8262, 499.7043, 548.0362, 562.8606, 608.7027, 691.1087, 834.4284, 867.3042, 963.3811, 1085.8598, 1104.6049, 1144.2205, 1161.0135, 1224.0376, 1245.0984, 1298.7728, 1347.3492, 1483.1006, 2994.8802, 3161.7102
IRC:	



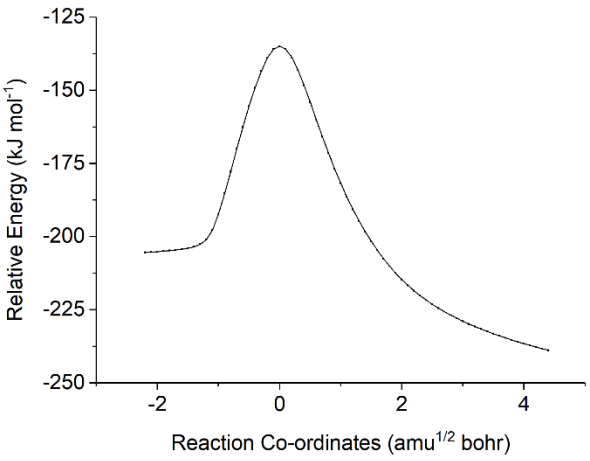
Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{SYN} 1	**Energy (Hartree)** -1099.784656778720
Reaction Coordinates: 6 2.737884 -0.093614 -0.000000 6 1.195520 -0.043340 0.000001 1 0.755736 0.966206 0.000001 8 0.531456 -1.042521 0.000001 9 3.200621 0.548397 1.088968 9 3.215427 -1.334284 -0.000000 9 3.200620 0.548397 -1.088968 6 -2.510733 -0.005119 0.000000 1 -1.574320 -0.559140 0.000001 17 -3.991815 -0.831924 -0.000000 8 -2.529942 1.242124 -0.000000 8 -1.302337 1.891083 0.000000	**Frequencies (cm^{-1}):** 19.0001, 27.7642, 56.3453, 63.4069, 95.6472, 104.4206, 129.2095, 233.5138, 266.1, 312.6967, 324.0951, 427.3231, 455.8691, 522.6357, 527.3453, 701.6504, 833.2318, 882.6348, 910.2688, 945.1757, 1008.1981, 1160.0357, 1178.9442, 1282.8255, 1336.4483, 1401.6061, 1485.6251, 1816.3094, 2996.9364, 3116.6598

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{ANTI} 2	**Energy (Hartree)** -1099.747027569040
Reaction Coordinates: 6 -1.513654 -0.395797 0.002887 6 -0.180442 -0.085281 -0.691779 6 1.150811 -0.233446 0.649301 1 0.774389 -1.149586 1.116263 17 2.665505 -0.691861 -0.308341 9 -2.516169 0.130737 -0.717608 9 -1.628237 0.025521 1.255627 9 -1.654045 -1.737168 0.000802 1 0.040525 -0.772293 -1.499392 8 -0.054856 2.013445 -0.065093 8 1.110879 0.848991 1.238294 8 0.108635 1.162421 -1.046566	**Frequencies (cm^{-1}):** -426.4395, 35.9052, 87.9176, 150.8103, 181.5555, 193.9187, 251.5827, 333.2695, 371.5811, 426.1663, 471.173, 528.9422, 548.4286, 577.3496, 646.1894, 668.3358, 768.6369, 890.338, 934.0581, 1042.068, 1098.7351, 1158.9891, 1171.5359, 1231.5024, 1245.3718, 1262.8063, 1425.0351, 1483.2258, 3013.7415, 3182.2486
IRC	



Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{ANTI} 2	**Energy (Hartree)** -1099.778251541460
Reaction Coordinates: 6 1.784448 -0.163867 -0.088304 6 0.970105 0.899690 0.683757 1 1.180187 1.929445 0.362396 8 0.288185 0.611290 1.629001 9 3.008080 -0.242656 0.488970 9 1.229794 -1.375761 -0.041775 9 1.967605 0.183589 -1.367538 6 -2.431934 0.409889 0.306630 1 -3.194061 0.704161 1.014448 17 -2.203411 -1.213467 -0.040980 8 -1.794637 1.341877 -0.236865 8 -0.782695 1.051146 -1.118333	**Frequencies (cm^{-1}):** 35.0067, 44.0839, 55.2409, 75.4857, 97.7973, 157.539, 199.4033, 246.2139, 257.0091, 362.8354, 428.4584, 465.3674, 520.9204, 531.9623, 655.7536, 701.3066, 809.6883, 832.0823, 860.9037, 895.4745, 952.3568, 1129.3181, 1188.2706, 1273.5248, 1336.8619, 1403.719, 1482.1805, 1802.1236, 3002.5106, 3211.2375

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{SYN} 2	**Energy (Hartree)** -1099.748405220490
Reaction Coordinates: 6 -1.513708 -0.394861 0.002619 6 -0.180853 -0.084458 -0.692416 6 1.150165 -0.235490 0.648404 17 2.665453 -0.691671 -0.308063 1 0.773805 -1.151710 1.115037 9 -1.633812 0.036755 1.251090 9 -2.517170 0.121090 -0.724750 9 -1.649203 -1.736800 0.011673 1 0.038591 -0.771687 -1.500292 8 -0.050792 2.012981 -0.063196 8 1.109280 0.846809 1.238793 8 0.109378 1.162868 -1.047026	**Frequencies (cm^{-1}):** -427.7395, 35.8602, 87.9803, 150.7817, 181.765, 194.2302, 251.8004, 333.1821, 371.9532, 426.8579, 471.0786, 529.0943, 548.9584, 577.722, 646.8298, 668.8404, 768.7379, 890.2811, 934.0925, 1041.2998, 1097.8373, 1158.429, 1170.6736, 1231.6597, 1245.4624, 1263.6583, 1424.809, 1480.9921, 3014.9339, 3181.9463
IRC	



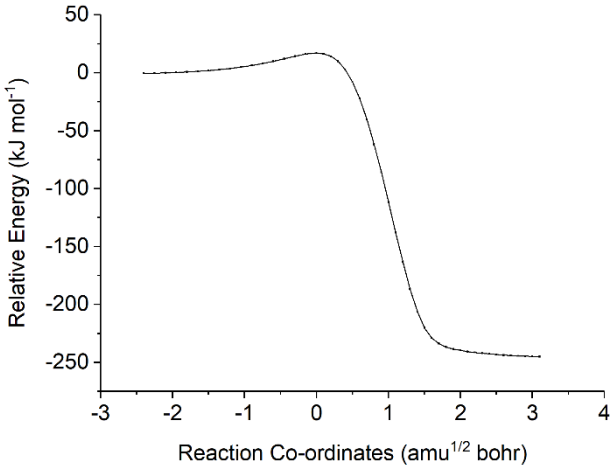
Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{SYN} 2	**Energy (Hartree)** -1099.786602698660
Reaction Coordinates: 6 -2.119779 -0.416894 -0.093052 6 -1.575344 0.575581 0.914608 1 -1.851829 0.505679 1.957069 8 -0.798593 1.515409 0.622578 8 -0.381795 1.681657 -0.648583 9 -2.864173 0.186193 -1.024296 9 -2.907370 -1.278730 0.578051 9 -1.153794 -1.115113 -0.690820 6 2.249947 0.093683 0.134454 17 3.933559 -0.331491 -0.309989 1 1.833235 0.814174 -0.574618 8 1.698787 -0.363303 1.074117	**Frequencies (cm^{-1}):** 13.1291, 24.0652, 38.7694, 57.8792, 67.3713, 82.9336, 112.2987, 182.9539, 249.4797, 326.2852, 447.7082, 478.5895, 505.9983, 535.5461, 588.9915, 710.0088, 757.9938, 797.2082, 882.2556, 926.6446, 972.7186, 1156.541, 1178.7399, 1243.144, 1321.9454, 1368.3674, 1556.7146, 1825.3675, 3070.4585, 3216.0234

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{POZ} 1	**Energy (Hartree)** -1099.777915798650
Reaction Coordinates: 6 -1.554608 -0.311060 0.007736 6 -0.124880 -0.173888 -0.546634 6 0.961849 -0.287146 0.524577 17 2.518143 -0.889302 -0.215338 1 0.735359 -0.956966 1.347822 1 -0.005809 -0.910056 -1.338516 9 -1.834292 0.560280 0.981471 9 -2.447764 -0.140568 -0.975975 9 -1.715367 -1.557615 0.504412 8 0.655787 1.910990 -0.031039 8 1.052487 0.986151 1.033607 8 0.134808 1.085215 -1.109044	**Frequencies (cm^{-1}):** -103.3462, 47.6043, 101.2299, 154.7137, 216.1124, 249.6566, 305.936, 381.9277, 395.367, 525.577, 552.3956, 653.7009, 711.5524, 750.9223, 777.5247, 858.0185, 886.6158, 896.6152, 973.0663, 1029.1639, 1094.289, 1144.5436, 1166.8418, 1243.2344, 1275.0457, 1281.9467, 1304.8115, 1378.8911, 3120.9837, 3142.8577
IRC Energy too low for IRC to take place	

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{POZ} 2	**Energy (Hartree)** -1099.770978070750
Reaction Coordinates: 6 -1.492268 -0.246953 0.004625 6 -0.155696 0.349271 -0.445698 6 1.056720 -0.074536 0.394229 17 1.809813 -1.595163 -0.132458 1 0.825670 -0.163638 1.453717 1 0.004953 0.104353 -1.498625 9 -1.707888 -0.073368 1.316505 9 -2.508777 0.316409 -0.662221 9 -1.507930 -1.565273 -0.248918 8 1.174508 2.167747 -0.051305 8 1.973438 0.961269 0.128818 8 -0.214026 1.734791 -0.211333	**Frequencies (cm^{-1}):** -212.1692, 47.7097, 101.9347, 138.5123, 219.3175, 235.7448, 330.6151, 379.1897, 408.5841, 486.5508, 555.2157, 576.5386, 685.5788, 708.603, 825.7592, 853.1021, 892.158, 906.8044, 1036.0657, 1071.1545, 1098.5329, 1155.6675, 1180.0767, 1256.3015, 1272.2581, 1304.4443, 1343.0164, 1404.4052, 3051.7001, 3097.6386
IRC Energy too low for IRC to take place	

S10.16 Ozonolysis of HFO-1234ze(E) (Alkene 14)

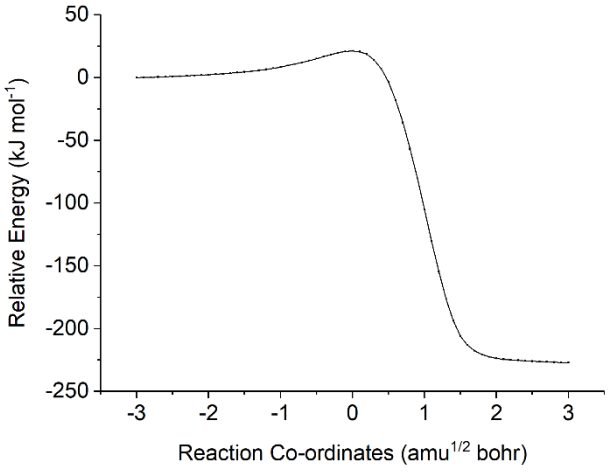
Compound: *E*-CF_3CHCHF + O_3 PRC1	**Energy (Hartree)** -739.703284627850
Reaction Coordinates: 6 -1.650945 -0.306763 -0.018338 6 -0.622713 0.630474 -0.552478 6 -0.026733 1.520569 0.219237 1 -0.198987 1.661027 1.276314 9 0.891810 2.358963 -0.274156 1 -0.402806 0.545570 -1.606650 9 -2.844800 -0.116720 -0.626706 9 -1.308519 -1.592769 -0.238216 9 -1.853623 -0.165119 1.306934 8 2.877900 -0.503195 -0.013235 8 2.313009 -1.046946 -0.993731 8 2.364132 -0.653793 1.123104	**Frequencies (cm^{-1}):** 4.8985, 12.6292, 22.7111, 26.1432, 38.8796, 94.8339, 105.985, 192.7761, 197.2378, 386.3606, 409.556, 419.2781, 555.1565, 577.4032, 691.3705, 745.1057, 868.5119, 879.7539, 961.8078, 1085.1441, 1119.6771, 1183.819, 1187.2852, 1241.4821, 1257.0108, 1318.8819, 1346.3541, 1735.9967, 3210.6938, 3219.0963

Compound: *E*-CF_3CHCHF + O_3 TS_{OZO} 1	**Energy (Hartree)** -739.689682804154
Reaction Coordinates: 6 1.419285 0.000042 0.014336 6 0.121245 0.471323 -0.570493 6 -0.766906 1.180052 0.183779 1 -0.637305 1.462953 1.215825 9 -1.751348 1.819674 -0.442068 1 0.073493 0.518754 -1.647519 9 2.373955 0.947162 -0.164839 9 1.333429 -0.231185 1.333889 9 1.862919 -1.114508 -0.581161 8 -2.020015 -1.102080 -0.174688 8 -1.914301 -0.509286 0.971199 8 -0.871751 -1.473697 -0.627314	**Frequencies (cm^{-1}):** -290.2803, 47.0046, 95.7327, 118.2241, 158.6037, 203.431, 240.3109, 344.6385, 375.0973, 411.3633, 456.6927, 531.2139, 563.8075, 576.1881, 696.1778, 753.3623, 876.707, 886.713, 923.5971, 1061.2793, 1095.4794, 1104.8871, 1130.8382, 1201.8657, 1255.8713, 1279.9515, 1330.5348, 1586.3292, 3220.608, 3238.2387
IRC:  	

Compound: *E*-$CF_3CHCHF + O_3$ POZ1	**Energy (Hartree)** -739.799128467212
Reaction Coordinates: 6 1.378940 0.046561 0.016352 6 -0.045567 -0.055917 -0.521609 6 -1.089193 0.741031 0.310137 9 -1.740430 1.620513 -0.524531 1 -0.696608 1.303143 1.155006 9 1.455821 -0.276226 1.314758 9 2.211038 -0.752440 -0.663023 9 1.810520 1.315649 -0.121266 1 -0.064039 0.299359 -1.553098 8 -1.884992 -1.263432 -0.211684 8 -1.933807 -0.229064 0.812425 8 -0.473322 -1.402506 -0.411321	**Frequencies (cm^{-1}):** 60.5452, 74.3865, 153.9635, 210.8506, 296.1848, 335.8249, 351.2962, 409.1283, 524.5177, 551.6113, 579.1047, 686.6407, 695.0589, 746.9879, 785.5228, 909.644, 938.9818, 1006.7012, 1037.1033, 1049.0572, 1070.631, 1153.7667, 1181.9293, 1271.4541, 1294.8085, 1307.7155, 1365.0142, 1403.4662, 3075.4681, 3120.7504

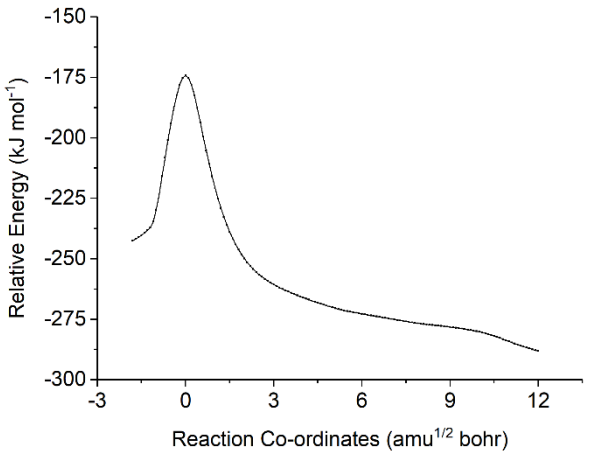
Compound: *E*-$CF_3CHCHF + O_3$ PRC 2	**Energy (Hartree)** -739.704017975154
Reaction Coordinates: 6 -1.514689 -0.376320 -0.023964 6 -0.663542 0.727051 -0.546537 6 -0.116785 1.626999 0.251828 1 -0.221380 1.665919 1.326106 9 0.641800 2.611457 -0.232782 9 -2.734903 -0.374353 -0.602646 9 -0.967756 -1.587414 -0.288741 9 -1.702803 -0.311298 1.309252 1 -0.514123 0.752145 -1.615942 8 2.409322 -1.148597 0.081561 8 2.382160 -0.359206 1.058701 8 2.380838 -0.658442 -1.073244	**Frequencies (cm^{-1}):** 15.9838, 16.9449, 23.9948, 30.1793, 47.1775, 94.6072, 119.9059, 192.6354, 198.3263, 387.002, 410.2886, 419.0111, 554.4183, 577.7799, 690.5176, 746.3248, 867.8081, 880.1144, 964.0518, 1085.004, 1113.9461, 1185.2165, 1193.6168, 1242.6261, 1258.1543, 1319.2618, 1347.6728, 1734.5187, 3210.5021, 3218.7069

Compound: *E*-$CF_3CHCHF + O_3$ TS_{OZO} 2	**Energy (Hartree)** -739.690068045272
Reaction Coordinates: 6 -1.381382 0.040928 0.020532 6 -0.110613 0.560985 -0.578236 6 0.827376 1.166245 0.205938 1 0.749638 1.303086 1.273748 9 1.770388 1.899755 -0.366997 9 -2.286569 1.039725 0.163952 9 -1.955346 -0.894030 -0.747418 9 -1.179123 -0.485408 1.245098 1 -0.110544 0.723826 -1.644402 8 1.415496 -1.492591 0.269456 8 2.156601 -0.496680 0.631215 8 0.953462 -1.345256 -0.921980	**Frequencies (cm^{-1}):** -274.3861, 44.2128, 93.1095, 114.6889, 162.2493, 199.2836, 257.7032, 343.0079, 382.5817, 415.0421, 443.5211, 507.8723, 559.9715, 579.4966, 694.7123, 751.4404, 874.9654, 882.5186, 928.2225, 1068.6525, 1096.9421, 1109.6482, 1132.1699, 1206.8847, 1243.4937, 1286.2774, 1339.7591, 1589.1863, 3222.0994, 3226.0896
IRC:	



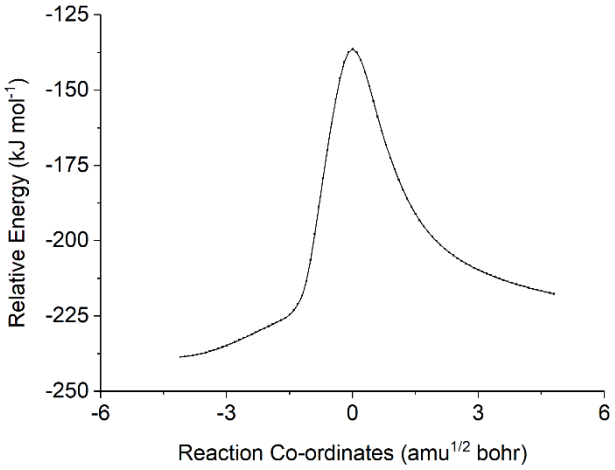
Compound: *E*-CF_3CHCHF + O_3 POZ 2	**Energy (Hartree)** -739.794731182167
Reaction Coordinates: 6 1.315638 0.126925 0.031010 6 −0.073099 0.211842 −0.618313 6 −1.181687 0.712690 0.319279 9 −2.133647 1.366200 −0.440351 1 −0.868015 1.394614 1.108504 9 1.325804 −0.538631 1.191189 9 2.185395 −0.462120 −0.798330 9 1.752457 1.382846 0.273165 1 0.007280 0.843175 −1.500583 8 −1.146873 −1.584141 0.150953 8 −1.714493 −0.426970 0.885602 8 −0.597941 −1.024038 −1.040408	**Frequencies (cm^{-1}):** 44.4138, 87.2889, 150.7713, 166.3573, 261.6313, 309.1999, 331.0583, 409.467, 488.7195, 528.8761, 567.5762, 685.3726, 709.8818, 768.1759, 870.5373, 887.5448, 915.5071, 972.2164, 1016.0725, 1045.1378, 1081.2547, 1142.3652, 1179.0545, 1276.3289, 1285.5176, 1302.1302, 1355.6254, 1393.0225, 3103.7767, 3123.0301

Compound: *E*-CF_3CHCHF + O_3 TS_{ANTI} 1	**Energy (Hartree)** -739.768398521593
Reaction Coordinates: 6 −1.401299 0.066028 0.015534 6 0.017686 −0.243656 −0.421743 6 1.355912 0.781542 0.401632 1 0.791762 1.244267 1.217796 9 1.583311 1.735172 −0.578134 9 −1.594858 −0.212898 1.310689 9 −2.294146 −0.637893 −0.700071 9 −1.646508 1.369905 −0.180485 1 0.271457 0.057819 −1.432879 8 1.662127 −1.658419 −0.404092 8 2.259655 −0.030627 0.652710 8 0.412317 −1.462722 −0.051799	**Frequencies (cm^{-1}):** -448.7486, 42.9496, 95.7915, 132.5415, 195.4736, 250.3922, 310.9982, 388.4779, 403.6771, 471.0522, 512.9073, 578.4309, 581.3856, 603.8158, 639.9277, 715.1346, 894.6684, 940.2153, 956.8633, 1113.3392, 1135.7124, 1161.8294, 1183.4475, 1235.2625, 1262.8909, 1298.824, 1409.8995, 1474.8955, 3035.7092, 3146.7313
IRC:	



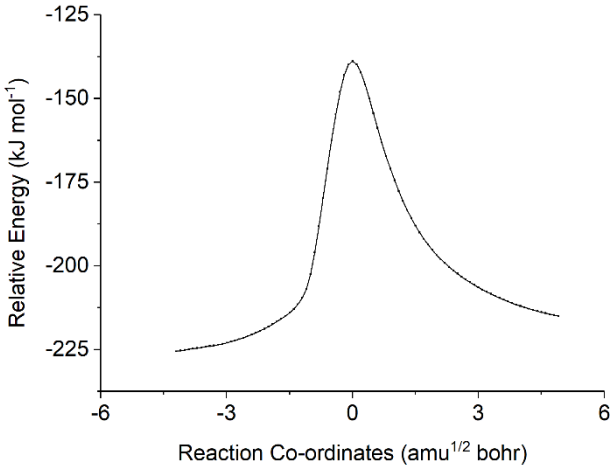
Compound: *E*-$CF_3CHCHF + O_3$ C_{ANTI} 1	**Energy (Hartree)** -739.811718375671
Reaction Coordinates: 6 1.805191 -0.184764 -0.060805 6 0.428206 0.326315 -0.417713 6 -2.636610 -0.435592 0.419496 1 -3.052729 0.215716 1.187229 9 -3.394008 -0.379769 -0.690955 9 2.252876 0.317518 1.086526 9 2.667010 0.149025 -1.041920 9 1.781650 -1.520950 0.023805 1 -0.111141 -0.062974 -1.271053 8 -1.278176 1.723444 -0.027125 8 -1.700715 -1.158403 0.502437 8 -0.044185 1.249845 0.279794	**Frequencies (cm^{-1}):** 22.8398, 37.3893, 55.0577, 75.5891, 134.8039, 158.4368, 195.9869, 247.5073, 250.6611, 388.0074, 407.923, 419.2533, 552.6533, 562.516, 667.4352, 700.8709, 887.0683, 900.0333, 960.0553, 1004.1026, 1067.3957, 1138.166, 1182.6463, 1270.5522, 1360.2933, 1368.1277, 1563.5239, 1828.7068, 3130.0091, 3204.1543

Compound: *E*-$CF_3CHCHF + O_3$ TS_{SYN} 1	**Energy (Hartree)** -739.756946242957
Reaction Coordinates: 6 -1.416495 0.056101 -0.032972 6 -0.127186 -0.014331 0.808340 6 1.261974 0.834771 -0.292212 1 0.870740 1.662063 -0.873059 9 2.134453 1.172253 0.641026 9 -1.633453 1.324664 -0.462022 9 -1.382269 -0.742020 -1.100891 9 -2.473154 -0.291889 0.720844 1 -0.073002 0.788436 1.559668 8 1.987626 -1.236023 -0.273504 8 1.517215 -0.240050 -1.005213 8 0.380448 -1.133529 1.056697	**Frequencies (cm^{-1}):** -429.6667, 41.2001, 93.1026, 141.865, 231.2141, 255.1767, 284.3394, 301.5314, 349.924, 434.4559, 509.3386, 530.0464, 566.6337, 647.9882, 699.4884, 777.9475, 841.4563, 876.4437, 1022.7121, 1083.8475, 1125.2987, 1166.0281, 1173.3267, 1250.3008, 1267.0655, 1338.4066, 1414.4067, 1507.834, 2961.687, 3181.4737
IRC:	



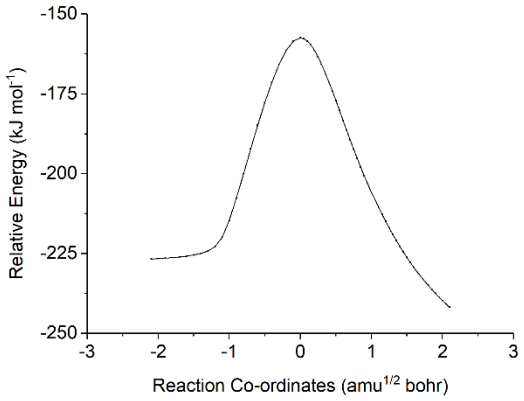
Compound: *E*-$CF_3CHCHF + O_3$ C_{SYN} 1	**Energy (Hartree)** -739.789802048716
Reaction Coordinates: 6 -1.310437 -0.493076 0.020906 6 -1.370217 0.906600 -0.643638 1 -0.820176 0.978637 -1.593096 8 -2.038622 1.777287 -0.174551 9 -0.257382 -1.210873 -0.431460 9 -1.230472 -0.429326 1.350372 9 -2.423353 -1.182553 -0.301112 6 2.603104 -0.340208 0.374894 1 3.118795 -0.995572 1.062996 9 2.799256 -0.512875 -0.888628 8 1.859035 0.546850 0.816288 8 1.201368 1.375574 -0.084916	**Frequencies (cm^{-1}):** 19.3457, 34.3577, 35.4825, 71.1917, 75.0499, 114.0954, 158.5361, 242.643, 295.349, 341.1491, 424.5251, 480.9683, 518.3991, 529.3147, 695.7802, 765.9299, 828.718, 832.6241, 834.9887, 950.9192, 1136.0438, 1163.6381, 1218.7279, 1271.6573, 1346.4634, 1396.3773, 1609.5661, 1834.244, 2995.2415, 3227.2839

Compound: *E*-$CF_3CHCHF + O_3$ TS_{ANTI} 2	**Energy (Hartree)** -739.756840898257
Reaction Coordinates: 6 -1.398570 0.016247 0.043500 6 -0.123011 -0.364554 -0.734958 6 1.250024 0.687744 0.236024 1 0.804487 0.648984 1.224417 9 1.408766 1.892765 -0.274657 9 -1.564785 1.357565 0.066062 9 -1.368318 -0.416669 1.311473 9 -2.477337 -0.511969 -0.553350 1 -0.027267 0.185298 -1.682594 8 2.266099 -0.104303 -0.026736 8 2.041987 -1.324586 0.444598 8 0.300313 -1.541879 -0.637233	**Frequencies (cm^{-1}):** -396.643, 49.3117, 75.4729, 141.1118, 228.3769, 242.4132, 310.9741, 358.3716, 408.6798, 440.9006, 488.4629, 516.7019, 556.8361, 596.2169, 620.6364, 693.2856, 834.9736, 913.977, 1080.183, 1114.8132, 1139.9608, 1163.2856, 1208.6758, 1241.5652, 1257.0001, 1354.044, 1387.0695, 1506.0419, 2974.2193, 3159.2806
IRC	



Compound: *E*-CF_3CHCHF + O_3 CPr_{ANTI} 2	**Energy (Hartree)** -739.790207230903
Reaction Coordinates: 6 -2.296863 0.008589 -0.000000 6 -0.755354 0.075085 0.000001 1 -0.237568 -0.896832 0.000002 8 -0.169487 1.122934 0.000001 9 -2.708784 -0.666389 1.089023 9 -2.866389 1.209717 -0.000002 9 -2.708782 -0.666391 -1.089023 6 2.895080 0.353330 0.000000 1 1.926361 0.851215 0.000002 9 3.976354 1.082023 -0.000000 8 3.048834 -0.870970 -0.000000 8 1.873458 -1.652846 0.000000	**Frequencies (cm^{-1}):** 22.3429, 28.8256, 61.2297, 82.1805, 98.1211, 110.115, 135.589, 268.577, 275.2861, 325.2231, 344.126, 428.2008, 523.0142, 527.5603, 571.1516, 702.0008, 834.2237, 877.7727, 989.4781, 1011.2292, 1161.4191, 1179.5574, 1223.9844, 1282.7178, 1360.1733, 1401.9915, 1593.874, 1813.3497, 2996.2364, 3119.6762

Compound: *E*-CF_3CHCHF + O_3 TS_{SYN}	**Energy (Hartree)** -739.765533937662
Reaction Coordinates: 6 -1.282551 -0.214067 0.017104 6 0.027391 -0.050471 -0.761908 6 1.403451 -0.715691 0.335157 1 0.908935 -1.634662 0.672425 9 2.362872 -1.050219 -0.607069 9 -2.204741 0.623466 -0.483584 9 -1.206690 -0.020417 1.327371 9 -1.707871 -1.478297 -0.191165 1 0.023475 -0.595507 -1.698812 8 0.674637 1.815283 0.194500 8 1.642204 0.204452 1.123585 8 0.556372 1.160358 -0.933799	**Frequencies (cm^{-1}):** -434.2081, 34.4039, 116.7645, 156.4385, 193.5575, 237.7254, 276.0766, 334.2677, 409.8321, 461.3927, 529.5368, 535.0495, 585.6571, 621.1691, 680.304, 768.4757, 892.1492, 915.6366, 966.3998, 1056.5562, 1109.937, 1158.9961, 1175.2459, 1236.5751, 1262.6982, 1294.1239, 1428.3821, 1498.3206, 3013.0146, 3172.9671
IRC	



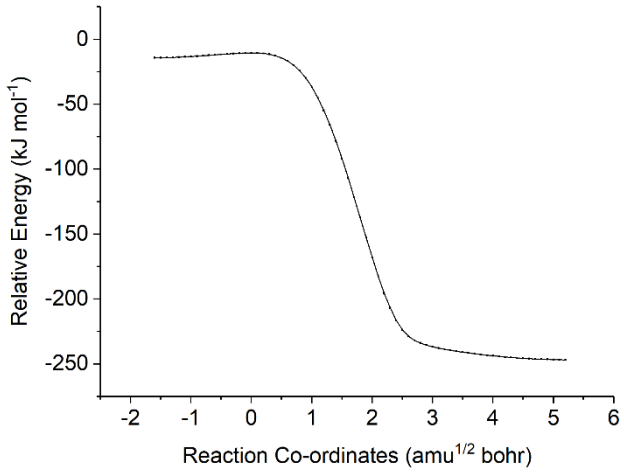
Compound: *E*-CF_3CHCHF + O_3 CPr_{SYN}	**Energy (Hartree)** -739.808552817472
Reaction Coordinates: 6 -1.668374 -0.375948 -0.081651 6 -1.033401 0.513484 0.968627 1 -1.242009 0.356492 2.017354 8 -0.258957 1.463517 0.707067 8 0.080355 1.731184 -0.570521 9 -2.464972 0.322155 -0.896849 9 -2.424746 -1.283152 0.565067 9 -0.765293 -1.031409 -0.810928 6 2.641303 -0.091388 -0.053514 9 3.872676 -0.469362 -0.454036 1 2.259975 0.708035 -0.693338 8 2.101838 -0.592889 0.869194	**Frequencies (cm^{-1}):** 17.9003, 28.7501, 43.7875, 67.6947, 76.6909, 87.9724, 111.7959, 183.141, 249.7382, 326.1957, 478.269, 505.8696, 535.6435, 588.5685, 664.2857, 757.8847, 798.2431, 881.8399, 924.7816, 1053.2791, 1055.5362, 1156.7697, 1178.1369, 1243.8193, 1359.1025, 1370.3575, 1558.5653, 1858.2746, 3102.8712, 3216.4218

Compound: *E*-CF_3CHCHF + O_3 TS_{POZ} 1	**Energy (Hartree)** -739.793338173632
Reaction Coordinates: 6 -1.334396 -0.096672 0.022788 6 0.053824 -0.178773 -0.631213 6 1.132847 -0.767150 0.280120 1 0.796272 -1.512436 0.998880 9 2.118520 -1.331403 -0.502613 9 -1.769863 -1.347417 0.293940 9 -1.337883 0.598684 1.164492 9 -2.210559 0.471886 -0.815755 1 -0.041647 -0.754124 -1.551361 8 0.577421 1.078823 -0.969372 8 1.453071 1.482258 0.132412 8 1.585731 0.313466 0.994678	**Frequencies (cm^{-1}):** -128.2522, 49.2648, 125.4765, 162.6181, 221.4459, 310.6157, 327.5195, 392.1092, 508.0751, 527.2178, 570.2736, 689.1202, 739.3659, 775.2732, 866.6245, 889.781, 903.0577, 974.8389, 1013.5754, 1056.6782, 1102.7176, 1144.1233, 1174.3029, 1276.2206, 1281.8243, 1310.4642, 1352.8677, 1388.5311, 3101.7388, 3115.7315
IRC Energy too low for IRC to take place	

S10.17 Ozonolysis of *E*-2-pentene (Alkene 15)

Compound: E-EtCHCHMe + O_3 PRC1.1	**Energy (Hartree)** -421.488584174397
Reaction Coordinates: 6 -1.740295 -0.585099 0.352968 6 -0.821547 0.406185 -0.283648 6 -0.042492 1.277148 0.375218 6 0.879374 2.254667 -0.275745 1 0.800355 2.221132 -1.361982 1 1.919934 2.051895 -0.004605 1 0.668871 3.274713 0.055365 1 -0.083216 1.293729 1.459895 1 -0.820252 0.430588 -1.370554 1 -1.398157 -1.590734 0.089446 6 -3.198945 -0.421645 -0.094226 1 -3.830124 -1.186904 0.358681 1 -3.291167 -0.513038 -1.177907 1 -3.592572 0.554398 0.192215 1 -1.667685 -0.508530 1.439462 8 1.721210 -0.751239 1.069423 8 2.111483 -0.862851 -0.130930 8 1.271987 -1.337759 -0.954420	**Frequencies (cm^{-1}):** 52.4086, 57.2729, 66.6782, 77.0619, 88.0584, 132.2452, 174.7364, 205.5678, 236.3251, 306.0925, 314.2166, 421.6036, 487.3069, 739.6599, 765.9261, 820.7085, 886.3627, 951.3048, 986.9944, 1028.1856, 1061.251, 1083.1677, 1103.0857, 1150.6436, 1170.3659, 1184.5195, 1274.1852, 1317.4957, 1330.4383, 1371.7929, 1410.1721, 1413.2998, 1475.8246, 1481.3627, 1488.8285, 1498.5984, 1505.9748, 1676.2265, 3010.4833, 3012.2186, 3025.559, 3050.2003, 3053.0606, 3087.1634, 3091.3595, 3094.7107, 3114.747, 3135.6153

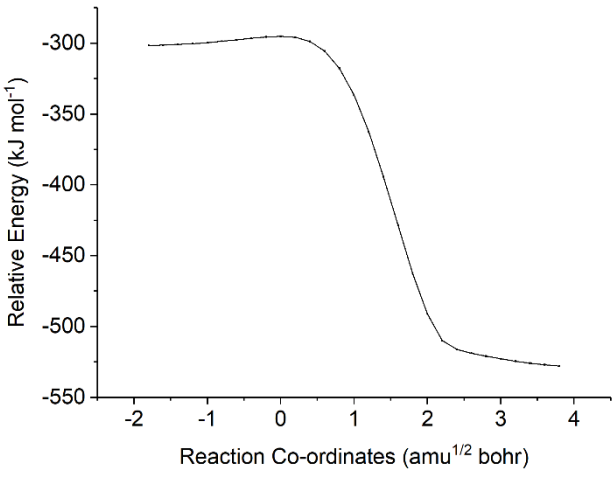
Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.1	**Energy (Hartree)** -421.484335971544
Reaction Coordinates: 6 -1.718366 -0.574154 0.285094 6 -0.639754 0.237996 -0.353853 6 0.180217 1.093402 0.332080 6 1.103712 2.059269 -0.336882 1 0.022995 1.211389 1.397100 1 2.010923 2.212969 0.245226 1 0.617601 3.034140 -0.444020 1 1.381633 1.719936 -1.334810 1 -0.644246 0.291379 -1.437517 1 -1.666646 -1.594651 -0.099247 6 -3.118478 -0.002846 0.012326 1 -3.882824 -0.638414 0.460343 1 -3.319145 0.055755 -1.058696 1 -3.226870 0.999673 0.427713 1 -1.540336 -0.634437 1.359943 8 1.696959 -0.485874 0.992779 8 1.895429 -0.959539 -0.192650 8 0.832978 -1.497054 -0.693708	**Frequencies (cm^{-1}):** -182.4056, 50.674, 77.3901, 97.0598, 140.42, 173.6853, 186.9526, 215.7021, 304.428, 326.4952, 454.0231, 474.6626, 502.8197, 739.7116, 780.9772, 836.0153, 885.2628, 951.9061, 956.6578, 1026.3492, 1046.9444, 1070.384, 1075.1744, 1104.4707, 1111.0102, 1187.1344, 1266.6054, 1304.4992, 1325.2135, 1362.7527, 1409.7649, 1410.2171, 1477.8087, 1487.8987, 1489.4171, 1498.4953, 1508.4053, 1597.7509, 3013.6713, 3026.5842, 3034.6722, 3065.5839, 3073.6044, 3091.0164, 3093.9823, 3110.3225, 3138.6547, 3161.7992
IRC:	



Compound: E-EtCHCHMe + O_3 POZ1.1	**Energy (Hartree)** -421.583943608976
Reaction Coordinates: 6 1.684696 -0.747268 0.211792 6 0.336624 -0.357350 -0.374311 6 -0.459868 0.737737 0.400490 6 -0.737339 1.988452 -0.413917 1 -1.311431 2.705640 0.171337 1 0.198448 2.463131 -0.715365 1 -1.301201 1.739134 -1.312539 1 0.031988 0.980075 1.343922 8 -1.666857 0.062812 0.784102 8 -1.826031 -0.915616 -0.266353 8 -0.518569 -1.502830 -0.308473 1 0.442560 -0.048565 -1.419504 1 1.547106 -0.997698 1.265563 1 2.019946 -1.658462 -0.287556 6 2.742814 0.344078 0.050703 1 2.463597 1.261807 0.571011 1 3.696943 0.014228 0.460521 1 2.902136 0.591894 -1.000135	**Frequencies (cm^{-1}):** 62.7112, 101.383, 192.4928, 225.0404, 233.675, 281.8098, 315.9847, 396.9137, 454.7088, 508.7768, 673.6165, 714.3245, 742.6936, 772.8453, 846.0353, 896.29, 930.1265, 953.2512, 997.072, 1037.6462, 1052.322, 1078.7669, 1116.089, 1153.23, 1180.432, 1279.9769, 1303.2886, 1322.6638, 1355.5458, 1377.9123, 1404.2388, 1410.0608, 1420.3887, 1487.3178, 1493.232, 1497.1963, 1503.9087, 1509.9617, 3003.7074, 3027.4916, 3032.9267, 3035.0219, 3054.828, 3063.7956, 3089.2092, 3095.8308, 3097.7117, 3113.6228

Compound: E-EtCHCHMe + O_3 PRC1.2	**Energy (Hartree)** -421.491497949549
Reaction Coordinates: 6 1.875424 -0.385929 0.681715 6 0.753230 0.601364 0.762251 6 0.205555 1.283753 -0.255317 6 -0.925875 2.247326 -0.106958 1 -1.211279 2.377239 0.936618 1 -1.806563 1.905648 -0.659437 1 -0.666102 3.225766 -0.518873 1 0.602744 1.156837 -1.255559 1 0.371957 0.787764 1.762276 1 2.655008 -0.070267 1.384374 6 2.484782 -0.613142 -0.698072 1 3.289683 -1.345934 -0.639777 1 2.904659 0.306849 -1.108124	**Frequencies (cm^{-1}):** 49.8705, 67.3768, 68.5854, 79.7483, 94.9353, 143.7213, 204.7577, 220.0862, 240.4633, 297.909, 318.817, 370.4692, 584.556, 715.9404, 739.6891, 836.9793, 856.637, 952.6201, 991.5418, 1041.6325, 1060.6622, 1086.8529, 1104.2934, 1149.1483, 1150.2937, 1168.6361, 1293.3128, 1323.8404, 1335.8443, 1383.7695, 1412.6411, 1417.242, 1465.8366, 1476.1338, 1489.1991, 1500.8061, 1510.4617, 1674.7055,

1 1.742257 -0.989644 -1.401468 1 1.505578 -1.337055 1.079948 8 -1.167912 -0.978271 -1.128868 8 -1.922014 -0.930556 -0.110796 8 -1.378404 -1.193352 1.004454	2996.4794, 3009.6975, 3012.9957, 3031.5562, 3049.2824, 3088.2777, 3094.4037, 3099.1246, 3121.698, 3156.3622

Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.2	**Energy (Hartree)** -421.483217596223
Reaction Coordinates: 6 -1.888878 0.025477 -0.625756 6 -0.492809 0.543541 -0.778729 6 0.253444 1.140152 0.203555 6 1.553328 1.824888 -0.073644 1 -0.189928 1.297107 1.176883 1 2.057904 1.388743 -0.936185 1 2.221968 1.775100 0.783872 1 1.383729 2.883546 -0.294297 1 -0.124464 0.606182 -1.796706 1 -2.541473 0.647851 -1.249695 6 -2.437538 -0.039153 0.796756 1 -2.512263 0.951273 1.248552 1 -1.804542 -0.656699 1.433065 1 -3.437681 -0.472201 0.793526 1 -1.925402 -0.969082 -1.078262 8 1.065576 -0.780037 1.139263 8 1.502782 -1.269644 0.025471 8 0.550001 -1.502975 -0.816464	**Frequencies (cm^{-1}):** -188.382, 67.2118, 84.8821, 96.1552, 151.1749, 178.3417, 220.713, 229.3139, 284.5453, 350.7869, 392.6666, 487.6771, 584.1714, 733.3562, 740.1909, 845.5988, 856.2946, 955.7994, 960.3943, 1043.1521, 1045.6115, 1071.7736, 1080.1009, 1102.0523, 1110.3965, 1152.4719, 1292.1589, 1304.6886, 1325.0636, 1385.498, 1410.0497, 1418.1713, 1461.4734, 1479.0089, 1488.6231, 1502.4927, 1511.3409, 1595.5623, 2993.8274, 3013.1463, 3030.8338, 3035.5302, 3072.4212, 3089.3299, 3105.5009, 3111.5825, 3143.5866, 3183.9673
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ1.2	**Energy (Hartree)** -421.583028237051
Reaction Coordinates: 6 1.742170 0.570256 -0.553846 6 0.289915 0.126070 -0.693240 6 -0.713617 0.634764 0.387138 6 -1.803817 1.528171 -0.177019 1 -2.483498 1.847771 0.611838	**Frequencies (cm^{-1}):** 59.1461, 89.215, 188.0411, 205.7193, 233.5142, 279.2846, 341.1988, 344.4109, 481.2354, 579.3189, 658.7938, 718.1129, 739.6046, 776.8728, 824.8245, 888.694, 925.8271, 943.0479, 958.8514, 1044.609,

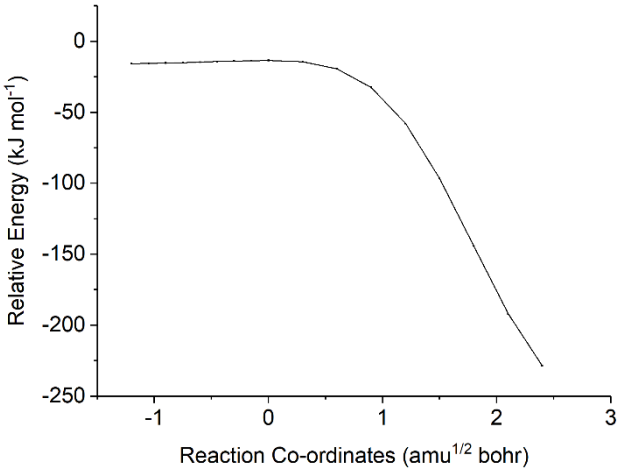
1 -1.366466 2.419604 -0.632017 1 -2.375119 0.998124 -0.938734 1 -0.193884 1.123839 1.210927 8 -1.237097 -0.574410 0.954214 8 -1.125318 -1.511451 -0.141375 8 0.227051 -1.297082 -0.566346 1 -0.090209 0.410446 -1.679110 1 2.297013 0.160058 -1.400472 1 1.759816 1.656057 -0.682502 6 2.432814 0.176414 0.751296 1 2.444175 -0.904234 0.879234 1 3.464272 0.529061 0.749104 1 1.942024 0.608770 1.623817	1056.2731, 1093.9126, 1115.3349, 1139.8958, 1165.6845, 1292.2375, 1300.8458, 1347.3392, 1355.8566, 1377.3026, 1407.1655, 1409.6545, 1425.6182, 1484.1471, 1486.5692, 1497.3083, 1500.8279, 1508.0073, 3007.9717, 3027.2193, 3031.0634, 3039.6811, 3053.8033, 3068.5564, 3093.2509, 3094.1744, 3114.3859, 3115.5146

Compound: E-EtCHCHMe + O_3 PRC1.3	**Energy (Hartree)** -421.488408351414
Reaction Coordinates: 6 -2.110866 0.458300 0.308163 6 -0.847938 0.949138 -0.327617 6 0.195465 1.476283 0.325040 6 1.436338 1.991358 -0.326229 1 0.143456 1.562002 1.406372 1 1.377078 1.929083 -1.412479 1 2.316706 1.427583 -0.001765 1 1.621626 3.032284 -0.049329 1 -0.805724 0.895527 -1.413040 1 -2.008738 0.486640 1.394801 6 -2.519408 -0.947770 -0.147438 1 -3.463460 -1.241606 0.312496 1 -1.760968 -1.680785 0.121748 1 -2.649694 -0.986102 -1.230342 1 -2.918790 1.154244 0.053090 8 1.207538 -1.031768 1.148805 8 1.735970 -1.211056 0.014520 8 0.959863 -1.525016 -0.934958	**Frequencies (cm^{-1}):** 34.1308, 50.7693, 60.3286, 69.4913, 86.4139, 127.4418, 180.2126, 205.1944, 226.1835, 275.1265, 302.7463, 412.7107, 484.0863, 739.8419, 758.852, 823.4271, 889.2012, 952.8856, 988.7214, 1032.253, 1062.896, 1088.0075, 1100.0182, 1158.5671, 1179.2669, 1183.345, 1278.4815, 1318.5258, 1331.8554, 1373.4184, 1411.6999, 1415.2813, 1475.1028, 1477.8603, 1490.1971, 1497.473, 1507.1125, 1684.6269, 2988.5311, 3008.1546, 3030.7855, 3047.8057, 3049.2737, 3087.499, 3093.9553, 3110.3614, 3112.1261, 3130.7571

Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.3	**Energy (Hartree)** -421.481896887431
Reaction Coordinates: 6 -1.702804 0.538697 0.588966 6 -0.462308 0.785366 -0.214088 6 0.737505 1.144840 0.329903 6 1.919813 1.558527 -0.484472 1 0.792747 1.309526 1.399345 1 1.823893 1.237980 -1.521576 1 2.845680 1.152880 -0.077600 1 2.019097 2.648476 -0.480098 1 -0.565227 0.823107 -1.293423 1 -1.457416 -0.148055 1.402837 6 -2.869610 -0.006710 -0.231163 1 -3.748164 -0.158472 0.395808 1 -2.611754 -0.961585 -0.687778 1 -3.147045 0.684923 -1.029047 1 -2.000778 1.479021 1.066594 8 1.370301 -0.991336 0.939272	**Frequencies (cm^{-1}):** -148.8838, 61.4492, 76.44, 108.7421, 138.1492, 162.8624, 188.6635, 212.2849, 268.2834, 357.7501, 425.4463, 463.5265, 472.9775, 726.2331, 739.2621, 839.8347, 893.3845, 956.0241, 960.0029, 1044.6301, 1053.7135, 1082.6521, 1088.0937, 1100.8369, 1113.12, 1171.5967, 1284.7341, 1294.1423, 1313.8097, 1376.9036, 1410.1944, 1416.4749, 1463.1431, 1477.3757, 1488.7903, 1500.0426, 1506.7703, 1604.6492, 2995.8308, 3014.1377, 3029.6537, 3041.6562, 3072.0552, 3088.1947, 3105.49, 3106.023, 3138.2489, 3157.3772

8 1.200161 -1.523504 -0.222041 8 -0.031288 -1.509174 -0.605974	

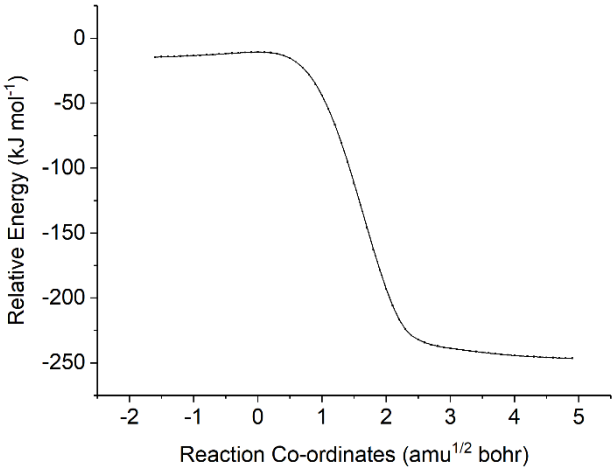
IRC:



Compound: E-EtCHCHMe + O_3 POZ1.3	**Energy (Hartree)** -421.584155305522
Reaction Coordinates: 6 1.629291 0.611131 0.480575 6 0.372590 0.147728 -0.235952 6 -0.970943 0.608446 0.403089 6 -1.761042 1.569258 -0.466468 1 -2.691029 1.854075 0.023680 1 -1.182583 2.476873 -0.652675 1 -1.997525 1.108358 -1.425265 1 -0.800178 1.024505 1.397486 8 -1.674675 -0.621463 0.636660 8 -1.100745 -1.515276 -0.347121 8 0.299340 -1.279439 -0.168079 1 0.390160 0.450939 -1.288137 1 1.609371 1.703998 0.505715 1 1.581713 0.268195 1.516576 6 2.920587 0.131701 -0.181100 1 2.986002 0.477972 -1.214188 1 3.791689 0.511118 0.353080 1 2.978124 -0.956191 -0.188830	**Frequencies (cm^{-1}):** 59.3892, 102.8335, 180.5783, 215.2143, 233.7539, 285.572, 301.7684, 395.3131, 479.1007, 503.0922, 646.6847, 723.1593, 748.222, 770.6378, 848.6494, 896.0402, 931.8441, 959.7328, 965.9326, 1045.3307, 1057.3865, 1095.5847, 1117.0301, 1143.4778, 1178.1827, 1286.5304, 1309.4065, 1332.4514, 1354.9259, 1378.5038, 1407.9144, 1410.7469, 1419.7996, 1478.1238, 1486.3193, 1497.4077, 1500.2126, 1507.2973, 3002.6981, 3022.5739, 3030.3067, 3031.3976, 3052.3587, 3058.6103, 3091.0241, 3093.4551, 3104.8712, 3113.9491

Compound: E-EtCHCHMe + O_3 PRC 2.1	**Energy (Hartree)** -421.488412063809
Reaction Coordinates: 6 1.681859 -0.571936 -0.353895 6 0.805693 0.462641 0.277701 6 0.002533 1.302166 -0.393169 6 -0.881277 2.328454 0.230648 1 -1.926017 2.136451 -0.025474 1 -0.641631 3.328518 -0.140125 1 -0.793076 2.329832 1.316366 1 0.001161 1.257089 -1.478366	**Frequencies (cm^{-1}):** 42.2677, 56.9293, 71.5651, 81.5233, 90.0497, 141.0423, 181.9032, 205.4046, 233.5044, 304.4492, 312.2162, 424.0715, 485.2367, 739.641, 763.1984, 822.6074, 888.2298, 951.7223, 986.2725, 1029.2267, 1062.9741, 1084.7685, 1103.6655, 1150.5181, 1170.1679, 1184.1695,

1 0.853849 0.540585 1.360446 1 1.322762 -1.566587 -0.065024 6 3.153759 -0.447676 0.061350 1 3.263624 -0.520844 1.144560 1 3.570009 0.510285 -0.252155 1 3.751840 -1.240636 -0.388617 1 1.591895 -0.515514 -1.440640 8 -1.979848 -0.600018 -0.914386 8 -1.583011 -1.456026 -0.066830 8 -1.383368 -1.031590 1.110368	1278.3249, 1316.8326, 1331.7104, 1373.5811, 1409.9642, 1411.1834, 1475.7629, 1479.2856, 1487.3538, 1498.5669, 1505.4007, 1676.1601, 2992.5755, 3016.4643, 3027.1847, 3047.8093, 3059.5013, 3088.9876, 3093.1187, 3098.3424, 3119.0874, 3131.689

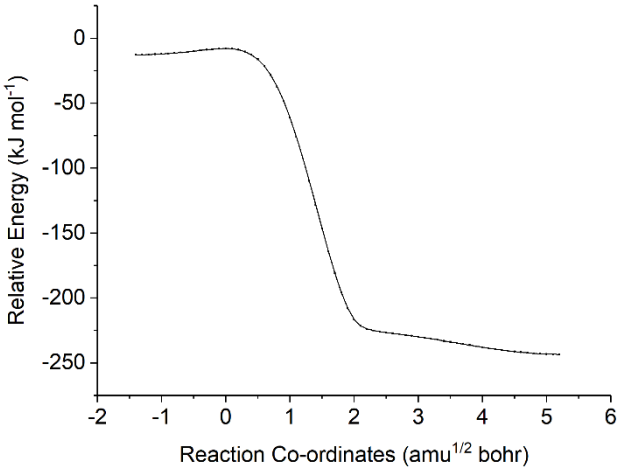
Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.1	**Energy (Hartree)** -421.482369557796
Reaction Coordinates: 6 1.645376 -0.638019 -0.159314 6 0.615525 0.273427 0.433529 6 -0.181487 1.096196 -0.317003 6 -1.046837 2.165327 0.256795 1 -0.045164 1.096119 -1.392583 1 -0.593052 3.147802 0.095170 1 -1.194373 2.026915 1.326824 1 -2.023640 2.177032 -0.226979 1 0.654259 0.431906 1.504956 1 1.673209 -1.570748 0.405339 6 3.047914 -0.007541 -0.155444 1 3.360648 0.249754 0.857610 1 3.073666 0.903167 -0.754559 1 3.779810 -0.704451 -0.565030 1 1.362792 -0.892004 -1.183115 8 -1.897463 -0.361807 -0.780436 8 -1.407236 -1.429552 -0.243076 8 -1.011690 -1.233869 0.971136	**Frequencies (cm^{-1}):** -181.5449, 46.5181, 77.5772, 120.546, 141.2679, 178.5368, 185.8023, 223.6371, 304.6912, 331.8079, 431.8882, 489.9109, 509.7112, 740.4161, 785.3186, 837.6203, 883.1986, 948.2282, 957.1135, 1024.7894, 1047.0982, 1069.0044, 1075.2178, 1105.2295, 1113.6094, 1186.8217, 1271.8589, 1299.0459, 1335.1025, 1360.8696, 1409.1053, 1410.8902, 1473.216, 1486.127, 1491.3066, 1497.5734, 1509.3064, 1597.8, 3016.6095, 3027.1487, 3033.4601, 3067.7716, 3074.3512, 3091.5597, 3096.3525, 3109.0755, 3144.7551, 3156.3794
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ 2.1	**Energy (Hartree)** -421.583851830179
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.588350 -0.805182 -0.142998 6 -0.309421 -0.309630 0.521206 6 0.481308 0.748207 -0.308605 1 0.051145 0.807670 -1.312623 6 0.606487 2.123785 0.313635 1 1.248533 2.761399 -0.293262 1 -0.373905 2.595676 0.378118 1 1.029826 2.054808 1.315280 8 1.793441 0.183975 -0.401706 8 1.518720 -1.219964 -0.432746 8 0.642403 -1.367392 0.709128 1 -0.515247 0.065226 1.526544 1 -1.958642 -1.651192 0.438473 1 -1.340632 -1.187850 -1.135361 6 -2.673298 0.268337 -0.237743 1 -2.934515 0.656609 0.748844 1 -3.580927 -0.140760 -0.680755 1 -2.362503 1.112364 -0.855644	64.7705, 111.9565, 195.1397, 218.8796, 225.1517, 282.1916, 317.9956, 389.4891, 465.4936, 504.4775, 660.794, 729.391, 748.6991, 766.3288, 859.5377, 894.1693, 921.5465, 936.9667, 987.7149, 1037.7992, 1050.9968, 1087.2358, 1131.2113, 1155.5538, 1179.0696, 1268.694, 1309.7594, 1338.9998, 1346.9399, 1380.7929, 1399.6796, 1414.5785, 1419.5094, 1487.3651, 1492.8972, 1500.2436, 1504.1552, 1509.6019, 3014.8514, 3025.2587, 3033.5754, 3039.8445, 3042.4624, 3065.1757, 3087.7622, 3094.7033, 3107.0054, 3112.3561

Compound: E-EtCHCHMe + O_3 PRC 2.2	**Energy (Hartree)** -421.487848822016
Reaction Coordinates: 6 1.819178 -0.387187 0.686960 6 0.736668 0.647177 0.758088 6 0.194562 1.308353 -0.275852 6 -0.892398 2.323443 -0.158790 1 -1.770567 2.007508 -0.727119 1 -0.575638 3.284768 -0.571974 1 -1.194900 2.473387 0.876902 1 0.573118 1.126382 -1.275302 1 0.380205 0.878827 1.757246 1 2.609907 -0.098510 1.388360 6 2.425741 -0.649508 -0.688671 1 2.882035 0.251191 -1.101809 1 1.677061 -1.001607 -1.398934 1 3.201189 -1.412469 -0.620452 1 1.420978 -1.324183 1.095078 8 -1.420991 -0.825579 -1.129254 8 -1.346955 -1.500539 -0.057747 8 -1.595290 -0.878753 1.017949	**Frequencies (cm^{-1}):** 52.9397, 58.1826, 68.8945, 81.5961, 89.4161, 153.5717, 204.2447, 219.9466, 239.8108, 292.9988, 317.0631, 369.9358, 583.6526, 716.9881, 739.2529, 835.4286, 855.6535, 951.981, 992.0281, 1041.9454, 1062.6787, 1087.4236, 1103.2847, 1150.3363, 1152.672, 1169.9164, 1290.3102, 1325.8236, 1334.7186, 1381.8094, 1410.6511, 1419.4712, 1469.0045, 1476.2265, 1487.8301, 1501.3044, 1509.7975, 1676.471, 2989.8577, 3005.4093, 3015.7424, 3031.5703, 3058.57, 3090.0874, 3094.7003, 3098.638, 3127.062, 3152.0201

Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.2	**Energy (Hartree)** -421.482448026458
Reaction Coordinates: 6 -1.816215 -0.235671 0.619683 6 -0.380106 -0.646950 0.772093 6 0.429611 -1.086962 -0.246339 6 1.769338 -1.699437 -0.016006 1 0.008172 -1.191523 -1.237070 1 1.702357 -2.789639 -0.083447 1 2.163014 -1.439293 0.965319 1 2.482332 -1.371165 -0.771989 1 -0.036591 -0.793182 1.788753	**Frequencies (cm^{-1}):** -217.6643, 57.3799, 82.4775, 126.0984, 154.0963, 184.6347, 218.1401, 241.5065, 282.0621, 360.5824, 403.1986, 491.4515, 587.8702, 733.6315, 745.8491, 842.8608, 858.3896, 951.0506, 957.8494, 1040.1506, 1044.4954, 1063.9249, 1080.8622, 1100.2809, 1110.2455, 1157.1246, 1291.9897, 1300.0723, 1320.309,

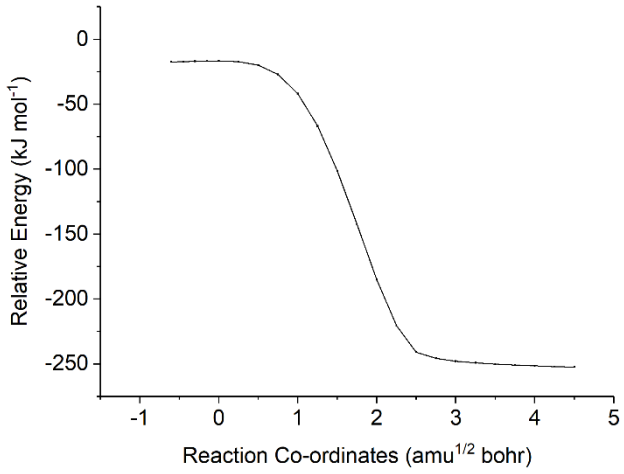
1 -2.417865 -0.936440 1.210158 6 -2.363368 -0.170698 -0.804869 1 -2.343689 -1.147539 -1.290325 1 -1.796317 0.524438 -1.423785 1 -3.399359 0.167259 -0.791239 1 -1.949824 0.731610 1.110263 8 1.225177 0.888078 -0.996082 8 0.575284 1.689506 -0.212120 8 0.668565 1.332889 1.030201	1381.1644, 1410.3168, 1421.0661, 1465.8541, 1473.1178, 1486.8735, 1503.3542, 1509.2003, 1589.6949, 2997.2193, 3016.1634, 3032.9582, 3039.6326, 3076.2247, 3091.5245, 3101.4563, 3111.7958, 3156.0066, 3178.452
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ 2.2	**Energy (Hartree)** -421.583083231273
Reaction Coordinates: 6 1.560747 -0.934347 0.381480 6 0.213357 -0.301243 0.727301 6 -0.880579 -0.433667 -0.370236 1 -0.414426 -0.702243 -1.321203 6 -2.017853 -1.377907 -0.041047 1 -1.639432 -2.396713 0.048429 1 -2.767990 -1.366893 -0.830927 1 -2.493071 -1.096119 0.898147 8 -1.408104 0.891630 -0.470412 8 -0.241943 1.690086 -0.261943 8 0.299643 1.114745 0.956858 1 -0.156607 -0.713723 1.668241 1 1.383012 -1.995889 0.178501 1 2.182000 -0.900162 1.278825 6 2.316762 -0.289796 -0.779642 1 1.777783 -0.370270 -1.723590 1 3.283890 -0.775313 -0.911612 1 2.493462 0.767396 -0.587969	**Frequencies (cm^{-1}):** 60.4282, 102.1048, 195.2891, 214.6022, 226.0847, 272.7123, 333.4032, 345.6821, 475.5063, 571.8655, 646.1119, 717.6559, 743.125, 788.0024, 827.8269, 888.2271, 916.95, 938.3956, 951.2646, 1045.3106, 1076.4613, 1091.3382, 1119.1613, 1158.7106, 1167.8806, 1278.1621, 1318.8674, 1336.854, 1356.0311, 1382.6477, 1406.4529, 1414.8674, 1424.1166, 1483.1315, 1486.7471, 1500.3015, 1502.8651, 1507.0398, 3008.361, 3029.3725, 3038.6341, 3040.7945, 3043.1664, 3053.2218, 3095.0621, 3104.0053, 3110.6241, 3113.2495

Compound: E-EtCHCHMe + O_3 PRC 2.3	**Energy (Hartree)** -421.488896111931
Reaction Coordinates:	**Frequencies (cm^{-1}):**

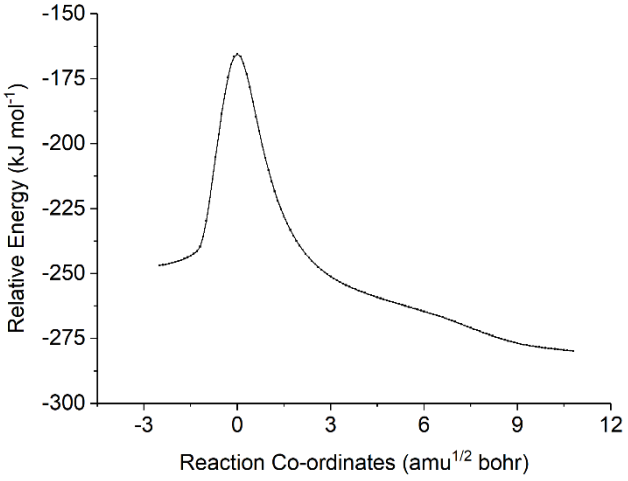
6 -1.916365 -0.608218 -0.502312 6 -0.681455 -1.046188 0.225096 6 0.478477 -1.392176 -0.352774 6 1.677916 -1.900869 0.374601 1 0.553818 -1.342020 -1.435206 1 2.544108 -1.264390 0.182137 1 1.939410 -2.906876 0.035055 1 1.510936 -1.933311 1.450701 1 -0.768964 -1.141122 1.304461 1 -1.666136 -0.356091 -1.535213 6 -2.656328 0.554328 0.168574 1 -2.036251 1.448637 0.217099 1 -2.941552 0.296597 1.189914 1 -3.566530 0.800196 -0.378968 1 -2.602063 -1.462594 -0.556227 8 1.676511 1.114686 -0.861086 8 0.870478 1.791045 -0.153699 8 0.655480 1.371733 1.020677	29.8602, 59.2189, 65.0918, 79.7001, 89.6354, 134.1471, 179.9143, 201.6077, 226.7766, 286.6027, 298.2473, 414.9852, 479.4264, 738.0541, 748.2966, 825.5325, 889.443, 953.489, 987.044, 1036.3263, 1064.2304, 1090.1374, 1098.0935, 1154.8251, 1173.649, 1181.9697, 1278.5475, 1314.1289, 1329.944, 1375.1521, 1410.6442, 1415.5444, 1475.2154, 1476.0086, 1489.1829, 1499.0961, 1504.611, 1676.172, 2984.2293, 3016.2331, 3031.541, 3043.7965, 3061.7515, 3089.1881, 3097.1921, 3103.9021, 3114.8445, 3129.56

Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.3	**Energy (Hartree)** -421.482791796432
Reaction Coordinates: 6 -1.585661 -0.534244 -0.636299 6 -0.368389 -0.863802 0.173208 6 0.863639 -1.069246 -0.374913 6 2.057215 -1.515920 0.396509 1 0.954642 -1.055699 -1.455450 1 2.920129 -0.889082 0.167492 1 2.324106 -2.542116 0.127620 1 1.878545 -1.474554 1.469911 1 -0.505152 -1.071593 1.227964 1 -1.357548 0.322574 -1.280512 6 -2.827385 -0.241512 0.201065 1 -2.656742 0.611443 0.857840 1 -3.092758 -1.098211 0.823282 1 -3.683079 -0.015175 -0.434806 1 -1.787379 -1.362941 -1.323978 8 1.509216 1.173702 -0.623256 8 0.439761 1.746755 -0.188795 8 0.072113 1.320006 0.969953	**Frequencies (cm^{-1}):** -124.7567, 48.7914, 87.1644, 128.8724, 140.229, 166.236, 190.3325, 220.0948, 276.1717, 351.9511, 425.3763, 465.2244, 474.2651, 726.2648, 738.8533, 839.1315, 895.0763, 958.5987, 959.6939, 1043.4284, 1055.3506, 1083.9675, 1091.6793, 1098.5971, 1116.795, 1172.8786, 1284.3789, 1296.2726, 1308.6784, 1379.2735, 1409.8176, 1416.6383, 1468.3369, 1473.9186, 1485.7609, 1499.2145, 1507.473, 1609.8296, 2994.0737, 3010.3495, 3017.5099, 3030.3872, 3070.2837, 3088.5578, 3101.883, 3106.6534, 3143.0212, 3155.6908
IRC:	



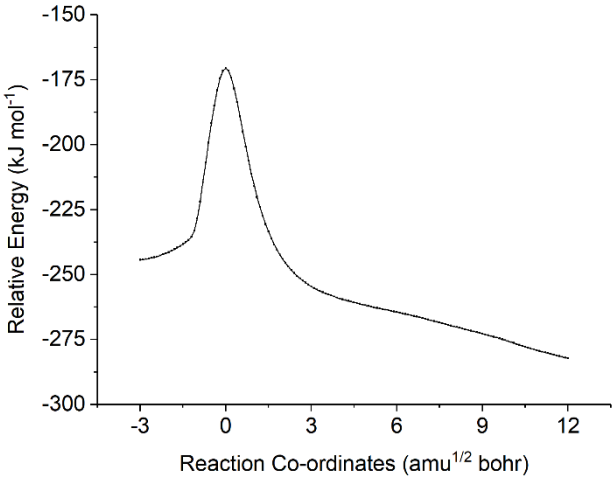
Compound: E-EtCHCHMe + O_3 POZ 2.3	**Energy (Hartree)** -421.584499116535
Reaction Coordinates: 6 1.535423 0.534084 0.575195 6 0.346354 0.223024 -0.322589 6 -1.030133 0.510142 0.347002 1 -0.873551 0.692253 1.414317 6 -1.848217 1.619904 -0.279454 1 -1.330390 2.572715 -0.164467 1 -2.818764 1.704467 0.208139 1 -2.005024 1.430568 -1.340947 8 -1.741304 -0.720384 0.186806 8 -0.689872 -1.687315 0.280851 8 0.267215 -1.168181 -0.673336 1 0.430336 0.745453 -1.278394 1 1.456382 -0.084383 1.472259 1 1.448129 1.574882 0.903863 6 2.882944 0.313046 -0.107378 1 2.988033 -0.721074 -0.434669 1 3.705455 0.535795 0.572381 1 2.992857 0.955158 -0.983697	**Frequencies (cm^{-1}):** 61.1127, 104.9018, 189.9569, 217.4095, 231.4799, 276.8662, 293.0606, 396.0192, 482.1328, 509.07, 649.8929, 712.2079, 744.8433, 778.4549, 866.8942, 890.9963, 924.3127, 940.3574, 963.6834, 1049.0934, 1066.1333, 1094.2115, 1121.8497, 1157.7834, 1174.0654, 1279.9548, 1293.1866, 1338.0158, 1356.4399, 1385.1085, 1402.1397, 1415.1632, 1417.5001, 1477.3576, 1486.6657, 1499.5593, 1501.5167, 1507.9329, 3008.1489, 3016.7029, 3028.0805, 3037.0783, 3039.5531, 3057.4536, 3087.9805, 3101.781, 3103.6298, 3112.9225

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.1	**Energy (Hartree)** -421.549380422627
Reaction Coordinates: 6 -1.674635 -0.867488 -0.211761 6 -0.293436 -0.568357 0.307925 6 0.628655 0.924535 -0.483910 6 0.346911 2.099820 0.444357 1 -0.716889 2.246898 0.626862 1 0.740734 3.008086 -0.014597 1 0.862033 1.954738 1.393318 6 -2.686646 0.259819 -0.009643 1 -2.757278 0.552643 1.038751 1 -2.432174 1.144078 -0.592068 1 -3.675009 -0.070092 -0.326809	**Frequencies (cm^{-1}):** -476.5859, 69.0866, 98.2151, 173.4452, 193.664, 229.5986, 270.8505, 290.1543, 378.5908, 424.5921, 482.2148, 491.7824, 555.8081, 612.0344, 783.1152, 870.1647, 927.6367, 968.4821, 982.2783, 1035.6195, 1063.2102, 1096.4126, 1116.3377, 1159.6463, 1179.3719, 1246.2126, 1301.2076, 1326.9905, 1330.9384, 1394.4486, 1412.5405, 1424.6189,

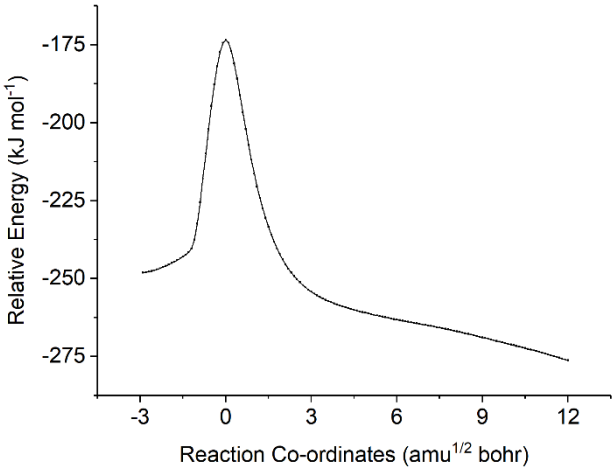
1 -0.191077 -0.202224 1.325975 1 -2.030226 -1.762642 0.308040 1 -1.601788 -1.131434 -1.267878 1 0.051168 0.914270 -1.422014 8 1.837020 0.515950 -0.574436 8 1.802280 -1.217582 0.421727 8 0.588877 -1.516405 -0.016215	1440.1641, 1481.5121, 1484.38, 1496.0891, 1504.9147, 1511.6844, 2926.7104, 3014.8747, 3035.1135, 3038.5385, 3064.6868, 3096.8382, 3099.8153, 3107.9825, 3112.4509, 3116.98
IRC:  	

Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.1	**Energy (Hartree)** -421.595845842666
Reaction Coordinates: 6 2.345438 0.222221 -0.299027 6 1.091165 0.690518 0.331503 6 -1.838594 -0.678247 0.473145 6 -2.793675 -0.576999 -0.676933 1 -3.688025 -1.162361 -0.442143 1 -2.343321 -0.955141 -1.592101 1 -3.102228 0.459887 -0.804976 6 2.569328 -1.284974 -0.097208 1 2.601094 -1.540293 0.961730 1 1.767272 -1.859702 -0.554426 1 3.517937 -1.576978 -0.545557 1 0.842494 0.501716 1.370197 1 3.170568 0.773716 0.167288 1 2.331840 0.486960 -1.355767 1 -2.193111 -0.243742 1.422246 8 -0.773328 -1.262694 0.428725 8 -0.895644 1.760291 0.286137 8 0.275662 1.362506 -0.341785	**Frequencies (cm^{-1}):** 42.0072, 52.9546, 72.5509, 80.5939, 130.0276, 132.9557, 176.1572, 205.3186, 240.4542, 278.5993, 325.0106, 424.9231, 514.6817, 535.9541, 776.1863, 791.908, 894.1458, 905.9834, 917.5901, 938.0548, 1022.5923, 1096.2713, 1115.3467, 1135.3901, 1182.1924, 1275.1886, 1325.5837, 1373.5271, 1376.2788, 1420.6604, 1424.5671, 1457.0395, 1467.5534, 1474.8352, 1496.5567, 1505.4297, 1579.346, 1748.2871, 2946.591, 2998.441, 3022.0867, 3045.7883, 3086.2788, 3091.8467, 3109.6546, 3129.1972, 3134.5785, 3166.9687

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.2	**Energy (Hartree)** -421.551877987989
Reaction Coordinates: 6 1.666366 0.642755 -0.541622 6 0.349755 -0.078508 -0.629117	**Frequencies (cm^{-1}):** -462.5283, 82.4136, 88.4235, 171.3083, 201.7565, 211.3323, 246.1585, 323.1904,

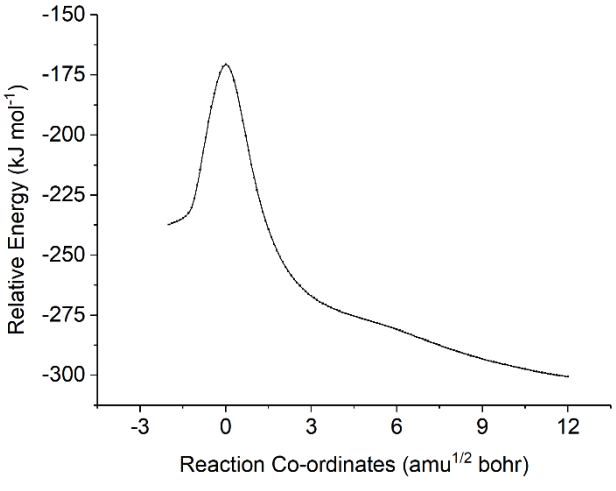
6 -0.999481 0.599490 0.510603 6 -1.606280 1.740897 -0.299949 1 -2.171875 1.345797 -1.142784 1 -0.848702 2.438411 -0.661116 1 -2.294521 2.295868 0.338984 6 2.511563 0.313349 0.688201 1 1.972970 0.523072 1.612349 1 2.799428 -0.736249 0.703613 1 3.420597 0.913659 0.686110 1 -0.224692 0.034974 -1.543734 1 1.451169 1.712656 -0.582701 1 2.230486 0.422433 -1.453599 1 -0.341343 0.924790 1.332321 8 -1.731191 -0.422753 0.753028 8 0.368482 -1.333860 -0.172494 8 -0.827923 -1.891302 -0.287802	373.8907, 413.9391, 480.548, 518.6697, 582.2787, 644.5958, 780.9312, 866.0714, 906.7746, 978.9033, 987.1634, 1031.6361, 1063.1129, 1093.1427, 1109.2807, 1140.3772, 1184.4143, 1254.9951, 1290.8773, 1335.9625, 1376.5717, 1391.6599, 1396.4297, 1428.3387, 1438.8091, 1477.1805, 1481.0628, 1497.0936, 1501.362, 1507.0533, 2924.3295, 3014.2757, 3028.6568, 3043.7387, 3053.8749, 3090.1287, 3103.0593, 3111.6702, 3114.9935, 3118.6321
IRC:  	

Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.2	**Energy (Hartree)** -421.596815811173
Reaction Coordinates: 6 -2.184680 0.573728 0.600706 6 -0.910369 -0.170058 0.706799 6 1.916700 0.531445 -0.546503 6 3.135941 0.122422 0.222744 1 3.067053 0.440062 1.260873 1 4.010803 0.590736 -0.239407 1 3.269622 -0.956828 0.162797 6 -3.040203 0.254671 -0.620306 1 -2.500942 0.467887 -1.541795 1 -3.331924 -0.794480 -0.638642 1 -3.945139 0.860056 -0.606095 1 -0.215970 -0.019558 1.524974 1 -1.911882 1.634801 0.627165 1 -2.737519 0.401553 1.532005 1 1.852194 0.137387 -1.573831 8 1.084251 1.322246 -0.142246 8 -0.606903 -1.024692 -0.156679 8 0.640073 -1.626912 -0.037160	**Frequencies (cm^{-1}):** 45.1866, 47.8048, 77.6404, 95.1931, 141.8753, 152.7521, 197.381, 201.1667, 261.3593, 269.3164, 299.1753, 425.6257, 513.417, 622.5573, 739.0062, 794.4318, 896.0498, 900.2705, 919.3153, 926.7113, 1027.3958, 1106.5996, 1112.7761, 1125.5387, 1134.0282, 1278.1834, 1350.0074, 1379.2513, 1392.5913, 1423.8789, 1424.2854, 1443.2306, 1457.7398, 1472.2245, 1499.5135, 1504.9112, 1584.3872, 1740.028, 2949.5137, 3001.8195, 3020.464, 3022.7196, 3048.5144, 3090.8625, 3112.5133, 3116.1148, 3134.3129, 3175.6459

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.3	**Energy (Hartree)** -421.552487519029
Reaction Coordinates: 6 1.608723 0.567044 0.487635 6 0.419190 -0.075428 -0.161504 6 -1.248708 0.594056 0.437475 6 -1.458189 1.832087 -0.430940 1 -1.662905 1.540740 -1.460181 1 -0.600945 2.506452 -0.402699 1 -2.325086 2.376906 -0.054731 6 2.922789 0.260020 -0.241598 1 3.130878 -0.809526 -0.239758 1 2.888024 0.595633 -1.278868 1 3.754313 0.767964 0.246609 1 0.242296 0.111317 -1.217248 1 1.661182 0.236210 1.525935 1 1.441345 1.645219 0.504718 1 -0.946270 0.811274 1.475333 8 -2.043900 -0.394257 0.276537 8 0.237678 -1.352436 0.186295 8 -0.824485 -1.859417 -0.418522	**Frequencies (cm^{-1}):** -452.7878, 66.9129, 92.1538, 163.8705, 201.0501, 211.9882, 242.2777, 307.8659, 356.7756, 468.8252, 478.9137, 518.1423, 543.5564, 616.1528, 776.8373, 873.1063, 921.3667, 979.9215, 994.1288, 1018.5205, 1056.6332, 1088.1927, 1129.4007, 1160.9558, 1181.0155, 1244.3065, 1302.2264, 1333.5361, 1353.1717, 1392.384, 1408.2269, 1425.4729, 1439.8994, 1478.3593, 1479.8696, 1498.71, 1499.8182, 1506.3758, 2915.4204, 3029.6751, 3034.0878, 3044.2574, 3075.7949, 3091.1753, 3098.096, 3106.6876, 3112.717, 3116.2338
IRC:  	

Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.3	**Energy (Hartree)** -421.592304735529
Reaction Coordinates: 6 2.016574 -0.716811 -0.494140 6 1.159297 0.282047 0.180685 6 -2.235987 -0.253200 0.124467 6 -3.687661 -0.542497 -0.106656 1 -3.862768 -1.606352 -0.249052 1 -4.031299 0.017654 -0.980293 1 -4.268892 -0.174142 0.742828 6 3.305366 -1.003894 0.292526 1 3.932962 -0.115860 0.359619 1 3.084368 -1.342492 1.305043 1 3.875915 -1.787032 -0.204806	**Frequencies (cm^{-1}):** 25.9963, 42.2362, 43.6952, 61.1989, 69.7843, 93.3085, 130.927, 163.3971, 204.6656, 209.5304, 326.6427, 417.1765, 511.891, 533.0139, 774.6084, 789.4365, 885.0835, 891.3136, 910.768, 942.1045, 1019.8716, 1093.9921, 1129.6983, 1154.9649, 1181.6657, 1275.0043, 1324.8872, 1374.3865, 1379.2058, 1417.0591, 1448.6431, 1460.828, 1468.1962, 1470.4036, 1500.7651,

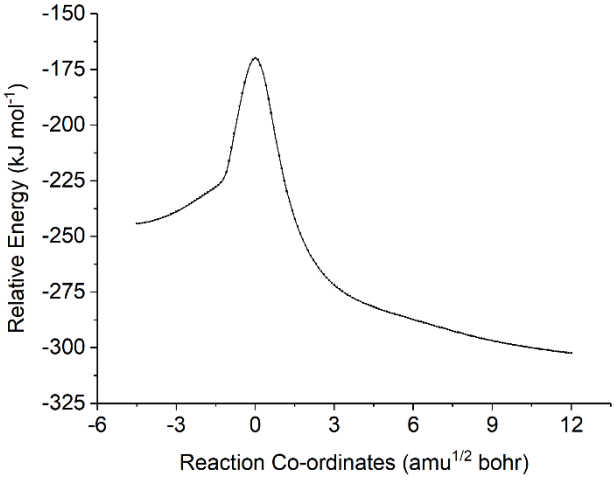
1 0.804329 0.164141 1.199658 1 2.235572 -0.375069 -1.505121 1 1.425480 -1.634871 -0.572223 1 -1.961356 0.805128 0.276268 8 -1.372744 -1.105615 0.144719 8 0.815896 1.320266 -0.426163 8 -0.015633 2.217226 0.237291	1505.5655, 1586.0273, 1765.1542, 2948.6456, 3021.5374, 3021.9536, 3038.7213, 3072.5224, 3086.7386, 3107.2711, 3109.7434, 3131.6861, 3156.9924

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.1	**Energy (Hartree)** -421.553099505068
Reaction Coordinates: 6 1.769289 -0.571468 0.100326 6 0.495268 -0.252246 -0.681838 6 -0.612804 0.819107 0.363802 6 -1.585307 1.469112 -0.577937 1 -1.938903 0.769859 -1.328851 1 -1.107848 2.320115 -1.060657 1 -2.443677 1.832176 -0.007381 6 2.723626 0.609979 0.254033 1 2.299577 1.411004 0.862387 1 2.985598 1.036243 -0.716817 1 3.650873 0.298629 0.734501 1 0.620287 0.529370 -1.453105 1 1.494892 -0.989215 1.070125 1 2.265334 -1.376574 -0.446590 1 0.002632 1.477237 0.969356 8 -1.044932 -0.190370 1.145452 8 -1.737761 -1.065972 0.436986 8 -0.288457 -1.213126 -1.004098	**Frequencies (cm^{-1}):** -455.5989, 68.353, 111.5629, 171.092, 189.3761, 240.9539, 254.6737, 288.5137, 334.6834, 392.9801, 486.0785, 548.8001, 609.7895, 697.3704, 786.1673, 860.5998, 902.7111, 938.7086, 996.0624, 1029.9804, 1049.1876, 1086.499, 1117.7416, 1145.4926, 1182.2283, 1215.7934, 1282.6978, 1304.0311, 1339.746, 1396.1577, 1417.1522, 1426.2771, 1440.8731, 1474.8601, 1482.88, 1496.5508, 1501.6978, 1503.726, 2892.8746, 3023.4513, 3035.5584, 3036.3321, 3062.4651, 3084.3281, 3093.147, 3103.5192, 3136.1778, 3154.7766
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.1	**Energy (Hartree)** -421.596446137597
Reaction Coordinates:	**Frequencies (cm^{-1}):**

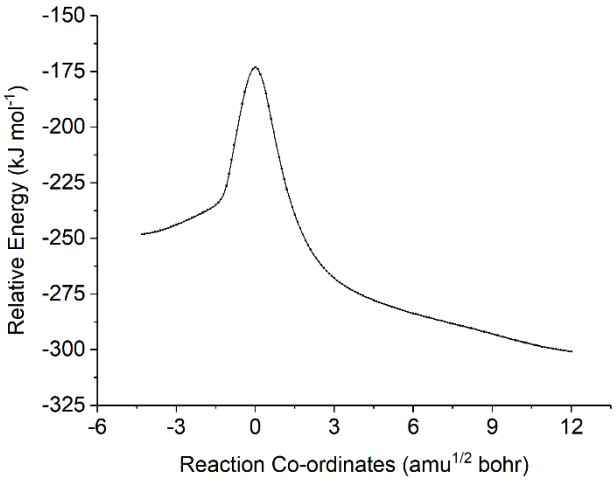
6 1.885569 -0.150819 -0.613871 6 1.665496 1.204534 -0.009417 6 -1.972738 0.222780 0.629340 6 -2.505478 0.730874 -0.637343 1 -1.689826 0.803151 -1.360245 1 -2.982768 1.697111 -0.502769 1 -3.201655 -0.003897 -1.051955 6 2.849405 -0.995521 0.231089 1 2.413916 -1.228212 1.202733 1 3.798399 -0.482032 0.396531 1 3.061957 -1.937542 -0.271798 1 2.592068 1.783612 0.191557 1 0.929757 -0.656703 -0.751598 1 2.333071 0.018405 -1.600804 1 -2.022408 0.755233 1.571191 8 -1.415518 -0.900272 0.730604 8 -1.272966 -1.641417 -0.425555 8 0.592731 1.689162 0.267246	28.6136, 36.8941, 52.8607, 72.3292, 79.5737, 93.7231, 104.2066, 160.6709, 209.1104, 296.3398, 331.5294, 453.4659, 518.627, 669.9734, 763.8095, 768.8914, 876.91, 881.8314, 924.7588, 985.8648, 1006.0905, 1055.4577, 1112.0018, 1135.4342, 1169.5424, 1280.4774, 1344.9298, 1354.1709, 1396.8592, 1410.5811, 1427.5763, 1440.2222, 1461.2682, 1478.0706, 1500.7573, 1505.7463, 1575.2569, 1782.5412, 2860.8282, 2996.6456, 3026.3718, 3031.1418, 3070.7638, 3077.3367, 3095.896, 3107.7674, 3143.4756, 3182.4111

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.2	**Energy (Hartree)** -421.552299326382
Reaction Coordinates: 6 1.739494 -0.878882 -0.138232 6 0.365480 -0.777460 0.531984 6 -0.921916 -0.377036 -0.726895 6 -2.233653 -0.842898 -0.159813 1 -3.047839 -0.364342 -0.709289 1 -2.320595 -1.920814 -0.285104 1 -2.324643 -0.585765 0.890671 6 2.420176 0.453899 -0.434635 1 3.436621 0.289212 -0.792801 1 2.468141 1.068227 0.462979 1 1.884096 1.021577 -1.194564 1 -0.073029 -1.766539 0.754521 1 1.655314 -1.487993 -1.042630 1 2.360908 -1.456954 0.553394 1 -0.620004 -0.803570 -1.679454 8 -0.676627 0.950325 -0.764079 8 -0.940398 1.503191 0.406880 8 0.162468 0.114138 1.433178	**Frequencies (cm^{-1}):** -441.6395, 72.0558, 112.4409, 176.2697, 199.7945, 243.5568, 269.0828, 288.3266, 302.4816, 393.9086, 536.8849, 548.6676, 674.0467, 702.7366, 792.628, 830.1472, 895.7149, 949.8234, 996.661, 1029.9834, 1046.6003, 1089.8941, 1104.8237, 1140.6727, 1188.0164, 1211.9866, 1291.8274, 1303.2324, 1347.7845, 1396.6285, 1409.4898, 1426.2491, 1447.4311, 1475.1692, 1485.7062, 1496.4683, 1497.3326, 1509.382, 2896.7239, 3009.1228, 3034.9724, 3037.0296, 3041.9061, 3098.5974, 3104.584, 3114.0203, 3127.4535, 3154.7772
IRC:	



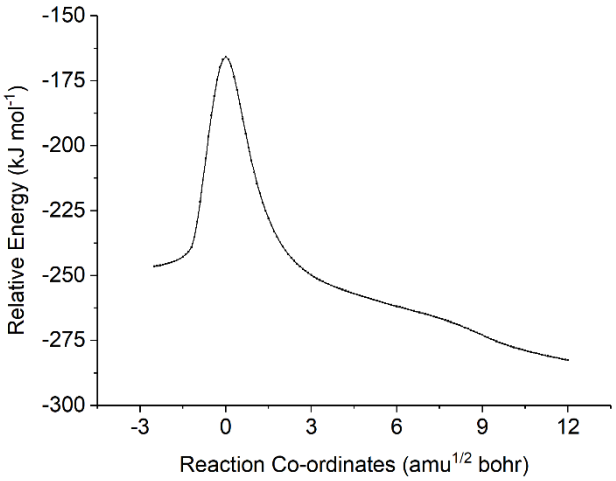
Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.2	**Energy (Hartree)** -421.596944298324
Reaction Coordinates: 6 2.525974 0.303166 -0.239626 6 1.873732 -1.033917 -0.437892 6 -1.967246 -0.653286 -0.256536 6 -2.167952 -0.457495 1.180978 1 -2.871815 0.364363 1.337315 1 -2.509020 -1.371976 1.657590 1 -1.223658 -0.128611 1.622889 6 1.873010 1.205142 0.797464 1 2.435312 2.133195 0.897976 1 1.844147 0.719625 1.773114 1 0.851607 1.452839 0.509622 1 2.358119 -1.675521 -1.202853 1 2.554041 0.780036 -1.226981 1 3.578523 0.098875 -0.005318 1 -2.067663 -1.604421 -0.764995 8 -1.651970 0.285159 -1.033510 8 -1.471712 1.533889 -0.479857 8 0.901844 -1.437806 0.155281	**Frequencies (cm^{-1}):** 19.6956, 35.2664, 45.7947, 64.0241, 73.9989, 78.1916, 161.7586, 162.9914, 244.9924, 256.2858, 296.2029, 456.0817, 663.7704, 670.7, 674.1578, 760.5124, 848.3052, 881.8958, 912.9134, 984.8543, 1008.7166, 1054.7273, 1113.8124, 1115.9216, 1151.6929, 1284.5835, 1353.5852, 1368.8002, 1395.9662, 1415.2611, 1426.7607, 1440.2789, 1444.9463, 1462.1051, 1499.2891, 1514.8318, 1572.7492, 1788.18, 2871.3864, 2995.4041, 3013.8909, 3025.8389, 3034.7747, 3068.2824, 3098.4348, 3105.8516, 3141.7506, 3180.9383

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.3	**Energy (Hartree)** -421.553488533986
Reaction Coordinates: 6 1.666181 0.206686 0.634242 6 0.528661 0.332833 -0.373832 6 -1.048605 0.630118 0.553826 6 -2.023270 1.206066 -0.432959 1 -1.819805 2.267263 -0.565724 1 -3.036183 1.094724 -0.038376 1 -1.965868 0.697015 -1.389807 6 3.019641 0.106907 -0.073650 1 3.043483 -0.761659 -0.731113 1 3.830207 0.011890 0.649341 1 3.216841 0.993357 -0.680100	**Frequencies (cm^{-1}):** -439.4293, 74.9712, 117.5825, 163.4788, 184.285, 235.5206, 275.1129, 289.9979, 313.9869, 380.3671, 502.319, 543.0404, 634.6056, 710.8916, 794.449, 858.891, 901.3207, 942.9218, 995.5055, 1014.1629, 1050.9656, 1087.6205, 1122.4807, 1148.4039, 1181.6662, 1214.6676, 1288.6972, 1296.2413, 1353.7458, 1395.8603, 1407.3544, 1425.9179,

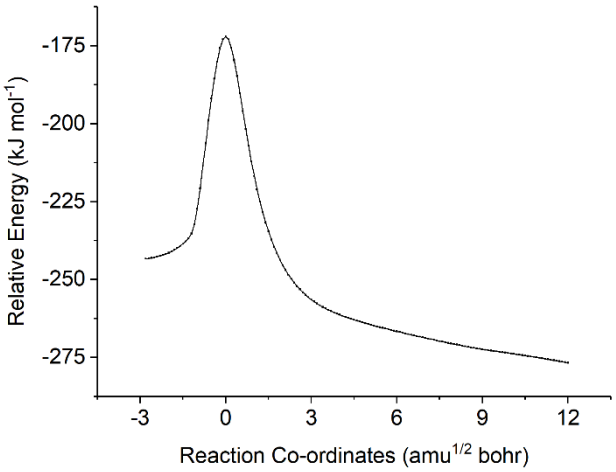
1 0.485715 1.309232 -0.889470 1 1.660836 1.070389 1.304994 1 1.494895 -0.685007 1.238496 1 -0.823675 1.225769 1.433932 8 -1.204232 -0.652315 0.940782 8 -1.398053 -1.435076 -0.106369 8 0.234524 -0.677439 -1.106654	1446.6551, 1475.2163, 1480.2614, 1496.1689, 1498.1925, 1505.7287, 2894.4403, 3018.7089, 3026.1407, 3035.7987, 3069.8406, 3088.4398, 3103.578, 3103.7855, 3129.1253
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.3	**Energy (Hartree)** -421.597591473391
Reaction Coordinates: 6 -2.071139 -0.008893 0.583128 6 -1.163705 0.373705 -0.551253 6 2.411333 0.150460 -0.387143 6 2.396554 0.757853 0.946109 1 3.128683 1.557201 1.019039 1 2.571581 -0.018859 1.694951 1 1.393673 1.147082 1.143291 6 -3.500608 -0.287432 0.103488 1 -3.964312 0.610141 -0.307410 1 -4.119366 -0.636223 0.929495 1 -3.515255 -1.058226 -0.668707 1 -1.163666 -0.332938 -1.403827 1 -1.645730 -0.916486 1.020457 1 -2.044530 0.777536 1.337300 1 2.987239 0.527548 -1.224372 8 1.758209 -0.885147 -0.678005 8 0.966487 -1.434112 0.307087 8 -0.482562 1.372893 -0.592355	**Frequencies (cm^{-1}):** 30.5976, 40.2006, 60.8459, 74.9248, 85.6753, 95.1958, 137.9676, 167.7147, 212.9328, 298.5853, 341.5353, 454.1851, 511.436, 670.4453, 759.3936, 766.0922, 876.0932, 883.7807, 920.2088, 982.1004, 1007.9798, 1058.7137, 1115.3856, 1131.1575, 1162.8557, 1272.0979, 1328.4197, 1353.9243, 1396.7576, 1410.2893, 1427.7266, 1441.3834, 1466.1072, 1469.4499, 1501.8416, 1505.4525, 1573.9096, 1777.975, 2899.6855, 3024.2393, 3029.8981, 3032.8514, 3068.3198, 3077.9606, 3098.1303, 3099.4953, 3139.3665, 3174.061

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.1	**Energy (Hartree)** -421.549557333725
Reaction Coordinates: 6 -1.664114 -0.839665 -0.252087 6 -0.379654 -0.651047 0.563542	**Frequencies (cm^{-1}):** -475.7885, 71.9645, 97.307, 148.3972, 217.6595, 231.5415, 240.4775, 315.4343,

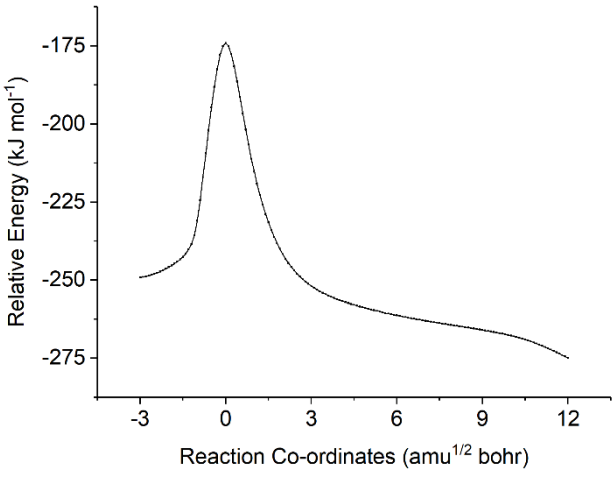
6 0.588907 0.781316 -0.282634 6 0.368099 2.146704 0.292157 1 0.830031 2.226736 1.274772 1 0.798600 2.910191 -0.359431 1 -0.695043 2.351155 0.388125 6 -2.650602 0.325306 -0.229662 1 -2.292503 1.188833 -0.791219 1 -3.600525 0.028104 -0.673832 1 -2.858143 0.651674 0.791746 1 -0.511098 -0.127907 1.526224 1 -1.386627 -1.106009 -1.273814 1 -2.145293 -1.726383 0.167538 1 0.213387 0.563089 -1.277724 8 1.823635 0.323408 -0.062243 8 1.974811 -0.901327 -0.539733 8 0.460479 -1.613977 0.561942	373.572, 393.4528, 477.8707, 514.9309, 562.2577, 623.0975, 770.7675, 862.8957, 907.499, 970.8542, 994.7688, 1032.352, 1054.2595, 1107.4535, 1118.9124, 1151.8491, 1180.4813, 1258.4082, 1286.2032, 1322.8348, 1347.6085, 1384.3431, 1414.9179, 1423.6612, 1443.2128, 1481.5857, 1484.722, 1492.7394, 1503.9163, 1510.0705, 2908.6597, 3025.6522, 3030.5374, 3036.8875, 3059.1189, 3085.5595, 3091.8356, 3102.1467, 3120.6752, 3139.1892
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.1	**Energy (Hartree)** -421.592887336933
Reaction Coordinates: 6 -1.947863 0.158963 -0.471952 6 -1.519455 -1.246505 -0.179510 6 1.897034 0.057497 0.405059 6 2.832289 -1.007369 -0.004265 1 3.256843 -0.802066 -0.983818 1 3.635400 -1.100336 0.731554 1 2.297352 -1.959075 -0.022590 6 -3.161713 0.568926 0.373073 1 -2.905281 0.609443 1.431894 1 -3.506494 1.558385 0.077111 1 -3.994879 -0.125967 0.251546 1 -2.326050 -2.007544 -0.238744 1 -1.107399 0.841580 -0.332364 1 -2.230343 0.178646 -1.531966 1 1.362129 0.050766 1.348026 8 1.705659 1.035256 -0.352434 8 0.806679 2.010102 0.061311 8 -0.397716 -1.599471 0.107989	**Frequencies (cm^{-1}):** 29.436, 50.3859, 71.4122, 76.7841, 100.3718, 104.5291, 132.4944, 197.5896, 210.1367, 269.7783, 325.1018, 332.7315, 521.929, 549.7382, 762.9334, 864.7927, 876.4414, 883.3442, 925.0513, 960.1427, 1008.5452, 1074.129, 1136.0436, 1162.6579, 1170.6192, 1282.8805, 1348.8374, 1359.0674, 1409.2952, 1411.2832, 1428.8512, 1459.2233, 1466.447, 1474.9059, 1500.8704, 1505.9838, 1592.7861, 1776.5071, 2866.0757, 2991.4436, 3026.223, 3029.6772, 3059.2132, 3076.5423, 3090.3431, 3106.7397, 3135.5724, 3171.0259

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.2	**Energy (Hartree)** -421.552392828301
Reaction Coordinates: 6 -1.691598 0.758841 0.326596 6 -0.454064 0.007847 0.850877 6 0.913084 0.490637 -0.349149 6 1.569522 1.794306 -0.020156 1 2.191540 1.700457 0.868359 1 2.190999 2.132992 -0.851193 1 0.813636 2.557186 0.159504 6 -2.413184 0.062354 -0.820870 1 -3.306769 0.620334 -1.101323 1 -2.707097 -0.945609 -0.535715 1 -1.786348 -0.024289 -1.709976 1 -0.012433 0.467067 1.751693 1 -1.418100 1.782713 0.057519 1 -2.366432 0.847062 1.183014 1 0.310269 0.425915 -1.249402 8 1.706425 -0.570024 -0.166955 8 1.066596 -1.690370 -0.460545 8 -0.454499 -1.270573 0.815466	**Frequencies (cm^{-1}):** -455.2172, 74.2402, 97.3318, 162.3392, 178.4687, 230.5036, 249.0991, 322.891, 357.0637, 374.4737, 489.3523, 529.459, 619.809, 637.3621, 786.8566, 826.7009, 906.8747, 983.3953, 1003.2031, 1030.4539, 1050.3595, 1097.0056, 1120.6748, 1152.9465, 1185.9323, 1260.7318, 1288.7282, 1328.7589, 1341.2467, 1385.6545, 1412.5751, 1422.8228, 1454.5993, 1481.296, 1488.7712, 1492.1226, 1495.5713, 1503.4234, 2905.6421, 3015.6992, 3033.5068, 3038.3852, 3041.7651, 3087.3697, 3098.9421, 3118.0155, 3119.3267, 3132.4769
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.2	**Energy (Hartree)** -421.593046039135
Reaction Coordinates: 6 -2.613139 0.150560 0.059691 6 -1.889859 -1.073793 0.535480 6 1.844747 -0.246405 0.291861 6 2.480589 -1.253799 -0.577504 1 2.838818 -0.806520 -1.501334 1 3.312019 -1.730879 -0.052411 1 1.749937 -2.034690 -0.801232 6 -1.860106 1.019848 -0.936402 1 -2.489897 1.846221 -1.265092 1 -1.570878 0.444626 -1.815956	**Frequencies (cm^{-1}):** 17.7044, 37.244, 63.1501, 69.0875, 81.6765, 120.1363, 164.4474, 185.5717, 245.9487, 258.7123, 268.921, 324.0153, 550.3206, 662.5874, 673.9513, 848.6607, 868.1376, 878.7414, 913.8014, 960.7304, 1010.075, 1075.2919, 1116.254, 1151.5121, 1162.811, 1284.3917, 1347.7404, 1369.7016, 1409.3151, 1416.1238, 1426.8359, 1444.4297,

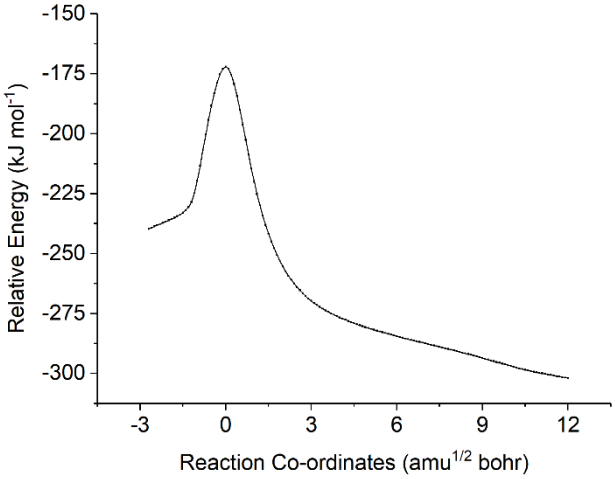
1 -0.958225 1.436123 -0.487892 1 -2.448241 -1.681606 1.276777 1 -2.887075 0.713851 0.960117 1 -3.572113 -0.202944 -0.341278 1 1.424806 -0.478359 1.264414 8 1.764167 0.941079 -0.094743 8 1.130699 1.853991 0.732763 8 -0.791434 -1.430607 0.177621	1459.827, 1464.4157, 1498.7334, 1518.468, 1592.4816, 1784.2264, 2875.3544, 2992.6708, 3012.7622, 3025.4207, 3034.4261, 3072.6458, 3099.4898, 3105.1407, 3135.32, 3167.9945

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.3	**Energy (Hartree)** -421.552491548523
Reaction Coordinates: 6 1.629964 0.405389 0.502142 6 0.537758 -0.165869 -0.407618 6 -1.051420 0.580516 0.307269 6 -1.351633 1.957729 -0.193535 1 -1.669366 1.930035 -1.234334 1 -2.140489 2.419692 0.403258 1 -0.465811 2.585480 -0.112783 6 3.020063 0.107886 -0.064159 1 3.140450 0.534668 -1.061694 1 3.796294 0.531216 0.574297 1 3.182846 -0.966937 -0.136512 1 0.484523 0.309861 -1.403022 1 1.502651 1.485627 0.613085 1 1.521938 -0.049985 1.487873 1 -0.773636 0.451651 1.348700 8 -1.901059 -0.349686 -0.134539 8 -1.582561 -1.543728 0.337762 8 0.322645 -1.424737 -0.371155	**Frequencies (cm^{-1}):** -444.222, 75.0725, 93.6383, 158.9987, 189.7572, 235.3774, 245.3922, 317.6951, 357.7265, 372.9298, 481.4654, 505.9212, 580.698, 621.2213, 788.7839, 869.2352, 909.4963, 988.143, 1008.4051, 1013.6967, 1064.6571, 1116.298, 1123.1731, 1152.4218, 1177.5094, 1262.3428, 1290.7836, 1329.6445, 1356.504, 1387.2132, 1408.9648, 1422.9765, 1448.1919, 1475.3279, 1481.5227, 1493.9068, 1496.8241, 1504.4106, 2897.1493, 3017.9865, 3027.6401, 3038.0557, 3066.0305, 3087.2328, 3099.0373, 3104.624, 3119.6249, 3132.3496
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.3	**Energy (Hartree)** -421.595100791669
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.051345 -0.085895 -0.564145 6 1.113731 0.329487 0.534249 6 -2.063768 0.010289 0.284461 6 -3.002990 0.914732 -0.403985 1 -3.128914 0.633779 -1.446450 1 -3.970852 0.907611 0.103088 1 -2.613927 1.934069 -0.342819 6 3.513811 0.158197 -0.166771 1 3.765471 -0.363415 0.758158 1 4.184890 -0.205970 -0.944040 1 3.713852 1.220179 -0.019911 1 1.269120 -0.180915 1.500908 1 1.887761 -1.150972 -0.739946 1 1.791156 0.457051 -1.472619 1 -1.812961 0.100396 1.334551 8 -1.527872 -0.922612 -0.357336 8 -0.601271 -1.704633 0.316380 8 0.284345 1.213161 0.436733	24.9661, 36.3675, 79.8801, 85.051, 117.7003, 137.1757, 195.3092, 217.8712, 239.7202, 288.5851, 331.0131, 375.8177, 512.8906, 554.0066, 776.215, 864.4793, 876.1346, 883.7518, 919.2619, 965.623, 1002.2612, 1072.2324, 1121.2311, 1162.3308, 1164.7847, 1269.4631, 1326.5173, 1352.6383, 1408.5293, 1410.0875, 1425.6943, 1457.6501, 1463.8446, 1476.3542, 1501.4739, 1505.7525, 1591.5707, 1745.0852, 2930.86, 3026.9634, 3029.4674, 3043.7528, 3074.2145, 3079.3903, 3098.1159, 3101.7584, 3137.5272, 3179.9323

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.1	**Energy (Hartree)** -421.552817024742
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.635617 0.320976 0.186542 6 -0.400464 0.081760 -0.647996 6 0.822811 -0.797904 0.420314 6 1.866751 -1.446277 -0.476205 1 2.444082 -0.687155 -1.001031 1 1.414118 -2.124484 -1.201227 1 2.554405 -2.022456 0.144696 6 -2.636888 -0.827527 0.091746 1 -2.960212 -0.996853 -0.936831 1 -2.219835 -1.762046 0.470543 1 -3.522940 -0.604870 0.685061 1 -0.532483 -0.489920 -1.563843 1 -2.085297 1.247257 -0.185624 1 -1.348678 0.513789 1.217616 1 0.068042 -1.496415 0.819921 8 1.192094 0.121019 1.235628 8 0.660612 1.806113 0.192406 8 0.408449 1.127491 -0.914995	-448.7841, 86.1757, 112.6357, 176.9164, 190.9359, 220.8673, 256.763, 277.1845, 372.8064, 385.4061, 488.0973, 537.3276, 593.9945, 710.1754, 785.36, 888.591, 915.6244, 944.5086, 987.6086, 1024.0983, 1064.3556, 1070.3482, 1109.8843, 1143.9378, 1185.5761, 1203.9772, 1282.0755, 1302.0812, 1334.6578, 1398.9077, 1418.786, 1427.2747, 1436.3273, 1482.0907, 1482.7554, 1495.9905, 1503.5483, 1505.0531, 2912.6405, 3019.6992, 3028.5025, 3031.378, 3079.2979, 3090.7257, 3098.7508, 3107.4046, 3117.5508, 3119.6179
IRC	

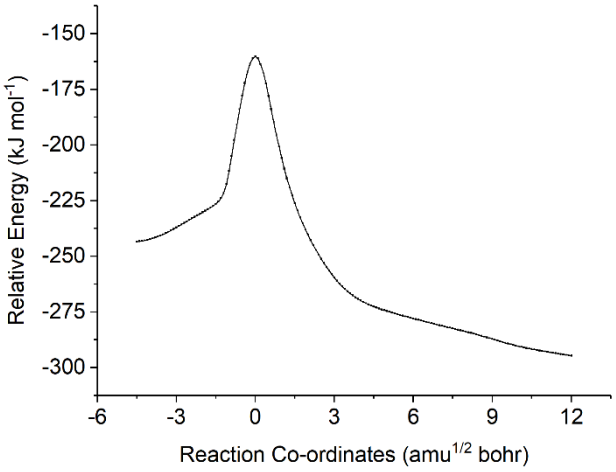


Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.1	**Energy (Hartree)** -421.596435832193
Reaction Coordinates: 6 1.675614 -0.282532 -0.537739 6 1.359132 0.628879 0.569750 6 -2.067320 -0.366123 0.514890 6 -2.860736 -0.508619 -0.746878 1 -2.564435 -1.397441 -1.299317 1 -2.712185 0.384495 -1.355852 1 -3.924781 -0.559789 -0.500241 6 2.858441 -1.203731 -0.254214 1 3.771548 -0.639241 -0.060596 1 2.663929 -1.843580 0.606878 1 3.045645 -1.850428 -1.109797 1 1.878408 0.624328 1.522952 1 1.821817 0.339735 -1.428753 1 0.759785 -0.842528 -0.754015 1 -2.317518 0.519016 1.128116 8 -1.220383 -1.144696 0.890183 8 -0.272829 1.588721 -0.652743 8 0.466585 1.513248 0.509531	**Frequencies (cm^{-1}):** 36.853, 45.3465, 67.437, 77.7763, 100.7234, 105.865, 119.8, 180.4349, 204.2004, 220.6665, 360.3963, 457.8005, 512.7642, 685.0171, 703.8188, 782.2635, 847.8696, 875.733, 891.114, 936.0878, 1047.8285, 1105.6493, 1130.5019, 1134.9002, 1141.2588, 1257.1687, 1326.0369, 1374.5668, 1378.0602, 1423.6171, 1425.4559, 1427.2401, 1460.3756, 1470.7763, 1503.4295, 1506.161, 1574.7377, 1781.3528, 2917.5182, 3008.5649, 3025.5961, 3032.4269, 3037.0121, 3086.1893, 3094.7245, 3108.5292, 3131.9677, 3155.8948

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.2	**Energy (Hartree)** -421.548726352612
Reaction Coordinates: 6 1.577500 -0.451707 0.816209 6 0.170544 0.093323 0.972746 6 -0.977975 -0.724066 -0.246747 6 -2.383994 -0.646310 0.331617 1 -2.711107 0.389351 0.406455 1 -2.446191 -1.120664 1.312145 1 -3.067161 -1.167195 -0.340980 6 2.136136 -0.802135 -0.562065 1 2.168382 0.066198 -1.211732 1 3.147948 -1.191511 -0.440904	**Frequencies (cm^{-1}):** -440.8988, 60.1082, 128.2652, 176.284, 200.375, 237.5097, 264.7053, 272.3935, 311.1051, 438.1377, 491.3508, 543.1412, 582.4567, 724.3799, 771.9594, 866.5055, 896.6203, 945.2631, 989.2353, 1010.7822, 1059.8268, 1089.1741, 1115.1152, 1130.6905, 1173.1832, 1226.0427, 1305.8307, 1315.8973, 1378.0793, 1397.5886,

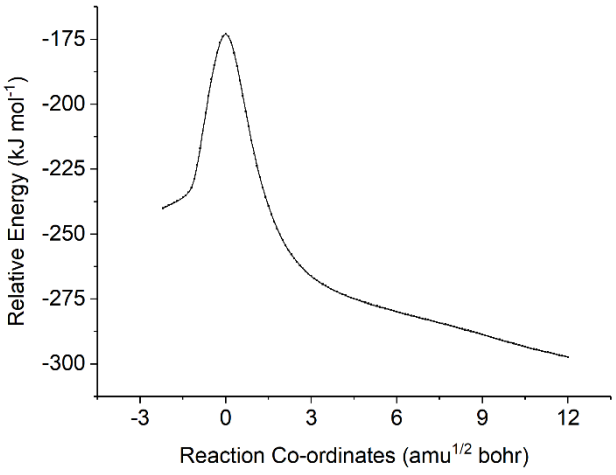
1 1.541995 -1.567736 -1.057718 1 -0.255127 -0.058067 1.961670 1 1.619932 -1.332926 1.460853 1 2.222974 0.298782 1.287800 1 -0.494698 -1.711422 -0.137348 8 -0.725869 -0.108345 -1.339132 8 0.245417 1.580634 -0.648535 8 -0.127074 1.350282 0.598816	1416.7276, 1432.5987, 1443.9895, 1464.6614, 1481.8242, 1495.5263, 1498.1068, 1503.4047, 2896.6268, 3000.2024, 3031.575, 3044.1848, 3048.7751, 3091.464, 3103.5638, 3117.3675, 3121.2128, 3150.0096

IRC



Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.2	**Energy (Hartree)** -421.593861868972
Reaction Coordinates: 6 -2.289340 0.667124 0.223020 6 -1.380521 -0.253540 0.928090 1 -1.034271 -0.101662 1.943518 8 -0.921544 -1.308237 0.416618 8 -1.255080 -1.600684 -0.890993 6 -1.558254 1.564742 -0.799842 1 -0.804702 2.180955 -0.313201 1 -1.079911 0.951502 -1.558758 1 -2.284551 2.217254 -1.282739 1 -2.801249 1.280757 0.964262 1 -3.016254 0.049843 -0.311017 6 2.109234 -0.051274 0.033901 6 3.551293 0.003408 -0.369730 1 4.054409 0.857372 0.077369 1 3.619173 0.052464 -1.459661 1 4.045376 -0.925006 -0.071482 1 1.527310 -0.894233 -0.382797 8 1.574148 0.752421 0.762109	**Frequencies (cm^{-1}):** 22.853, 26.0031, 43.8889, 49.7757, 70.4458, 80.2237, 112.819, 161.9233, 199.2529, 243.914, 318.6642, 513.2774, 532.5313, 649.5875, 782.8472, 811.6095, 841.0502, 868.4889, 891.6661, 906.886, 1015.0018, 1086.0657, 1131.7504, 1144.6879, 1147.6118, 1290.5496, 1333.8152, 1375.6581, 1380.1994, 1402.8184, 1439.7307, 1460.0967, 1461.2279, 1468.4263, 1492.7702, 1513.9816, 1570.0011, 1785.4563, 2926.4545, 3022.7495, 3030.4738, 3049.5588, 3073.2538, 3086.2388, 3114.8273, 3134.2045, 3137.9692, 3176.7519

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.3	**Energy (Hartree)** -421.553174717087
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.417198 -0.687853 0.536451 6 -0.316526 -0.462936 -0.469455 6 1.284319 -0.500849 0.472457 6 2.408267 -0.770940 -0.516527 1 2.250192 -1.699999 -1.066422 1 3.346853 -0.857191 0.033091 1 2.505351 0.054950 -1.219141 6 -2.797807 -0.374662 -0.052422 1 -3.008762 -0.985106 -0.931781 1 -3.570739 -0.577433 0.688742 1 -2.873442 0.673658 -0.337320 1 -0.252219 -1.173228 -1.290329 1 -1.229669 -0.077895 1.416367 1 -1.368135 -1.735422 0.838278 1 0.980539 -1.375891 1.071667 8 1.267564 0.617063 1.098731 8 -0.106090 1.675898 -0.004864 8 -0.129760 0.774163 -0.972140	-444.9487, 74.9216, 124.9824, 167.0417, 185.3857, 215.3436, 260.9597, 275.883, 351.4307, 418.2267, 485.2143, 551.4887, 612.677, 676.3137, 797.9259, 885.7834, 900.547, 945.8479, 990.6047, 991.7042, 1058.9089, 1077.1946, 1105.323, 1141.7259, 1185.9153, 1206.4877, 1298.8354, 1306.8728, 1353.2693, 1398.2586, 1408.5676, 1432.2777, 1436.2517, 1481.7266, 1483.2642, 1496.2087, 1498.6676, 1505.9064, 2912.4073, 3030.8051, 3033.9521, 3050.2013, 3090.1644, 3090.3847, 3108.3851, 3114.4963, 3117.3564, 3128.6289
IRC  	

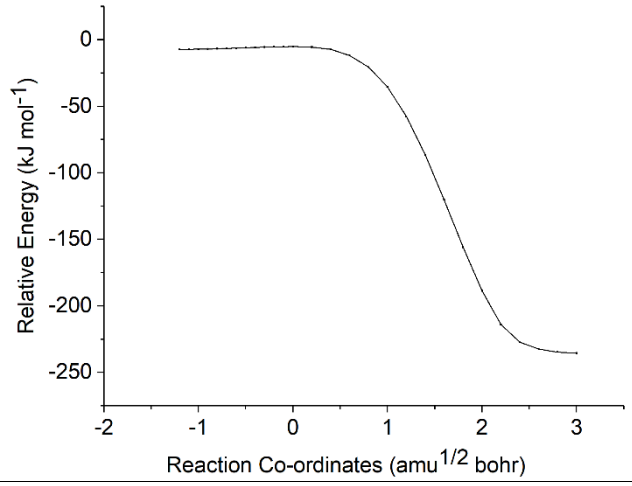
Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.3	**Energy (Hartree)** -421.597649635912
Reaction Coordinates: 6 1.600425 -0.789202 0.456010 6 1.291458 0.611512 0.790171 6 -2.178308 0.105372 0.327895 6 -2.779359 -0.660224 -0.810701 1 -2.349063 -0.296457 -1.745022 1 -3.854010 -0.462060 -0.850522 1 -2.603423 -1.728080 -0.702155 6 2.750006 -0.889736 -0.571403 1 3.675271 -0.470993 -0.176148 1 2.926937 -1.938067 -0.807636 1 2.485014 -0.365909 -1.486497 1 1.615409 1.096673 1.704856 1 0.698389 -1.231015 0.033449 1 1.860260 -1.314109 1.374492 1 -2.314102 1.201200 0.278710 8 -1.599242 -0.394304 1.265551	**Frequencies (cm^{-1}):** 34.3343, 50.4259, 62.445, 78.5207, 93.396, 108.8934, 124.0889, 184.5023, 202.1773, 247.1415, 323.6472, 512.1253, 530.2569, 649.3045, 782.5202, 808.0057, 852.8218, 875.4383, 890.4967, 905.6274, 1008.3437, 1083.7874, 1129.5219, 1134.0319, 1149.4922, 1281.4845, 1331.5976, 1374.3901, 1377.4555, 1402.4769, 1426.9531, 1460.3532, 1466.6299, 1471.1677, 1496.5973, 1511.4618, 1572.4543, 1780.859, 2919.2627, 3025.4484, 3043.2422, 3057.7005, 3085.9501, 3099.8593,

8 0.164176 0.904091 -1.152243 8 0.654314 1.395523 0.039772	3110.9962, 3131.7359, 3132.6979, 3162.3001

S10.18 Ozonolysis of *Z*-2-pentene (Alkene 16)

Compound: Z-EtCHCHMe + O_3 PRC1.1	**Energy (Hartree)** -421.485915987591
Reaction Coordinates: 6 1.690064 -0.580681 -0.464478 6 0.754076 -0.056575 0.581561 6 0.148956 1.144028 0.619170 6 0.239489 2.242063 -0.391680 1 0.853972 1.981390 -1.250184 1 -0.754359 2.507941 -0.757122 1 0.658560 3.143270 0.064103 1 -0.443884 1.374398 1.497639 1 0.609621 -0.711825 1.435080 6 3.109933 -0.792147 0.081851 1 3.105640 -1.471869 0.935629 1 3.550001 0.150149 0.410230 1 3.758551 -1.221211 -0.682782 1 1.723823 0.084451 -1.326579 1 1.307398 -1.537419 -0.828989 8 -2.458488 0.365242 -0.119871 8 -2.355915 -0.852044 0.211952 8 -1.438651 -1.518123 -0.349027	**Frequencies (cm^{-1}):** 16.3461, 33.9606, 62.951, 77.2082, 94.849, 98.7302, 107.8881, 215.0195, 267.3096, 279.4655, 308.9347, 485.8696, 570.9152, 738.2921, 744.9766, 794.9528, 863.127, 935.113, 1005.3333, 1019.9495, 1054.5782, 1062.4593, 1091.283, 1158.4361, 1175.8812, 1179.4621, 1280.6143, 1299.6119, 1338.398, 1405.5231, 1409.8654, 1444.9284, 1481.5746, 1483.5515, 1494.8062, 1498.3462, 1508.3192, 1661.2401, 3021.2104, 3025.3238, 3027.6121, 3063.5139, 3069.8607, 3089.9603, 3092.7421, 3114.6609, 3123.9899, 3147.9352

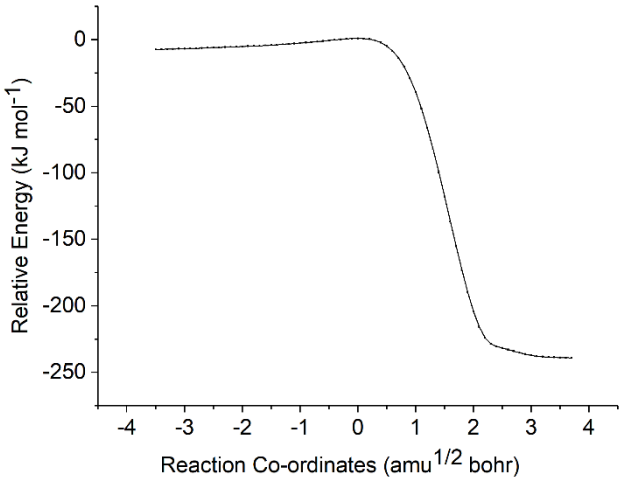
Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.1	**Energy (Hartree)** -421.481920649981
Reaction Coordinates: 6 1.537073 -0.711988 -0.410332 6 0.545964 -0.235037 0.606613 6 -0.041306 1.001289 0.636802 6 0.176339 2.097263 -0.356088 1 0.426058 1.717199 -1.344409 1 -0.712974 2.719312 -0.444805 1 0.994634 2.746859 -0.030281 6 2.987602 -0.466429 0.036310 1 3.685998 -0.858832 -0.703625 1 3.195991 -0.959133 0.987145 1 3.190643 0.597543 0.161642 1 -0.575098 1.276466 1.537311 1 1.360594 -0.226410 -1.369761 1 1.390243 -1.780796 -0.570841 1 0.437240 -0.856941 1.486873 8 -2.157619 0.450121 -0.215537 8 -2.199464 -0.779285 0.158471 8 -1.221338 -1.481568 -0.291568	**Frequencies (cm^{-1}):** -139.2013, 45.7237, 62.0983, 93.8126, 128.9555, 163.8692, 195.094, 217.4619, 293.3005, 303.0398, 432.3547, 523.0694, 571.2071, 738.0359, 781.5139, 794.1595, 861.0797, 933.6821, 993.8774, 1022.4919, 1050.874, 1054.0495, 1088.3243, 1095.0381, 1113.2647, 1176.2111, 1272.7227, 1292.8308, 1340.1243, 1403.2789, 1410.6896, 1446.0296, 1475.2666, 1485.3282, 1497.4079, 1498.7036, 1511.2308, 1586.0258, 3017.3027, 3027.6856, 3046.047, 3073.9682, 3082.8548, 3092.2204, 3097.3822, 3118.8816, 3150.1332, 3171.5845
IRC:	



Compound: Z-EtCHCHMe + O_3 POZ1.1	**Energy (Hartree)** -421.580622944704
Reaction Coordinates: 6 -1.553649 -0.584625 -0.492720 6 -0.244001 -0.561739 0.280899 6 0.517018 0.798878 0.459114 6 0.076409 1.986478 -0.375029 1 0.051749 1.737697 -1.434389 1 -0.908424 2.334351 -0.065086 1 0.777839 2.808751 -0.236077 6 -2.743768 -0.094372 0.333660 1 -2.622607 0.939096 0.659495 1 -3.661693 -0.147624 -0.251103 1 -2.882468 -0.708324 1.224950 1 -0.391742 -1.000074 1.272486 1 -1.456093 -0.007112 -1.411757 1 -1.730050 -1.618896 -0.794525 1 0.523345 1.058280 1.521065 8 1.858646 0.483099 0.044703 8 1.936787 -0.952528 0.168923 8 0.703079 -1.363554 -0.428701	**Frequencies (cm^{-1}):** 39.003, 115.5644, 182.3987, 228.9281, 234.0677, 285.15, 353.1717, 390.0921, 443.0518, 496.8085, 695.2308, 707.2439, 723.3158, 776.0962, 826.4231, 888.076, 938.0483, 942.8503, 996.0758, 1046.2614, 1058.2113, 1070.9476, 1116.9519, 1171.6633, 1188.7505, 1282.578, 1320.2756, 1332.9801, 1367.7061, 1384.4634, 1405.737, 1420.5157, 1424.941, 1483.8785, 1496.5478, 1500.2911, 1505.2034, 1513.4434, 3003.3032, 3025.9169, 3032.7374, 3042.6299, 3046.2986, 3074.0422, 3096.27, 3098.4244, 3106.9382, 3121.0695

Compound: Z-EtCHCHMe + O_3 PRC1.2	**Energy (Hartree)** -421.486538211307
Reaction Coordinates: 6 1.779046 -1.077094 -0.136753 6 1.201636 -0.066142 0.804319 6 1.047226 1.251419 0.611672 6 1.423053 2.050749 -0.594315 1 1.798082 1.439144 -1.411749 1 0.563460 2.617172 -0.960108 1 2.194128 2.783389 -0.340406 1 0.626736 1.824953 1.430786 1 0.885262 -0.465169 1.764430 6 0.926237 -2.347264 -0.245536 1 -0.062625 -2.118669 -0.642859 1 0.792792 -2.814051 0.732065 1 1.400604 -3.078109 -0.901222	**Frequencies (cm^{-1}):** 17.983, 28.1298, 42.6776, 61.2296, 78.7215, 103.1846, 131.5227, 198.4799, 220.6543, 264.4991, 306.272, 455.65, 579.03, 714.4045, 736.9095, 800.6033, 869.9845, 938.6042, 998.4331, 1029.5138, 1056.1354, 1064.2333, 1092.0364, 1162.117, 1174.8367, 1188.8683, 1280.208, 1298.7537, 1337.3589, 1409.7277, 1412.0548, 1445.9767, 1474.6914, 1482.8954, 1489.5188, 1499.6188, 1506.5024, 1680.477,

1 2.774185 -1.358675 0.228769 1 1.930294 -0.646423 -1.126377 8 -1.571613 1.051512 -0.249519 8 -2.390002 0.246652 0.270933 8 -2.434148 -0.929860 -0.197620	2985.2115, 3018.627, 3027.0897, 3057.104, 3065.4498, 3088.5795, 3100.1847, 3110.6328, 3115.4909, 3143.7423

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.2	**Energy (Hartree)** -421.476885591147
Reaction Coordinates: 6 1.679182 -0.864164 0.505697 6 0.487846 -0.127589 1.054031 6 0.013721 1.117827 0.744532 6 0.562756 2.080729 -0.264959 1 -0.032790 2.991119 -0.284867 1 1.592141 2.359835 -0.026312 1 0.560693 1.657530 -1.267710 6 2.027455 -0.701934 -0.976023 1 2.412822 0.288706 -1.207730 1 1.158315 -0.888937 -1.604204 1 2.799567 -1.422369 -1.247952 1 -0.741940 1.514716 1.409354 1 1.522092 -1.924018 0.713736 1 2.545951 -0.580413 1.116799 1 0.064878 -0.582430 1.941426 8 -1.846089 0.511094 -0.601017 8 -2.101812 -0.621288 -0.051518 8 -1.115536 -1.445176 -0.087741	**Frequencies (cm^{-1}):** -126.4689, 30.33, 62.5429, 107.4037, 134.127, 162.5276, 183.0648, 219.4792, 272.8367, 323.0429, 431.8665, 452.6057, 666.4433, 729.0285, 745.6078, 784.0458, 824.6833, 943.34, 980.0162, 1045.4895, 1054.949, 1060.5751, 1096.9769, 1104.239, 1118.7334, 1138.9058, 1282.5462, 1307.8236, 1389.145, 1402.6045, 1413.9986, 1454.5312, 1468.6294, 1483.6732, 1490.7571, 1505.9371, 1517.8441, 1588.1979, 2980.8597, 3026.9433, 3044.3464, 3049.2838, 3090.5147, 3100.3669, 3117.2101, 3121.9256, 3149.0335, 3173.2118
IRC:  	

Compound: Z-EtCHCHMe + O_3 POZ1.2	**Energy (Hartree)** -421.579310920700
Reaction Coordinates: 6 -1.688587 -0.010523 0.557950 6 -0.217169 -0.274690 0.883741 6 0.862963 0.726409 0.365555 1 1.650149 0.783536 1.122288 6 0.434022 2.122044 -0.032372	**Frequencies (cm^{-1}):** 48.1535, 122.0777, 173.958, 206.0727, 238.8542, 266.616, 318.1005, 361.8957, 482.9635, 532.5013, 691.5148, 716.3085, 743.4831, 754.8398, 809.0164, 880.4181, 915.9471, 937.6895, 958.426, 1036.5619,

1 1.298162 2.689194 -0.375997 1 -0.312217 2.114698 -0.822375 1 0.020125 2.638884 0.833691 8 1.396368 0.048574 -0.772207 8 1.497223 -1.282315 -0.268810 8 0.165570 -1.518591 0.272459 1 -0.100472 -0.360650 1.968309 1 -1.936025 0.986245 0.932705 1 -2.282994 -0.704839 1.156222 6 -2.091923 -0.153975 -0.910249 1 -1.931333 -1.172263 -1.257863 1 -3.149444 0.083723 -1.029932 1 -1.525072 0.504536 -1.566333	1081.759, 1098.3757, 1118.9318, 1141.546, 1196.8561, 1282.4425, 1329.8854, 1336.4482, 1370.482, 1398.2098, 1400.5574, 1421.1929, 1428.1523, 1481.424, 1492.9937, 1496.3208, 1503.7782, 1514.2391, 3000.3475, 3021.475, 3030.1411, 3044.2734, 3049.5474, 3050.9091, 3101.7669, 3106.6684, 3118.7516, 3135.9776

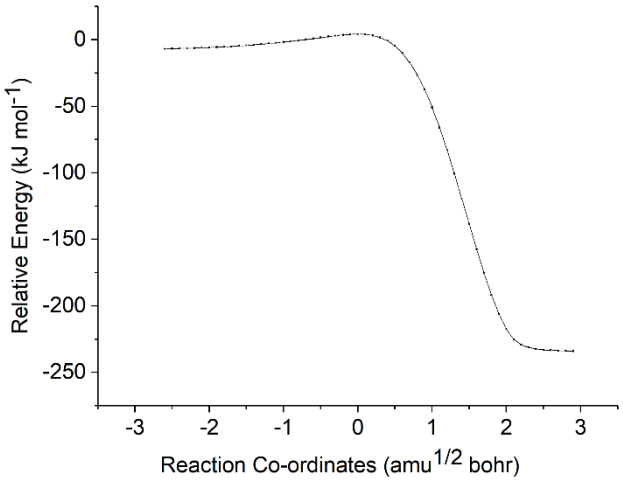
Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.3	**Energy (Hartree)** -421.482637679565
Reaction Coordinates: 6 1.682482 0.473886 -0.305652 6 0.571891 0.390221 0.698002 6 -0.568220 1.137983 0.663222 6 -0.876929 2.170559 -0.372441 1 -0.501858 1.884675 -1.353945 1 -1.949536 2.338345 -0.450695 1 -0.413795 3.126611 -0.107468 6 2.789696 -0.552307 -0.075821 1 3.579534 -0.447913 -0.819632 1 2.397698 -1.567333 -0.138970 1 3.242780 -0.428377 0.909549 1 -1.223136 1.100914 1.523921 1 2.107061 1.484328 -0.280878 1 1.265978 0.354208 -1.309254 1 0.756987 -0.208182 1.581699 8 -2.049920 -0.449790 -0.300061 8 -1.514792 -1.533165 0.129014 8 -0.292192 -1.686961 -0.228726	**Frequencies (cm^{-1}):** -95.8156, 57.1143, 66.6457, 91.4541, 136.9122, 155.0359, 172.306, 206.7368, 244.2774, 351.4562, 420.2222, 450.2199, 599.6161, 706.1163, 739.4924, 803.8615, 878.8389, 948.0656, 983.8884, 1044.4223, 1053.7588, 1055.6652, 1094.9748, 1104.4175, 1122.3205, 1160.0784, 1267.2129, 1290.6675, 1339.7159, 1405.7511, 1416.7323, 1446.1349, 1462.7882, 1476.1303, 1490.8253, 1500.6767, 1506.2546, 1592.7954, 2991.6312, 3013.2051, 3028.7823, 3034.344, 3080.0874, 3088.1929, 3101.249, 3115.3023, 3151.0948, 3173.7999
IRC:	

Compound: Z-EtCHCHMe + O_3 POZ1.3	**Energy (Hartree)** -421.582011869880
Reaction Coordinates: 6 -1.511892 0.691824 -0.147310 6 -0.373175 -0.091623 0.483980 6 1.062248 0.544585 0.463019 6 1.241259 1.893475 -0.203858 1 0.888895 1.879954 -1.233317 1 0.699155 2.662171 0.346934 1 2.296042 2.166362 -0.204986 6 -2.855904 -0.030922 -0.049644 1 -3.119336 -0.233763 0.990104 1 -3.651409 0.575550 -0.482746 1 -2.831120 -0.982260 -0.579720	**Frequencies (cm^{-1}):** 40.1952, 106.0324, 182.2964, 221.9801, 232.3694, 289.0288, 330.6208, 409.2705, 458.8236, 475.2868, 696.5606, 705.349, 752.6953, 776.3765, 818.4988, 891.9646, 934.897, 943.3704, 964.1349, 1052.9824, 1056.5677, 1085.6373, 1125.1043, 1167.4514, 1185.254, 1295.6435, 1324.4308, 1338.6855, 1353.5213, 1385.6238, 1411.1699, 1416.9465,

1 -0.621148 -0.344498 1.519629 1 -1.576970 1.656983 0.360713 1 -1.271151 0.894932 -1.191672 1 1.435759 0.577513 1.490063 8 1.833462 -0.407426 -0.280510 8 1.166717 -1.648477 0.002709 8 -0.203171 -1.306219 -0.258714	1426.3987, 1475.4189, 1490.2773, 1500.0055, 1504.478, 1507.893, 2998.9044, 3024.0488, 3030.3206, 3030.9631, 3045.4689, 3069.4776, 3091.7494, 3104.8795, 3106.2006, 3122.4955

Compound: Z-EtCHCHMe + O_3 PRC 2.1	**Energy (Hartree)** -421.487538592535
Reaction Coordinates: 6 1.695993 -0.601860 -0.537355 6 0.802956 -0.061714 0.538783 6 0.298439 1.175493 0.647263 6 0.511856 2.338538 -0.271744 1 1.095424 2.085784 -1.154402 1 -0.443809 2.749168 -0.603701 1 1.030152 3.145598 0.253637 1 -0.313757 1.383428 1.517400 1 0.570969 -0.761651 1.334906 6 3.049666 -1.075259 0.011894 1 2.915626 -1.833940 0.784652 1 3.604668 -0.246598 0.453097 1 3.660500 -1.509524 -0.780462 1 1.857573 0.137722 -1.321356 1 1.198398 -1.452722 -1.013520 8 -2.506490 0.462945 -0.036225 8 -2.318500 -0.698359 -0.490110 8 -1.841160 -1.558143 0.300924	**Frequencies (cm^{-1}):** 8.7818, 35.7762, 40.3933, 47.6769, 69.3407, 94.4089, 128.1644, 213.1579, 224.6509, 266.6179, 302.9068, 483.5177, 572.0087, 732.5615, 742.5733, 796.3762, 863.3594, 934.1974, 1008.1776, 1021.2217, 1053.5112, 1065.1447, 1090.9361, 1170.3615, 1174.1367, 1194.8837, 1283.077, 1302.1533, 1339.5978, 1406.4936, 1410.4433, 1444.5333, 1482.8075, 1483.7888, 1494.3507, 1498.2498, 1506.9293, 1677.0231, 3008.7474, 3019.2479, 3025.9334, 3060.1784, 3065.5138, 3089.526, 3091.967, 3110.6595, 3130.262, 3153.3472

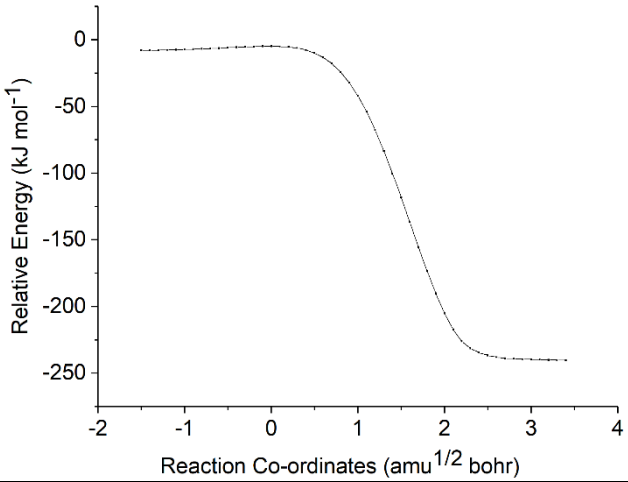
Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.1	**Energy (Hartree)** -421.478927651676
Reaction Coordinates: 6 1.510495 -0.734284 -0.368736 6 0.544529 -0.235458 0.666017 6 -0.060441 0.998046 0.658017 6 0.085628 2.017463 -0.429575 1 0.071770 1.564395 -1.420826 1 -0.712070 2.755268 -0.381953 1 1.036100 2.551419 -0.331973 6 2.960173 -0.345647 -0.031206 1 3.645525 -0.744472 -0.779909 1 3.256871 -0.743902 0.940031 1 3.087191 0.736779 0.000137 1 -0.516841 1.331927 1.578740 1 1.250357 -0.344752 -1.353762 1 1.439435 -1.819895 -0.431752 1 0.503653 -0.796539 1.589987 8 -2.229954 0.357023 0.197369 8 -1.932415 -0.645526 -0.557170 8 -1.250669 -1.547866 0.062823	**Frequencies (cm^{-1}):** -185.8554, 37.7874, 74.1741, 116.2373, 132.513, 175.4102, 182.9449, 214.9733, 292.3001, 301.6991, 467.0825, 540.8411, 580.5906, 739.7251, 782.7614, 795.5139, 861.8555, 937.0212, 990.7083, 1022.9191, 1047.6194, 1051.6373, 1081.3036, 1088.0966, 1103.5319, 1173.255, 1265.2907, 1293.8288, 1341.2785, 1401.2572, 1411.2227, 1440.3576, 1477.9975, 1486.5151, 1496.2587, 1498.2512, 1510.8248, 1567.8158, 3013.5218, 3028.5461, 3044.9321, 3072.6854, 3075.811, 3091.9832, 3098.5813, 3116.8195, 3167.3658, 3188.293
IRC:	



Compound: Z-EtCHCHMe + O_3 POZ 2.1	**Energy (Hartree)** -421.579764023369
Reaction Coordinates: 6 -1.566130 -0.559220 -0.465196 6 -0.302042 -0.569722 0.385547 6 0.489909 0.763607 0.536177 6 0.303965 1.808233 -0.551952 1 0.550045 1.402491 -1.531183 1 -0.719930 2.179691 -0.575661 1 0.964003 2.651451 -0.351839 6 -2.749797 0.112889 0.232966 1 -2.559780 1.164869 0.450353 1 -3.642022 0.064092 -0.390820 1 -2.980579 -0.382448 1.177947 1 -0.539510 -0.946600 1.383871 1 -1.363811 -0.090433 -1.428604 1 -1.818335 -1.599855 -0.675724 1 0.318132 1.193860 1.522950 8 1.839889 0.289147 0.578634 8 1.829515 -0.670169 -0.479286 8 0.672641 -1.490458 -0.150166	**Frequencies (cm^{-1}):** 41.4595, 131.5617, 185.2356, 230.8316, 239.3666, 284.7816, 290.7138, 407.705, 467.6656, 504.4749, 686.9927, 715.1293, 752.6265, 767.4205, 835.9035, 892.262, 910.9456, 947.2209, 977.7365, 1030.1813, 1052.7483, 1068.8779, 1101.892, 1158.7002, 1173.1139, 1276.3252, 1301.076, 1325.7568, 1358.426, 1371.7144, 1401.677, 1415.4427, 1420.0279, 1486.4189, 1497.6168, 1499.8777, 1504.3428, 1512.4406, 3021.4901, 3028.7451, 3044.4945, 3048.185, 3070.3359, 3074.0248, 3092.5004, 3096.024, 3109.4634, 3125.0629

Compound: Z-EtCHCHMe + O_3 PRC 2.2	**Energy (Hartree)** -421.487538592535
Reaction Coordinates: 6 2.078715 -0.278347 -0.065732 6 0.969689 0.298643 0.762733 6 0.297207 1.440079 0.555489 6 0.469563 2.408069 -0.573512 1 1.143653 2.046667 -1.347335 1 -0.492223 2.636527 -1.037528 1 0.867012 3.357607 -0.203171 6 1.980074 -1.797226 -0.242671 1 1.071975 -2.071226 -0.779827 1 1.956174 -2.303406 0.723829	**Frequencies (cm^{-1}):** 23.5576, 31.0201, 38.0319, 61.8044, 68.3488, 98.3679, 121.1293, 214.3459, 224.723, 264.3391, 314.6344, 458.7348, 580.7507, 708.7569, 741.1838, 800.1846, 868.5019, 938.3971, 1002.6201, 1034.81, 1054.4252, 1063.0705, 1092.505, 1168.4664, 1171.91, 1191.2559, 1281.6948, 1297.8266, 1339.0757,

1 2.836259 -2.180284 -0.798854 1 -0.434837 1.725535 1.301750 1 3.029307 -0.050332 0.431968 1 2.129209 0.205847 -1.041400 1 0.723065 -0.264352 1.657246 8 -2.410517 0.325180 0.221786 8 -2.109324 -0.677953 -0.481892 8 -1.430294 -1.588464 0.069540	1409.7959, 1412.4017, 1444.883, 1474.6623, 1483.5566, 1490.9211, 1498.0583, 1504.7358, 1674.3616, 2984.3962, 3016.652, 3028.0911, 3057.1837, 3059.3456, 3089.0117, 3096.8555, 3109.1064, 3129.6205, 3155.8443

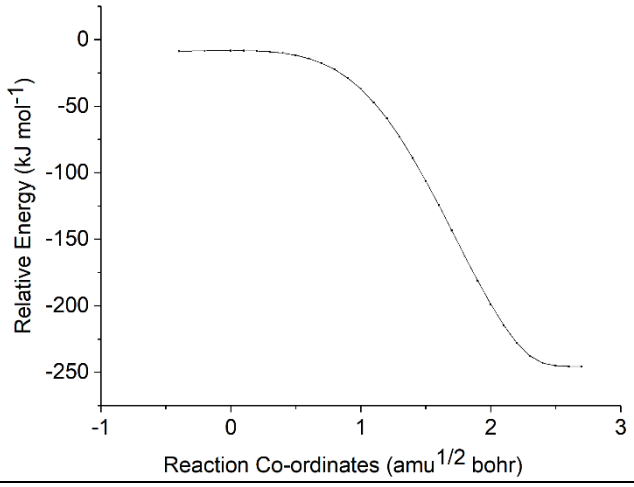
Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.2	**Energy (Hartree)** -421.475493403939
Reaction Coordinates: 6 1.873971 -0.070063 0.387875 6 0.541612 0.244056 1.021567 6 -0.310895 1.236219 0.587453 6 -0.034170 2.151529 -0.565802 1 0.461818 1.644901 -1.391297 1 -0.953385 2.596264 -0.940775 1 0.618508 2.970101 -0.243440 6 1.857177 -0.985271 -0.845915 1 1.224052 -0.589512 -1.639677 1 1.482443 -1.973555 -0.588865 1 2.867592 -1.086779 -1.242910 1 -1.092257 1.542969 1.267105 1 2.512605 -0.523679 1.146782 1 2.352951 0.874387 0.110979 1 0.365519 -0.152058 2.010474 8 -1.993247 0.034267 -0.288360 8 -1.361093 -1.072279 -0.515636 8 -0.821412 -1.557221 0.554065	**Frequencies (cm^{-1}):** -229.0107, 64.0517, 78.9177, 129.2482, 162.4993, 177.4459, 197.5797, 216.8561, 279.3811, 332.6511, 475.5939, 515.4286, 624.6646, 737.2053, 787.5741, 794.488, 845.2854, 929.7366, 991.7578, 1034.1803, 1045.4619, 1064.2902, 1071.9528, 1088.5727, 1106.9105, 1157.3854, 1263.042, 1299.6186, 1357.4185, 1398.7445, 1414.4435, 1437.4029, 1472.2841, 1485.7327, 1497.1251, 1502.3955, 1512.747, 1555.0945, 3007.4365, 3008.9832, 3039.9373, 3060.6074, 3086.3798, 3098.3772, 3120.8139, 3123.6175, 3180.7038, 3197.9474
IRC:  	

Compound: Z-EtCHCHMe + O_3 POZ 2.2	**Energy (Hartree)** -421.577414763780
Reaction Coordinates: 6 -1.601125 0.417075 0.575694 6 -0.234671 -0.169540 0.951115 6 1.063253 0.553678 0.447193	**Frequencies (cm^{-1}):** 47.4175, 118.1233, 195.748, 221.1323, 240.6022, 280.0724, 330.2283, 389.9908, 478.8777, 556.265, 693.249, 708.3074,

1 1.741299 0.685514 1.291993 6 0.900861 1.875591 -0.282525 1 1.882377 2.245821 -0.575931 1 0.292594 1.773935 -1.177573 1 0.445064 2.622901 0.368660 8 1.707244 -0.438392 -0.372723 8 0.622926 -1.296849 -0.775253 8 -0.057116 -1.508819 0.473687 1 -0.180304 -0.261587 2.036737 1 -1.590133 1.486541 0.799564 1 -2.327193 -0.021049 1.264117 6 -2.089685 0.172915 -0.852861 1 -2.132522 -0.892859 -1.069834 1 -3.094515 0.579906 -0.970799 1 -1.452899 0.635032 -1.604327	748.3374, 783.3273, 818.9452, 866.3148, 911.437, 936.1644, 952.8634, 1040.8849, 1063.5519, 1087.3183, 1101.3445, 1136.0476, 1163.9872, 1278.5798, 1310.0643, 1335.6261, 1353.439, 1389.5589, 1398.8705, 1414.9147, 1423.8093, 1480.2656, 1495.3771, 1497.3148, 1501.359, 1512.4381, 3025.7765, 3041.9281, 3044.0656, 3045.3223, 3052.7977, 3065.0729, 3100.3185, 3102.4637, 3118.4534, 3135.592

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.3	**Energy (Hartree)** -421.480940628349
Reaction Coordinates: 6 1.577252 0.593434 -0.331464 6 0.518968 0.454347 0.721638 6 -0.702978 1.073025 0.671916 6 -1.129752 2.008027 -0.417127 1 -0.830936 1.651497 -1.402857 1 -2.208243 2.148454 -0.416754 1 -0.666123 2.990328 -0.276808 6 2.786577 -0.312333 -0.116193 1 3.537722 -0.150681 -0.889296 1 2.491049 -1.360822 -0.141624 1 3.256504 -0.117636 0.849539 1 -1.312354 1.047282 1.563826 1 1.902865 1.640991 -0.360851 1 1.138866 0.404760 -1.316147 1 0.806710 -0.017882 1.651130 8 -2.027569 -0.720797 0.033071 8 -1.120169 -1.416085 -0.560006 8 -0.154320 -1.755031 0.222838	**Frequencies (cm^{-1}):** -164.7987, 49.0223, 78.0182, 130.553, 139.7573, 167.103, 175.635, 211.1543, 246.3096, 351.3945, 460.319, 476.1011, 602.7169, 723.512, 739.3675, 805.6246, 876.8665, 947.5148, 985.2007, 1046.5174, 1050.9305, 1054.0613, 1085.1637, 1093.3173, 1108.9112, 1161.0518, 1259.1384, 1287.9661, 1338.8972, 1407.7528, 1415.6271, 1440.8839, 1464.2203, 1478.7768, 1489.8112, 1499.3211, 1507.9139, 1571.0574, 2980.7896, 3008.0896, 3019.543, 3031.3402, 3072.8116, 3089.0237, 3103.8828, 3117.3074, 3169.1895, 3189.7965

IRC:



Compound: Z-EtCHCHMe + O_3 POZ 2.3	**Energy (Hartree)** -421.581360460904
Reaction Coordinates: 6 -1.422163 0.686450 -0.239577 6 -0.380240 -0.044094 0.597870 6 1.086067 0.514640 0.554928 6 1.335760 1.735640 -0.314006 1 1.060509 1.549666 -1.350365 1 0.774462 2.597753 0.047736 1 2.394933 1.987217 -0.280178 6 -2.819409 0.090063 -0.075765 1 -3.156240 0.150062 0.961291 1 -3.543262 0.624669 -0.690930 1 -2.834134 -0.958101 -0.372655 1 -0.718225 -0.117995 1.633497 1 -1.435344 1.738560 0.054977 1 -1.122536 0.654705 -1.288104 1 1.439131 0.696229 1.570751 8 1.853935 -0.613245 0.104495 8 0.909055 -1.329990 -0.709328 8 -0.220413 -1.409136 0.176493	**Frequencies (cm^{-1}):** 38.1236, 106.4651, 194.9527, 222.8799, 247.6416, 286.9838, 309.4444, 433.3448, 457.2585, 514.6987, 695.0401, 716.5112, 758.7964, 764.8899, 845.3108, 882.7421, 917.5293, 938.6717, 965.0015, 1049.1385, 1054.262, 1059.2291, 1105.7839, 1142.7719, 1169.6196, 1289.5342, 1291.9887, 1315.4559, 1351.1668, 1379.0314, 1401.1074, 1413.0908, 1417.6865, 1475.6873, 1493.3709, 1498.9986, 1502.2109, 1508.9637, 3027.9321, 3029.4778, 3042.1709, 3043.8476, 3062.0927, 3070.1698, 3089.9162, 3103.1012, 3105.1662, 3122.2873

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.1	**Energy (Hartree)** -421.552501616669
Reaction Coordinates: 6 -1.667754 -0.596109 -0.421243 6 -0.295935 -0.670430 0.188979 6 0.586842 0.965512 0.451080 6 0.401005 1.838943 -0.780213 1 -0.648385 2.051277 -0.985626 1 0.855230 1.371828 -1.652551 1 0.908834 2.789035 -0.607947 6 -2.683005 0.120495 0.469411 1 -2.741390 -0.342745 1.455335 1 -2.433124 1.171967 0.606926 1 -3.674861 0.071721 0.022157 1 -0.216907 -1.033382 1.210073 1 -1.607879 -0.124746 -1.402586 1 -2.002406 -1.624118 -0.590942 1 -0.050354 1.230197 1.311364 8 1.768609 0.576760 0.749867 8 1.790088 -1.322453 0.020157 8 0.636843 -1.193245 -0.621809	**Frequencies (cm^{-1}):** -450.0294, 91.4302, 114.878, 172.9944, 179.5044, 206.6829, 258.5214, 317.0113, 346.6393, 422.3487, 482.3502, 514.905, 585.8273, 614.6184, 782.6311, 851.1901, 926.9331, 957.1878, 1023.132, 1035.1318, 1057.1777, 1112.1293, 1116.963, 1160.2349, 1177.8288, 1241.8886, 1299.7796, 1309.543, 1333.3556, 1396.9342, 1411.2643, 1425.1988, 1438.3836, 1478.0755, 1485.5915, 1498.5172, 1504.1062, 1508.7575, 2915.2916, 3018.3756, 3035.7268, 3037.6692, 3071.7089, 3094.3685, 3099.2615, 3106.6701, 3116.9107, 3117.3735
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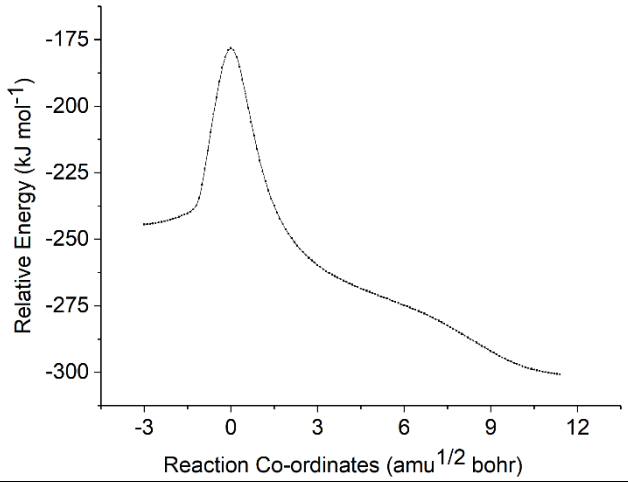
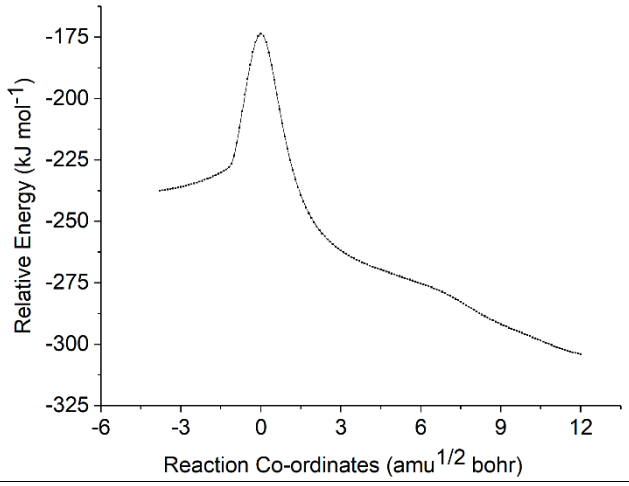


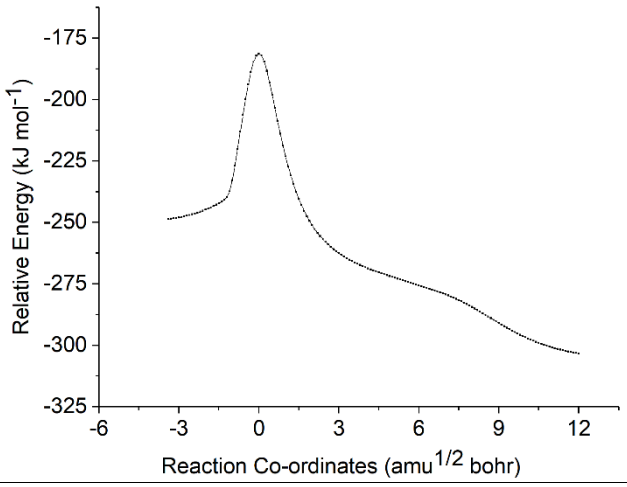
Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.1	**Energy (Hartree)** -421.591705369877
Reaction Coordinates: 6 -2.378148 -0.090769 0.169545 6 -1.188993 0.627316 -0.346030 6 2.215901 -1.228810 0.014316 6 2.866776 0.108015 0.149070 1 3.381974 0.152544 1.113585 1 2.144433 0.920450 0.062945 1 3.645561 0.201178 -0.613786 6 -2.275893 -1.614920 0.024560 1 -2.118895 -1.902579 -1.014956 1 -1.445259 -2.009515 0.604454 1 -3.199963 -2.078395 0.367613 1 -0.735748 0.419205 -1.310197 1 -2.547057 0.205798 1.204589 1 -3.239971 0.265890 -0.409097 1 2.898316 -2.101605 0.072512 8 1.031588 -1.417762 -0.147327 8 0.381686 2.252896 -0.202189 8 -0.690930 1.555121 0.331213	**Frequencies (cm^{-1}):** 18.355, 37.982, 71.8795, 74.4901, 94.6839, 116.6462, 137.8392, 178.2563, 202.1971, 217.8623, 314.0613, 420.1788, 527.4796, 531.8243, 764.5768, 779.8635, 896.2511, 898.8132, 911.4336, 936.8395, 1030.636, 1097.4494, 1145.4745, 1152.5863, 1177.7462, 1276.184, 1325.6832, 1373.589, 1388.2182, 1422.7758, 1425.6546, 1463.6346, 1464.5937, 1481.6193, 1497.9401, 1503.517, 1577.4011, 1783.6574, 2874.266, 2986.8342, 2999.9241, 3045.712, 3059.6874, 3081.3696, 3097.8496, 3106.9369, 3131.1692, 3156.9083

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.2	**Energy (Hartree)** -421.550522919038
Reaction Coordinates: 6 -1.709302 -0.038328 0.767777 6 -0.275448 -0.494166 0.654954 6 1.019442 0.827337 0.468768 6 0.558645 1.895322 -0.512470 1 -0.380188 2.358610 -0.208729 1 0.456986 1.480326 -1.513614 1 1.319782 2.676206 -0.550621 6 -2.475555 0.110415 -0.547290 1 -2.007881 0.830227 -1.215588 1 -2.539849 -0.839411 -1.075705 1 -3.490036 0.450809 -0.342303	**Frequencies (cm^{-1}):** -453.2759, 101.0517, 107.8832, 185.3135, 208.2626, 222.4456, 238.7892, 288.7735, 354.5828, 434.8191, 485.8356, 569.7036, 588.5365, 649.5598, 780.5226, 841.9272, 906.067, 966.8712, 1007.184, 1051.7089, 1072.2076, 1107.9662, 1122.0021, 1131.6047, 1190.8897, 1250.5314, 1293.2576, 1309.984, 1375.7417, 1392.7874, 1397.6494, 1427.946,

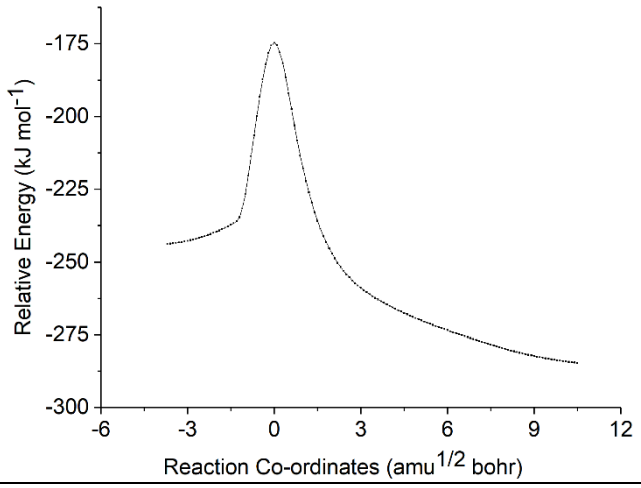
1 0.156042 -0.964978 1.532980 1 -1.716663 0.901917 1.323653 1 -2.225703 -0.759539 1.408247 1 0.948658 1.124642 1.528922 8 2.059649 0.138297 0.166908 8 1.265565 -1.612562 -0.424956 8 0.021305 -1.158521 -0.476660	1432.2042, 1480.6771, 1482.417, 1498.675, 1501.987, 1510.5701, 2906.7921, 3018.6873, 3035.1643, 3049.2286, 3051.1604, 3092.6788, 3108.855, 3119.5132, 3120.2971, 3122.6671
IRC:  	

Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.2	**Energy (Hartree)** -421.593801885446
Reaction Coordinates: 6 -1.962661 -0.783962 -0.499882 6 -0.991550 0.313241 -0.709935 6 2.369011 -1.065233 0.062503 6 2.788974 0.328495 0.394386 1 3.139895 0.352472 1.430609 1 1.981981 1.048227 0.249032 1 3.654100 0.591118 -0.222149 6 -2.695095 -0.771443 0.837496 1 -1.994856 -0.847259 1.668035 1 -3.269532 0.144435 0.969040 1 -3.380959 -1.615551 0.891854 1 -0.393392 0.397662 -1.611067 1 -1.403044 -1.714664 -0.638464 1 -2.670007 -0.749035 -1.337712 1 3.148883 -1.843119 0.190555 8 1.269825 -1.393295 -0.324331 8 0.090694 2.204703 -0.094309 8 -0.843662 1.202232 0.156497	**Frequencies (cm^{-1}):** 35.4228, 42.8486, 79.8051, 98.6999, 101.4857, 117.143, 175.1613, 181.173, 195.3352, 223.0269, 281.3285, 416.8592, 533.044, 618.6424, 741.441, 781.7961, 892.989, 896.8663, 905.0053, 927.1014, 1026.6217, 1109.4606, 1124.0407, 1145.4685, 1152.675, 1279.563, 1346.3248, 1389.7477, 1392.3987, 1423.4905, 1425.0139, 1447.3798, 1468.2239, 1480.5158, 1499.0874, 1504.6434, 1588.9356, 1781.9202, 2880.6668, 2997.5999, 2997.9413, 3032.4312, 3047.3283, 3059.688, 3092.8242, 3111.7056, 3113.0959, 3161.5725

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.3	**Energy (Hartree)** -421.552964279408
Reaction Coordinates: 6 -1.589612 0.727157 -0.007695 6 -0.449226 -0.186278 0.333972	**Frequencies (cm^{-1}):** -442.1928, 80.0073, 110.4935, 161.1972, 184.1964, 210.9157, 248.6438, 286.6601,

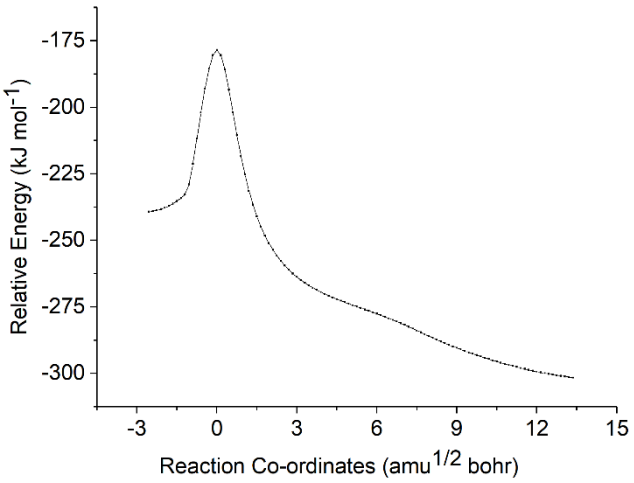
6 1.216989 0.635842 0.531749 6 1.401594 1.670292 -0.568647 1 0.628827 2.438961 -0.546569 1 1.412995 1.191635 -1.546551 1 2.366566 2.158340 -0.424267 6 -2.953060 0.036203 0.126437 1 -3.034406 -0.806045 -0.559938 1 -3.110710 -0.336648 1.139160 1 -3.755749 0.737517 -0.100832 1 -0.473223 -0.687557 1.297550 1 -1.454698 1.105954 -1.021054 1 -1.544594 1.585909 0.664427 1 0.949747 1.053516 1.517791 8 2.007267 -0.370882 0.561018 8 0.860037 -1.840398 -0.259478 8 -0.085412 -1.006330 -0.665868	350.73, 462.3242, 483.1396, 517.9774, 604.2923, 617.6594, 780.5891, 850.2464, 925.2345, 962.1581, 996.5967, 1037.3785, 1054.745, 1115.3351, 1124.477, 1159.4245, 1172.1227, 1240.4848, 1300.2444, 1315.9062, 1345.5932, 1397.1244, 1406.7005, 1424.0185, 1436.7811, 1479.4835, 1483.0613, 1497.643, 1499.5715, 1506.4466, 2903.9589, 3034.7796, 3035.3372, 3044.8617, 3079.5011, 3094.8024, 3099.4746, 3107.4466, 3117.3383, 3118.9542
IRC:  	

Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.3	**Energy (Hartree)** -421.592763619681
Reaction Coordinates: 6 -1.927792 -0.599929 0.477028 6 -0.989512 0.332694 -0.185640 6 2.392000 -1.186273 0.004957 6 2.939923 0.202329 -0.022783 1 3.519493 0.369624 0.890222 1 2.154969 0.953953 -0.117845 1 3.651679 0.283175 -0.850013 6 -3.231439 -0.772388 -0.319525 1 -3.782072 0.165492 -0.384478 1 -3.033080 -1.122134 -1.332974 1 -3.868752 -1.508206 0.169123 1 -0.627999 0.189175 -1.198713 1 -2.126194 -0.246771 1.488388 1 -1.415704 -1.563545 0.551690 1 3.144611 -1.995392 0.097604 8 1.219548 -1.479365 -0.064128 8 0.289236 2.200520 -0.235549 8 -0.598289 1.355849 0.420025	**Frequencies (cm^{-1}):** 36.2591, 45.1843, 69.7326, 83.0776, 101.8862, 111.8572, 146.8604, 179.9158, 205.4241, 221.5528, 331.091, 417.7094, 531.2702, 535.5493, 777.3848, 781.8696, 893.7283, 897.3574, 911.2546, 940.9086, 1018.62, 1093.6334, 1145.2497, 1152.1486, 1181.2257, 1276.3212, 1324.1559, 1372.9321, 1389.7383, 1416.2506, 1424.9786, 1467.7567, 1472.6765, 1480.4433, 1500.6015, 1505.5614, 1582.0114, 1782.0364, 2880.8381, 2998.7018, 3029.8939, 3038.2448, 3059.9994, 3086.8366, 3093.9029, 3106.7803, 3109.2429, 3159.6008

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.1	**Energy (Hartree)** -421.550754676428
Reaction Coordinates: 6 1.426705 -0.629905 -0.559256 6 0.345583 -0.680722 0.527739 6 -0.783787 0.815501 0.404070 6 -0.111330 2.128327 0.151688 1 0.391981 2.143172 -0.812939 1 -0.849857 2.932501 0.168548 1 0.615847 2.329251 0.935853 6 2.735871 0.004856 -0.093377 1 3.134933 -0.516650 0.778754 1 3.490417 -0.044231 -0.878651 1 2.615246 1.054422 0.177246 1 0.694028 -0.389000 1.535391 1 1.600407 -1.665040 -0.856153 1 1.043050 -0.126043 -1.448716 1 -1.291787 0.678213 1.353241 8 -1.496995 0.360191 -0.637423 8 -2.138709 -0.751898 -0.305444 8 -0.504610 -1.636410 0.500646	**Frequencies (cm^{-1}):** -456.5309, 76.2024, 106.812, 172.8893, 202.5363, 222.4548, 272.4678, 293.2747, 353.7351, 368.2323, 487.0462, 529.9655, 606.7228, 631.8152, 783.1452, 836.0845, 907.3963, 971.5368, 1004.268, 1031.4462, 1084.185, 1114.8078, 1121.7341, 1148.493, 1176.8374, 1260.8923, 1283.2688, 1310.6288, 1339.5636, 1386.2307, 1413.4168, 1421.7528, 1437.4152, 1481.9637, 1484.9268, 1497.9121, 1502.6216, 1505.6484, 2887.3654, 3028.629, 3038.3705, 3039.1503, 3065.7214, 3088.4416, 3093.6681, 3101.1853, 3123.4699, 3137.0609
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.1	**Energy (Hartree)** -421.595241321489
Reaction Coordinates: 6 -2.135609 0.178117 0.487146 6 -1.071013 -0.308518 -0.455432 6 1.964290 -0.025222 0.420383 6 3.104462 -0.892367 0.071376 1 3.582540 -0.564562 -0.848138 1 3.831613 -0.904381 0.886651 1 2.738532 -1.914942 -0.050576 6 -3.529905 -0.227569 -0.014065 1 -3.641865 -1.311969 -0.037424	**Frequencies (cm^{-1}):** 29.5056, 44.9132, 76.0531, 89.7766, 128.5953, 142.2844, 207.5987, 219.6339, 241.4023, 295.8674, 331.1586, 381.4413, 510.2165, 555.8819, 787.3946, 865.3856, 879.6719, 887.4779, 921.5283, 968.107, 999.728, 1071.489, 1115.9627, 1162.1742, 1165.0033, 1270.6198, 1325.3949, 1352.4912, 1407.3042, 1409.7775,

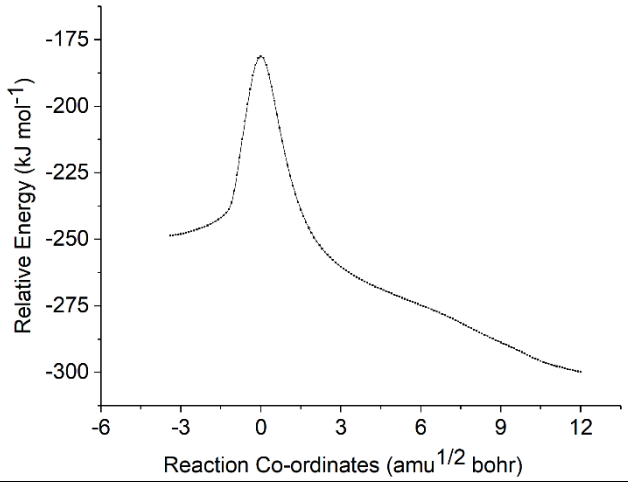
1 -4.301576 0.177520 0.639985 1 -3.715774 0.152671 -1.019990 1 -1.095001 0.143556 -1.462136 1 -1.942760 -0.230380 1.479017 1 -2.063016 1.265527 0.539933 1 1.369124 -0.156574 1.315738 8 1.663199 0.925523 -0.338956 8 0.533593 1.659577 -0.013024 8 -0.291187 -1.210489 -0.210459	1423.6526, 1457.1875, 1463.9607, 1475.7504, 1501.1711, 1505.9131, 1589.7386, 1737.2285, 2934.4546, 3027.2871, 3029.4081, 3046.0195, 3074.7101, 3080.2197, 3097.2101, 3103.4173, 3137.7024, 3182.43

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.2	**Energy (Hartree)** -421.552628851513
Reaction Coordinates: 6 -1.581968 0.732140 -0.359363 6 -0.459488 -0.090414 -0.999764 6 1.191679 0.351509 -0.266992 6 1.400728 1.804045 0.027122 1 0.785329 2.134801 0.861158 1 2.448513 1.989159 0.271454 1 1.154628 2.399516 -0.850773 6 -2.026007 0.253685 1.019853 1 -1.240990 0.380909 1.765037 1 -2.900464 0.813027 1.353119 1 -2.283720 -0.803561 0.993152 1 -0.169915 0.279255 -2.000226 1 -1.301235 1.787750 -0.340173 1 -2.424357 0.663922 -1.055143 1 1.806883 -0.100186 -1.038936 8 1.096809 -0.420212 0.830338 8 0.997739 -1.694751 0.485354 8 -0.472590 -1.366335 -0.876167	**Frequencies (cm^{-1}):** -438.7923, 63.812, 111.6364, 186.2891, 188.6131, 236.8966, 245.5334, 324.8111, 342.0849, 372.7971, 519.2866, 527.0752, 622.721, 683.251, 790.9445, 801.4111, 900.4654, 973.6562, 1009.0764, 1031.1071, 1077.2358, 1105.7587, 1121.034, 1147.4765, 1189.2073, 1262.2017, 1292.9759, 1309.6959, 1347.3079, 1387.5792, 1409.2023, 1421.62, 1449.473, 1477.2059, 1489.3336, 1494.4392, 1497.5487, 1510.0199, 2886.5649, 3013.9567, 3039.0285, 3040.2595, 3045.8022, 3096.9794, 3099.5492, 3115.2202, 3119.9478, 3134.0814
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.2	**Energy (Hartree)** -421.596921970227

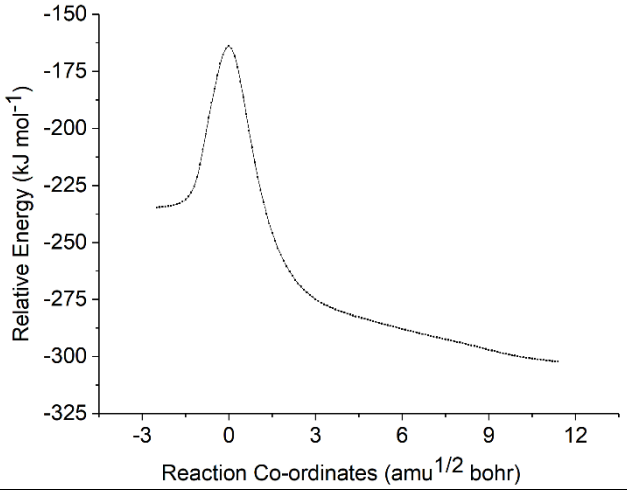
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.362459 0.260935 -0.255183 6 -1.105422 -0.112448 -0.990552 6 1.737710 -0.120585 0.479878 6 2.929029 -0.920829 0.141533 1 3.554928 -0.409254 -0.585172 1 3.505713 -1.136751 1.044029 1 2.599968 -1.879222 -0.267998 6 -2.622428 -0.527101 1.020509 1 -1.842075 -0.336576 1.756825 1 -3.577086 -0.239823 1.460855 1 -2.642810 -1.598805 0.826148 1 -0.874391 0.522917 -1.862145 1 -2.315303 1.335577 -0.065839 1 -3.180466 0.127085 -0.975268 1 0.996889 -0.434264 1.205096 8 1.562691 0.985162 -0.083141 8 0.390905 1.666743 0.207767 8 -0.414089 -1.080744 -0.738830	36.3684, 49.7967, 78.127, 106.1801, 133.0478, 142.5792, 202.0803, 231.6806, 255.3723, 278.2227, 295.6679, 332.6072, 554.7849, 657.2547, 697.5214, 849.9052, 866.1274, 885.2998, 910.1057, 966.9598, 1007.964, 1071.5065, 1109.78, 1134.7997, 1164.6349, 1284.216, 1352.507, 1369.4147, 1408.3148, 1409.8591, 1422.7164, 1449.8084, 1457.5247, 1463.8707, 1493.8912, 1503.508, 1590.6049, 1743.5182, 2939.8785, 2992.6478, 3026.8335, 3040.2196, 3057.7379, 3073.9362, 3099.8241, 3105.676, 3137.4574, 3182.1094

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.3	**Energy (Hartree)** -421.553201394595
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.428450 0.549724 -0.425231 6 0.532521 -0.128511 0.606236 6 -1.234949 0.443148 0.372601 6 -1.409582 1.903347 0.095848 1 -1.039287 2.167285 -0.892443 1 -2.466156 2.171811 0.156531 1 -0.874840 2.489451 0.841724 6 2.897028 0.180308 -0.196960 1 3.035764 -0.897659 -0.271146 1 3.537417 0.661128 -0.936982 1 3.235881 0.495855 0.791962 1 0.594157 0.304438 1.621514 1 1.115912 0.229203 -1.420082 1 1.310643 1.634233 -0.369422 1 -1.626431 0.050357 1.305554 8 -1.504983 -0.349046 -0.676895 8 -1.414121 -1.623687 -0.329000 8 0.406121 -1.401541 0.563124	-435.7698, 74.7693, 110.9366, 171.9122, 191.1959, 237.8586, 250.4272, 309.4136, 350.531, 365.7514, 507.8113, 518.1431, 624.4095, 628.5492, 790.8912, 840.832, 905.666, 972.7448, 1006.3154, 1015.6856, 1079.4347, 1118.0988, 1140.6912, 1149.3417, 1174.4585, 1261.6082, 1290.2781, 1305.1364, 1353.0096, 1387.7668, 1407.5843, 1421.989, 1449.0227, 1480.4676, 1483.1515, 1494.0364, 1498.1887, 1506.3233, 2886.8147, 3026.4462, 3028.9737, 3038.1568, 3070.2946, 3087.8145, 3098.887, 3105.7428, 3121.9309, 3135.8716
IRC:	



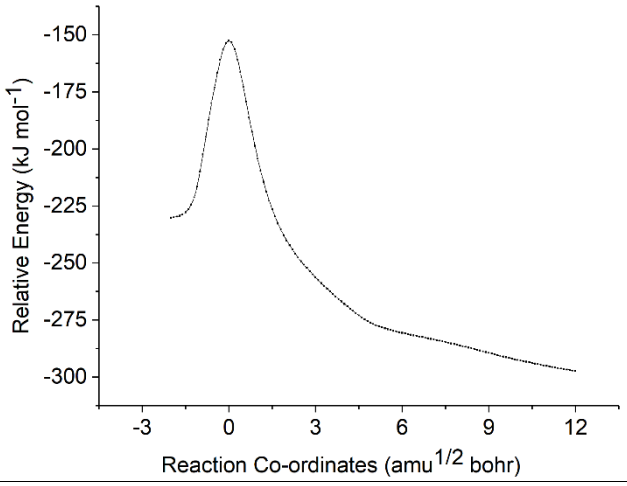
Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.3	**Energy (Hartree)** -421.595100791669
Reaction Coordinates: 6 2.051350 0.085931 0.564133 6 1.113728 -0.329468 -0.534248 6 -2.063766 -0.010296 -0.284463 6 -3.002986 -0.914745 0.403978 1 -3.128924 -0.633789 1.446440 1 -3.970844 -0.907636 -0.103105 1 -2.613913 -1.934078 0.342820 6 3.513809 -0.158229 0.166770 1 3.765488 0.363334 -0.758181 1 4.184899 0.205947 0.944025 1 3.713812 -1.220225 0.019957 1 1.269107 0.180924 -1.500914 1 1.887803 1.151020 0.739892 1 1.791142 -0.456971 1.472628 1 -1.812955 -0.100401 -1.334551 8 -1.527878 0.922607 0.357338 8 -0.601277 1.704632 -0.316374 8 0.284352 -1.213150 -0.436718	**Frequencies (cm^{-1}):** 24.97, 36.3681, 79.8813, 85.0518, 117.7021, 137.1761, 195.3116, 217.8739, 239.7259, 288.5853, 331.0133, 375.8215, 512.8901, 554.0073, 776.2214, 864.4798, 876.1359, 883.7525, 919.2635, 965.6231, 1002.2593, 1072.2316, 1121.2301, 1162.331, 1164.7844, 1269.4636, 1326.5168, 1352.6407, 1408.5293, 1410.0894, 1425.6937, 1457.6505, 1463.8441, 1476.3559, 1501.4738, 1505.7527, 1591.5727, 1745.0838, 2930.8569, 3026.9663, 3029.4667, 3043.753, 3074.2177, 3079.39, 3098.1153, 3101.7586, 3137.5302, 3179.9309

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.1	**Energy (Hartree)** -421.547763213279
Reaction Coordinates: 6 -1.213292 -0.609037 -0.483452 6 -0.219218 -0.453030 0.647084 6 0.899352 1.000321 0.329053 6 -0.039598 2.174568 0.038939 1 -0.567010 2.044926 -0.902825 1 -0.751532 2.328571 0.849562 1 0.577693 3.069724 -0.042200 6 -2.629685 -0.185201 -0.098445 1 -2.689491 0.876196 0.140615 1 -3.314916 -0.374391 -0.924512 1 -2.991951 -0.745119 0.765332	**Frequencies (cm^{-1}):** -467.5539, 98.9511, 106.1755, 192.0707, 222.0799, 244.533, 257.5907, 302.6104, 341.7176, 396.3764, 487.1542, 533.4525, 579.8498, 709.6385, 782.0742, 883.7748, 910.6977, 969.4444, 1001.524, 1027.1177, 1073.6382, 1080.0511, 1108.7138, 1146.5508, 1191.767, 1201.6391, 1281.1749, 1333.3232, 1348.2452, 1389.7876, 1416.903, 1425.8669,

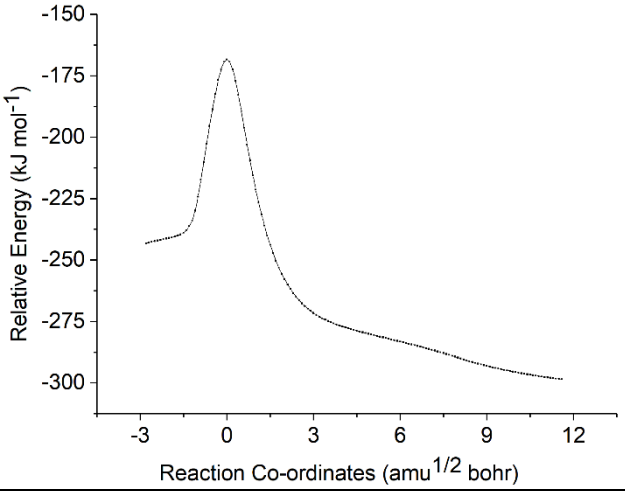
1 -0.624826 -0.330875 1.648881 1 -0.869806 -0.086049 -1.372948 1 -1.192315 -1.670162 -0.748833 1 1.371692 1.079694 1.322229 8 1.644396 0.581197 -0.627482 8 1.347630 -1.455594 -0.490617 8 0.791363 -1.345384 0.701302	1435.9346, 1477.756, 1484.4594, 1500.7022, 1505.9066, 1507.7766, 2913.338, 3028.8068, 3033.5229, 3039.23, 3084.8474, 3098.17, 3101.8014, 3105.5528, 3115.5306, 3131.8946
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.1	**Energy (Hartree)** -421.594302014611
Reaction Coordinates: 6 -1.613697 0.574527 -0.343989 6 -1.874865 -0.587352 0.509903 6 2.214155 0.215268 -0.007807 6 3.703898 0.054287 0.034096 1 4.196776 0.987275 0.297521 1 3.962365 -0.726509 0.754208 1 4.055784 -0.296984 -0.939501 6 -2.573553 1.738351 -0.110783 1 -2.524034 2.095828 0.918532 1 -2.313426 2.573277 -0.758982 1 -3.606439 1.460635 -0.324830 1 -2.597756 -0.593621 1.320237 1 -0.566709 0.870827 -0.174335 1 -1.614616 0.217440 -1.380319 1 1.627739 -0.686464 -0.264227 8 1.641157 1.257921 0.222617 8 -0.331406 -1.800002 -0.604404 8 -1.279166 -1.691943 0.389683	**Frequencies (cm^{-1}):** 31.3852, 48.6145, 68.2796, 73.3178, 85.8861, 103.1177, 120.4182, 166.9355, 199.6125, 219.6591, 359.5018, 470.9166, 514.3039, 685.5906, 716.4343, 798.6364, 850.1149, 878.4964, 890.3537, 937.177, 1050.8862, 1105.2622, 1128.9864, 1143.6434, 1159.6472, 1264.3814, 1334.7979, 1377.1138, 1378.9465, 1424.1461, 1437.1939, 1448.7442, 1461.0831, 1468.8266, 1502.6254, 1505.8906, 1566.056, 1772.4749, 2925.8497, 2950.9292, 3015.3422, 3021.7002, 3034.7808, 3072.2688, 3090.7093, 3109.3763, 3131.008, 3149.5679

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.2	**Energy (Hartree)** -421.542983956151
Reaction Coordinates: 6 -0.945569 1.199696 0.585627 6 -0.278626 -0.089314 1.022906	**Frequencies (cm^{-1}):** -462.2323, 90.9978, 128.6762, 184.9448, 233.2946, 259.5594, 265.1407, 297.4194,

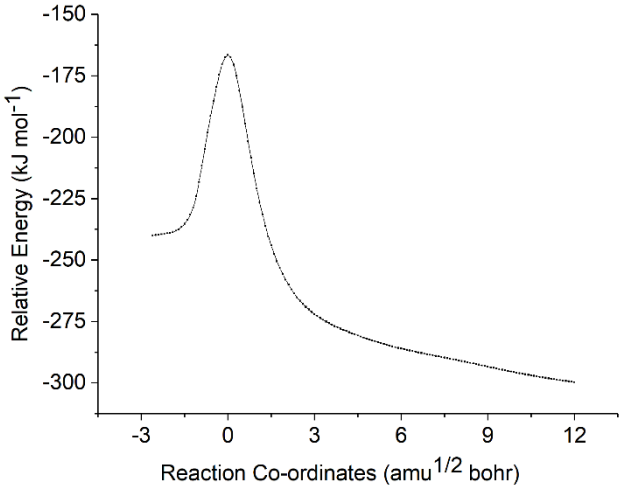
6 1.340793 -0.394289 0.097491 6 2.036087 0.968064 0.058016 1 1.542786 1.654449 -0.624836 1 2.105067 1.414969 1.050081 1 3.051247 0.801528 -0.304849 6 -1.345894 1.419634 -0.873174 1 -2.145198 0.748251 -1.171583 1 -1.696774 2.446306 -0.990600 1 -0.513560 1.256477 -1.552840 1 -0.014493 -0.099481 2.078391 1 -0.291738 2.005526 0.922050 1 -1.837653 1.272904 1.220122 1 1.802289 -1.078556 0.829818 8 0.957999 -0.917545 -1.005087 8 -1.008021 -1.424951 -0.571934 8 -0.805317 -1.288144 0.726902	333.8751, 395.9951, 481.5867, 520.6181, 561.8054, 740.9344, 783.2709, 843.1437, 886.8322, 971.485, 997.0958, 1012.4722, 1059.225, 1082.6595, 1114.3745, 1140.4581, 1192.0703, 1222.6964, 1304.0793, 1351.587, 1372.3337, 1393.2254, 1419.0711, 1439.059, 1446.1546, 1469.3424, 1489.2539, 1492.6871, 1500.177, 1511.571, 2902.8746, 2991.4313, 3036.764, 3042.8423, 3062.8233, 3093.9537, 3109.1742, 3115.1174, 3136.5386, 3143.1911
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.2	**Energy (Hartree)** -421.593861868972
Reaction Coordinates: 6 2.242592 -0.173882 -0.543721 6 1.137718 0.836646 -0.662151 1 0.805370 1.035905 -1.697294 8 0.631297 1.426554 0.265886 6 2.702541 -0.463722 0.877868 1 3.052498 0.442007 1.372212 1 3.515210 -1.189807 0.876760 1 1.886842 -0.868945 1.475396 1 1.880076 -1.076129 -1.046007 1 3.067522 0.191073 -1.167861 6 -1.969147 -0.245984 0.803176 6 -2.612250 0.818160 0.028930 1 -3.324040 1.368093 0.638342 1 -3.085712 0.384315 -0.854957 1 -1.835122 1.494597 -0.340021 1 -2.074461 -0.370898 1.874762 8 -1.235626 -1.128503 0.285476 8 -1.007785 -1.052741 -1.070855	**Frequencies (cm^{-1}):** 34.4011, 39.2154, 66.1622, 84.5421, 88.4878, 98.6929, 171.7936, 172.4224, 245.1941, 255.1205, 300.6495, 454.8323, 668.5725, 671.3097, 672.7391, 764.6795, 850.9917, 884.604, 907.242, 980.9781, 1006.1276, 1058.1955, 1110.3202, 1117.4683, 1142.537, 1285.7294, 1353.0135, 1368.8011, 1395.0399, 1411.8714, 1424.8578, 1441.6054, 1449.6731, 1467.3696, 1494.612, 1501.1559, 1572.6431, 1775.2655, 2917.6717, 3001.9437, 3021.6891, 3039.803, 3041.6395, 3068.314, 3102.3263, 3105.6145, 3138.6306, 3173.1756

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.3	**Energy (Hartree)** -421.549091178838
Reaction Coordinates: 6 -1.039768 0.917984 -0.325141 6 -0.320199 0.108530 0.724457 6 1.504685 0.035992 0.289584 6 1.890495 1.481247 -0.035253 1 1.473982 1.796104 -0.988655 1 1.586330 2.171273 0.752341 1 2.977916 1.516878 -0.112094 6 -2.560829 0.752689 -0.200735 1 -2.919908 1.064298 0.781183 1 -3.059781 1.366944 -0.950190 1 -2.858306 -0.282212 -0.361688 1 -0.395546 0.462513 1.750122 1 -0.771823 1.964168 -0.184706 1 -0.705568 0.614282 -1.313400 1 1.892509 -0.297317 1.266575 8 1.540186 -0.821720 -0.661389 8 -0.311546 -1.720604 -0.485417 8 -0.486904 -1.227124 0.727185	**Frequencies (cm^{-1}):** -462.0059, 78.6617, 110.5305, 186.7328, 219.9061, 226.174, 260.4617, 306.3856, 358.6679, 406.9177, 481.0186, 543.8094, 588.7721, 675.2071, 802.4534, 877.0357, 896.7579, 967.6062, 987.3409, 1002.8773, 1058.0108, 1080.4393, 1104.4544, 1163.1897, 1187.3988, 1206.2578, 1306.7073, 1336.7326, 1358.5944, 1387.171, 1408.4392, 1430.4143, 1437.8437, 1478.22, 1488.4517, 1498.1817, 1500.3636, 1506.0343, 2912.0228, 3035.0807, 3035.6809, 3070.2728, 3091.9893, 3094.818, 3110.3328, 3114.9711, 3132.3192, 3133.7843
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.3	**Energy (Hartree)** -421.592825799532
Reaction Coordinates: 6 2.248000 0.749929 0.561103 6 0.873717 0.270950 0.330847 6 -3.199591 0.588453 -0.060676 6 -3.116826 -0.892604 -0.258530 1 -2.091552 -1.249737 -0.203226 1 -3.730515 -1.390311 0.497250 1 -3.553872 -1.150112 -1.227139 6 3.057735 0.845713 -0.751412 1 2.614386 1.568221 -1.436079 1 4.072673 1.170122 -0.525520 1 3.101810 -0.126254 -1.236131	**Frequencies (cm^{-1}):** 22.9373, 32.1715, 37.327, 59.2534, 71.561, 93.8392, 118.8651, 164.6629, 198.9975, 246.9829, 324.8511, 516.2707, 542.1093, 654.1262, 777.949, 812.6897, 873.4806, 891.0133, 891.654, 909.0511, 1012.3516, 1087.4547, 1138.2663, 1140.4523, 1146.4308, 1289.0478, 1335.2074, 1383.9711, 1385.9446, 1401.8166, 1426.1193, 1461.052, 1461.9211, 1471.5507, 1495.7878,

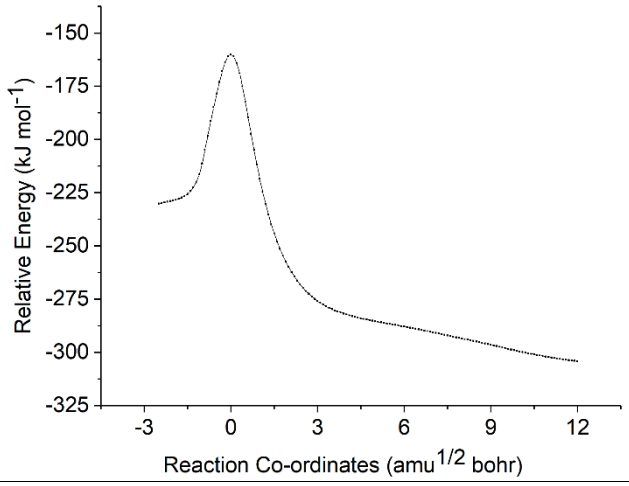
1 -0.013050 0.897515 0.322515 1 2.201037 1.723072 1.049401 1 2.736380 0.027802 1.219842 1 -4.220596 1.017382 -0.106164 8 -2.256128 1.316594 0.138057 8 1.621975 -1.858122 0.087626 8 0.597290 -0.941265 0.113975	1511.8383, 1562.8442, 1792.5829, 2888.2096, 3021.8259, 3032.7374, 3043.8229, 3070.8711, 3088.0617, 3105.6064, 3133.7957, 3139.5042, 3153.9733

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.1	**Energy (Hartree)** -421.549271906827
Reaction Coordinates: 6 1.736066 -0.482490 -0.451520 6 0.393698 -0.841356 0.215327 6 -0.492103 0.791587 0.471927 6 -0.491085 1.544633 -0.827466 1 0.447071 2.079958 -0.951617 1 -1.302334 2.276519 -0.795498 1 -0.659563 0.888348 -1.674857 6 2.670220 0.354013 0.417238 1 2.308640 1.373453 0.559293 1 3.657523 0.421464 -0.039823 1 2.798360 -0.094099 1.404352 1 0.520472 -1.141450 1.270566 1 2.206208 -1.446023 -0.660698 1 1.553337 -0.018212 -1.419160 1 -0.043612 1.278804 1.332454 8 -1.647775 0.222159 0.863823 8 -2.198095 -0.439853 -0.136657 8 -0.452489 -1.509442 -0.474422	**Frequencies (cm^{-1}):** -463.2804, 95.0495, 113.2382, 191.1886, 202.3046, 234.5614, 266.1292, 308.0648, 336.0689, 406.3467, 484.428, 528.4982, 580.6257, 702.0924, 777.3758, 859.563, 897.4619, 945.3965, 1019.3711, 1025.0573, 1053.6429, 1089.7359, 1113.2695, 1150.3938, 1195.9869, 1214.5781, 1280.2288, 1332.6324, 1357.7014, 1395.4697, 1415.3882, 1428.528, 1435.4679, 1472.2276, 1487.783, 1496.4134, 1503.6249, 1506.0536, 2896.2426, 3027.7849, 3036.3855, 3038.3606, 3076.3835, 3091.763, 3098.4442, 3111.6904, 3133.6415, 3157.73
IRC  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.1	**Energy (Hartree)** -421.598002966569
Reaction Coordinates:	**Frequencies (cm^{-1}):**

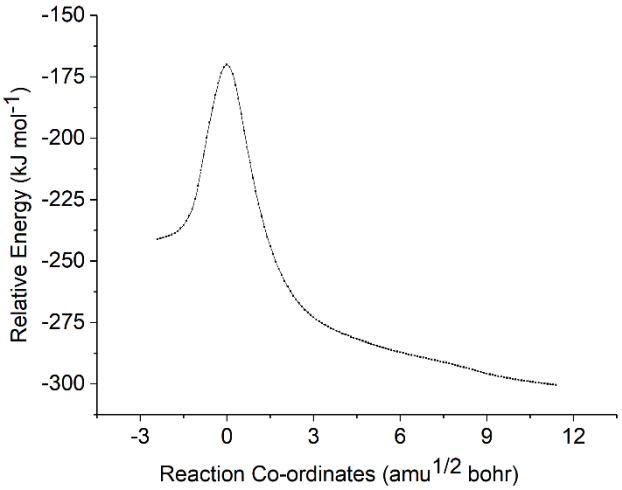
6 -2.262030 0.376069 -0.407011 6 -1.126531 1.008893 0.352349 6 2.112765 -0.134127 -0.653402 6 2.657194 0.443484 0.577728 1 3.555466 1.019700 0.373946 1 2.844213 -0.356886 1.297646 1 1.893728 1.086303 1.025508 6 -2.748147 -0.940444 0.198393 1 -1.951734 -1.682670 0.190605 1 -3.598595 -1.329059 -0.361245 1 -3.068994 -0.802613 1.232629 1 -1.133588 0.834618 1.445676 1 -3.073461 1.115202 -0.394833 1 -1.958903 0.265739 -1.448634 1 2.471889 0.100220 -1.648907 8 1.178475 -0.977358 -0.665059 8 0.620769 -1.325469 0.545740 8 -0.271685 1.706102 -0.145772	36.1159, 43.5273, 69.6185, 81.0122, 86.0921, 93.5975, 164.707, 169.4145, 215.2777, 301.8551, 320.6325, 453.5753, 520.3452, 670.2184, 699.816, 765.3163, 879.8852, 886.6142, 917.8593, 981.4554, 1026.7299, 1058.5703, 1117.1084, 1130.3546, 1157.4048, 1277.5943, 1331.6724, 1353.1368, 1395.0174, 1414.2266, 1428.5259, 1441.7608, 1452.4014, 1467.1711, 1497.9546, 1512.5515, 1574.1802, 1773.1909, 2900.3553, 2992.4337, 3024.0757, 3032.209, 3070.0018, 3071.9048, 3092.2088, 3114.4803, 3138.8741, 3173.8597

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.2	**Energy (Hartree)** -421.546725604641
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.780302 -0.024703 0.689968 6 0.384315 -0.697603 0.638887 6 -0.869276 0.676408 0.643693 6 -0.521350 1.696509 -0.402076 1 0.330648 2.292068 -0.084721 1 -1.377917 2.366501 -0.515531 1 -0.316387 1.233750 -1.360309 6 2.477907 0.153570 -0.653052 1 2.548870 -0.797006 -1.178271 1 3.486145 0.539148 -0.496635 1 1.955774 0.847353 -1.308393 1 0.121222 -1.148874 1.610257 1 1.731948 0.915663 1.243079 1 2.375775 -0.699949 1.310879 1 -0.939790 1.034060 1.667706 8 -1.922846 -0.130517 0.403393 8 -1.826283 -0.668760 -0.799714 8 0.070669 -1.376698 -0.402753	-465.3972, 83.1955, 112.7145, 173.4238, 205.0201, 245.1094, 263.6383, 306.5101, 315.0381, 371.0628, 523.2907, 552.3252, 640.4458, 698.5914, 779.0574, 819.1216, 889.9091, 960.8098, 1005.3205, 1030.7925, 1059.9733, 1090.2942, 1104.1572, 1157.3531, 1207.7375, 1210.4091, 1290.5772, 1314.1744, 1360.0036, 1394.7551, 1411.5037, 1423.3327, 1451.7662, 1473.8377, 1486.3895, 1495.7252, 1501.8017, 1506.9454, 2903.75, 3020.1905, 3034.0802, 3044.8696, 3047.9559, 3104.2681, 3113.6435, 3120.9821, 3121.8964, 3170.7739
IRC	



Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.2	**Energy (Hartree)** -421.598881244841
Reaction Coordinates: 6 2.242592 -0.173882 -0.543721 6 1.137718 0.836646 -0.662151 1 0.805370 1.035905 -1.697294 8 0.631297 1.426554 0.265886 6 2.702541 -0.463722 0.877868 1 3.052498 0.442007 1.372212 1 3.515210 -1.189807 0.876760 1 1.886842 -0.868945 1.475396 1 1.880076 -1.076129 -1.046007 1 3.067522 0.191073 -1.167861 6 -1.969147 -0.245984 0.803176 6 -2.612250 0.818160 0.028930 1 -3.324040 1.368093 0.638342 1 -3.085712 0.384315 -0.854957 1 -1.835122 1.494597 -0.340021 1 -2.074461 -0.370898 1.874762 8 -1.235626 -1.128503 0.285476 8 -1.007785 -1.052741 -1.070855	**Frequencies (cm^{-1}):** 34.4011, 39.2154, 66.1622, 84.5421, 88.4878, 98.6929, 171.7936, 172.4224, 245.1941, 255.1205, 300.6495, 454.8323, 668.5725, 671.3097, 672.7391, 764.6795, 850.9917, 884.604, 907.242, 980.9781, 1006.1276, 1058.1955, 1110.3202, 1117.4683, 1142.537, 1285.7294, 1353.0135, 1368.8011, 1395.0399, 1411.8714, 1424.8578, 1441.6054, 1449.6731, 1467.3696, 1494.612, 1501.1559, 1572.6431, 1775.2655, 2917.6717, 3001.9437, 3021.6891, 3039.803, 3041.6395, 3068.314, 3102.3263, 3105.6145, 3138.6306, 3173.1756

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.3	**Energy (Hartree)** -421.549400028304
Reaction Coordinates: 6 1.668858 0.574212 -0.003248 6 0.541350 -0.413522 0.342411 6 -0.955481 0.663123 0.605561 6 -1.101048 1.588553 -0.568885 1 -0.438867 2.443448 -0.457370 1 -2.131631 1.952413 -0.587113 1 -0.900999 1.083276 -1.507761 6 3.018277 -0.147382 0.017056 1 3.210240 -0.602983 0.989955 1 3.828786 0.553183 -0.187856 1 3.045167 -0.935176 -0.734960 1 0.648212 -0.826591 1.361043	**Frequencies (cm^{-1}):** -447.1446, 92.8643, 105.2922, 181.1188, 194.2728, 235.7871, 288.3123, 305.1581, 316.2272, 363.268, 491.0615, 531.8951, 606.4045, 709.3256, 792.075, 862.8779, 901.0758, 953.2958, 998.8875, 1025.8471, 1066.8904, 1097.8707, 1119.9234, 1150.9869, 1189.9971, 1212.4343, 1286.9133, 1331.0319, 1356.592, 1395.3581, 1409.3749, 1424.3784, 1438.2018, 1473.5369, 1482.6427, 1494.4735,

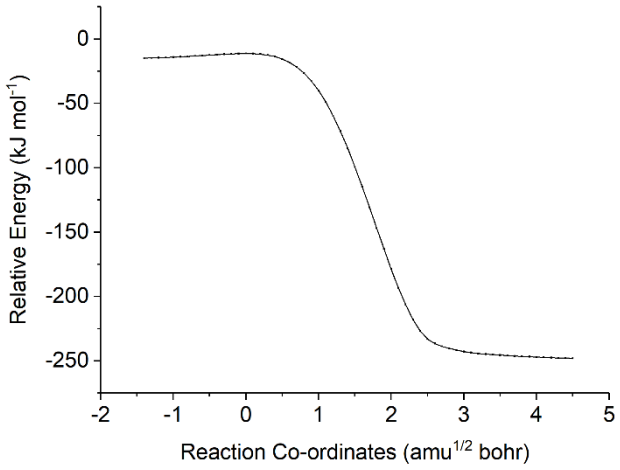
1 1.484873 0.991902 -0.991624 1 1.677925 1.393230 0.720208 1 -0.855214 1.118707 1.586977 8 -1.817138 -0.367974 0.701885 8 -1.912647 -0.999098 -0.453420 8 0.154757 -1.228093 -0.567074	1495.9127, 1504.2816, 2896.6084, 3024.2406, 3028.991, 3036.4732, 3080.7535, 3096.029, 3108.0724, 3113.1669, 3125.1493, 3159.7198
IRC  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.3	**Energy (Hartree)** -421.597666248278
Reaction Coordinates: 6 -2.081170 -0.279867 -0.420192 6 -1.126153 0.653042 0.268217 6 2.265923 -0.051798 -0.633879 6 2.682980 0.763726 0.509109 1 3.482446 1.444902 0.231141 1 2.977923 0.106923 1.330928 1 1.816324 1.329332 0.864856 6 -3.486922 -0.215923 0.188174 1 -3.463849 -0.422705 1.259334 1 -4.138253 -0.955291 -0.276480 1 -3.938472 0.766399 0.044302 1 -1.093176 0.554347 1.369949 1 -2.090897 -0.051875 -1.485951 1 -1.668680 -1.284587 -0.288183 1 2.603939 0.104266 -1.651904 8 1.476212 -1.026981 -0.533108 8 0.958650 -1.301327 0.713873 8 -0.436769 1.477459 -0.289087	**Frequencies (cm^{-1}):** 34.0085, 41.9796, 58.9497, 77.72, 85.0036, 98.3234, 154.1378, 171.5929, 213.2412, 300.7512, 344.636, 455.0148, 512.4946, 669.8224, 756.9535, 765.2295, 875.3512, 884.4651, 919.1895, 981.2262, 1009.0809, 1058.5425, 1117.1317, 1129.3386, 1162.4371, 1273.7295, 1329.8178, 1353.1604, 1395.2041, 1410.6231, 1428.8666, 1441.7341, 1467.1374, 1469.9637, 1501.8379, 1505.5438, 1572.7884, 1774.7958, 2906.6795, 3021.7024, 3027.2645, 3031.0964, 3068.0737, 3077.5953, 3097.4632, 3099.4044, 3138.8147, 3173.3747

S10.19 Ozonolysis of *E*-2-butene (Alkene 17)

Compound: E-MeCHCHMe + O_3 PRC	**Energy (Hartree)** -382.236446263383
Reaction Coordinates: 6 0.899353 -2.059761 -0.233507 6 1.126348 -0.702981 0.346488 6 1.258616 0.421787 -0.373015 6 1.470945 1.783677 0.195458 1 2.396089 2.225974 -0.183389 1 1.515791 1.763446 1.283676 1 0.656295 2.449612 -0.099113 1 1.235012 0.346561 -1.456194 1 1.204206 -0.641103 1.427355 1 1.663445 -2.764642 0.103887 1 -0.061902 -2.468878 0.091693 1 0.906912 -2.038565 -1.322928 8 -1.456886 0.685232 -0.949545 8 -1.865483 -0.144804 -0.081511 8 -1.433558 0.018479 1.098866	**Frequencies (cm^{-1}):** 58.3586, 69.5577, 81.0762, 90.1568, 126.5186, 163.9061, 242.876, 264.4227, 289.7316, 318.6782, 502.6586, 739.653, 771.3887, 874.9868, 984.0216, 991.5663, 1053.6945, 1069.9653, 1083.077, 1149.6834, 1169.4477, 1174.1439, 1328.1025, 1335.5889, 1410.0842, 1413.3125, 1475.7148, 1475.9204, 1482.5652, 1493.5208, 1679.165, 3011.0538, 3016.6008, 3050.4858, 3059.6857, 3094.4754, 3098.2549, 3125.7921, 3139.1112

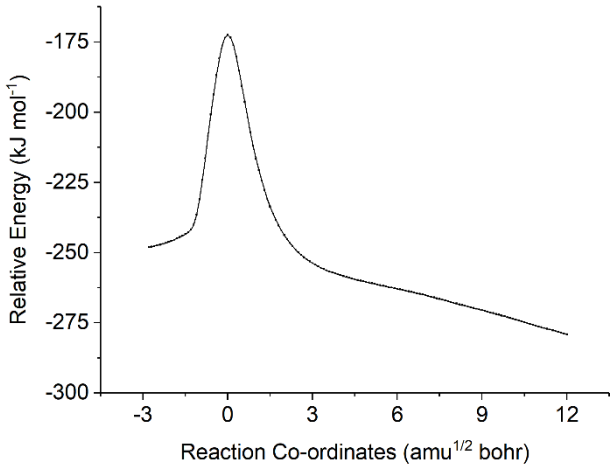
Compound: E-MeCHCHMe + O_3 TS_{OZO}	**Energy (Hartree)** -382.225772463065
Reaction Coordinates: 6 -1.046677 1.897412 -0.332661 6 0.059065 1.141408 0.329336 6 1.033198 0.474964 -0.364221 6 2.248105 -0.111637 0.268324 1 3.123758 0.509393 0.056798 1 2.452687 -1.105067 -0.131445 1 2.136225 -0.192016 1.348558 1 1.016920 0.527941 -1.446770 1 0.194916 1.288004 1.393561 1 -0.780048 2.955219 -0.422601 1 -1.242606 1.521364 -1.336818 1 -1.967711 1.845308 0.245864 8 -0.053144 -1.525471 -0.703149 8 -1.197710 -1.224115 -0.185209 8 -1.086182 -0.720791 0.999382	**Frequencies (cm^{-1}):** -188.3547, 81.9622, 90.3163, 135.352, 162.7455, 180.6841, 254.1221, 294.6378, 379.805, 479.5723, 503.7301, 739.6787, 803.6502, 872.6806, 956.0153, 996.0356, 1034.6915, 1053.4335, 1074.5121, 1094.6569, 1106.8957, 1177.6518, 1300.688, 1331.9812, 1409.7198, 1410.9994, 1471.1451, 1477.8972, 1484.5723, 1492.2466, 1602.8403, 3013.7441, 3016.9005, 3073.6073, 3073.8089, 3108.7869, 3109.9587, 3148.9688, 3164.9979
IRC:	



Compound: E-MeCHCHMe + O_3 POZ	**Energy (Hartree)** -382.327078857588
Reaction Coordinates: 6 1.552802 -1.393379 -0.388665 6 0.570268 -0.556745 0.410087 6 -0.755976 -0.254690 -0.350420 6 -2.006228 -0.877494 0.234351 1 -2.126000 -0.592138 1.279081 1 -1.943863 -1.964386 0.171272 1 -2.889129 -0.559370 -0.318865 1 -0.632648 -0.532809 -1.401312 1 0.361936 -1.010346 1.380563 1 1.114307 -2.362878 -0.635399 1 1.816169 -0.887667 -1.317411 1 2.462291 -1.568202 0.184421 8 -0.873681 1.167117 -0.258536 8 0.495158 1.582108 -0.306378 8 1.087491 0.747229 0.718105	**Frequencies (cm^{-1}):** 64.8038, 220.309, 232.5758, 267.1186, 287.8715, 341.1056, 467.6735, 515.0555, 646.2952, 716.2727, 744.8524, 803.9528, 890.906, 899.2291, 937.0789, 1010.3096, 1051.2288, 1090.2497, 1117.0373, 1157.8789, 1172.3666, 1301.6783, 1337.0446, 1366.9887, 1399.4585, 1410.2449, 1415.6693, 1485.2531, 1487.4438, 1497.608, 1501.3611, 3014.0789, 3030.515, 3038.9844, 3052.9045, 3093.5058, 3103.9515, 3112.8106, 3114.6029

Compound: E-MeCHCHMe + O_3 TS_{ANTI}	**Energy (Hartree)** -382.295161272590
Reaction Coordinates: 6 1.982012 0.808100 0.391907 6 0.987127 0.034970 -0.470264 6 -0.686210 0.470036 0.311440 6 -1.266063 1.757674 -0.181327 1 -1.614813 1.657476 -1.207646 1 -0.514404 2.544412 -0.140648 1 -2.103645 2.067487 0.446608 1 -0.344016 0.411206 1.339913 1 0.797515 0.482601 -1.460054 1 2.966448 0.744557 -0.073579 1 1.720916 1.863857 0.478890 1 2.047834 0.362715 1.383574 8 -1.358055 -0.612924 -0.086607 8 -0.789511 -1.715009 0.375186 8 1.015437 -1.241941 -0.423278	**Frequencies (cm^{-1}):** -461.3129, 91.8994, 163.6875, 194.3116, 232.996, 289.5988, 353.4411, 373.2795, 478.6797, 491.976, 547.6361, 622.021, 866.0536, 916.347, 971.0719, 1004.3841, 1020.9138, 1088.6455, 1119.7499, 1152.6565, 1187.8778, 1262.5048, 1340.2856, 1386.3372, 1393.6048, 1423.3211, 1439.6029, 1479.2885, 1480.8882, 1494.1293, 1499.375, 2914.4882, 3030.1394, 3038.0648, 3091.4781, 3098.7484, 3113.2483, 3119.6802, 3132.2864

IRC:

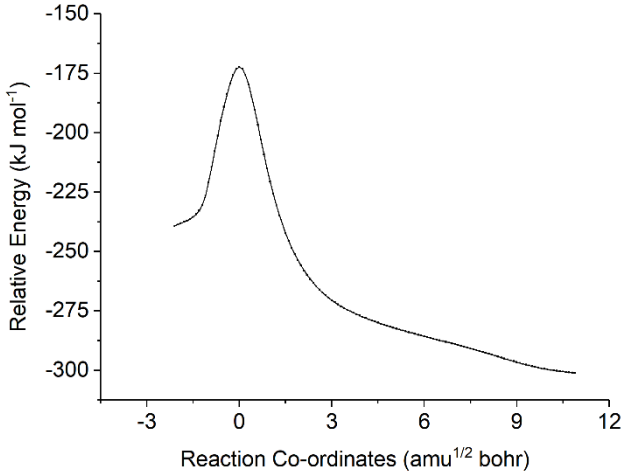


Compound: E-MeCHCHMe + O_3 C_{ANTI}	**Energy (Hartree)** -382.336226600511
Reaction Coordinates: 6 -3.254952 -0.033203 -0.203001 6 -1.786166 -0.012313 0.090147 1 -1.310158 0.981262 0.158031 8 -1.114416 -1.010819 0.245567 1 -3.785193 0.529793 0.569664 1 -3.440921 0.488432 -1.145558 1 -3.635213 -1.050752 -0.254613 6 1.626486 -0.184485 0.340862 6 2.261185 -1.406324 -0.187642 1 2.614081 -1.258390 -1.205145 1 1.531600 -2.219316 -0.163555 1 3.095391 -1.701772 0.453602 1 1.217081 -0.112318 1.342510 8 1.539705 0.830109 -0.384929 8 0.903963 1.950835 0.139721	**Frequencies (cm^{-1}):** 28.4429, 48.3231, 64.7263, 73.094, 87.4988, 122.5109, 163.4894, 188.7282, 264.6646, 323.2547, 512.331, 548.2417, 789.2904, 858.9501, 874.6003, 890.8356, 957.8616, 1075.5635, 1130.1522, 1154.8462, 1163.031, 1350.6001, 1379.4436, 1409.4662, 1448.5499, 1459.1851, 1460.7838, 1464.6933, 1468.236, 1596.7031, 1764.9877, 2949.6237, 3022.0973, 3026.0529, 3072.6207, 3073.4064, 3132.0938, 3136.0207, 3167.7308

Compound: E-MeCHCHMe + O_3 TS_{SYN}	**Energy (Hartree)** -382.296226059565
Reaction Coordinates: 6 2.132171 0.359796 0.464386 6 0.931909 0.400328 -0.468626 6 -0.597681 0.619543 0.556405 6 -1.672387 1.105775 -0.372864 1 -1.644973 0.577929 -1.320843 1 -1.549797 2.174421 -0.540871 1 -2.647102 0.938567 0.091855 1 -0.354940 1.250341 1.406966 1 0.790782 1.361140 -0.992451 1 2.088969 -0.519937 1.104142 1 3.041521 0.295586 -0.135078 1 2.195684 1.256652 1.082583	**Frequencies (cm^{-1}):** -453.6742, 125.4624, 173.6081, 179.8899, 239.9279, 287.1788, 293.3539, 377.7335, 486.9587, 541.0982, 594.4834, 698.8899, 861.5047, 917.26, 942.6928, 975.2381, 1029.3112, 1072.3249, 1106.1106, 1142.2371, 1184.7656, 1213.9764, 1300.9619, 1395.7229, 1398.5453, 1425.5087, 1434.8039, 1473.7058, 1481.8844, 1495.727, 1496.9769, 2910.6552, 3031.1764,

8 -0.639885 -0.660664 0.979123 8 -0.847443 -1.479948 -0.037499 8 0.651801 -0.640307 -1.163137	3036.1403, 3090.7214, 3103.5445, 3117.6852, 3127.8814, 3153.5131

IRC

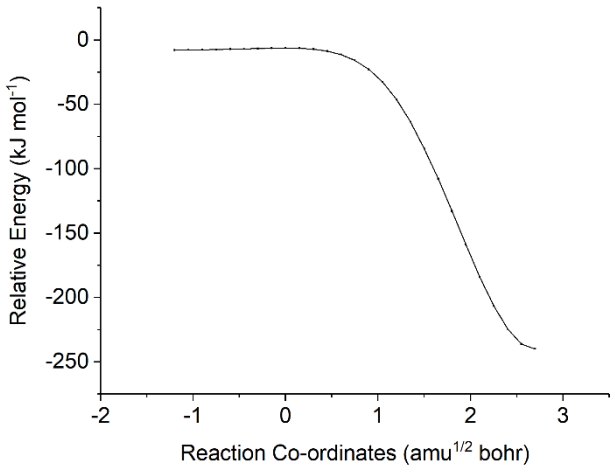


Compound: E-MeCHCHMe + O_3 CPr_{SYN}	**Energy (Hartree)** -382.340232237893
Reaction Coordinates: 6 -2.172479 -0.960228 0.293099 6 -2.286877 0.487923 -0.061300 1 -3.322654 0.867678 -0.177628 8 -1.357784 1.244593 -0.223801 1 -1.136696 -1.275381 0.412009 1 -2.738558 -1.146179 1.210525 1 -2.658302 -1.553438 -0.487401 6 1.530365 0.521866 -0.556862 6 1.830951 1.029386 0.784156 1 0.970935 0.845622 1.432052 1 2.069402 2.088660 0.758532 1 2.651532 0.445553 1.210916 1 1.514447 1.131220 -1.452260 8 1.275161 -0.688463 -0.784525 8 1.237390 -1.540808 0.300663	**Frequencies (cm^{-1}):** 40.5603, 56.762, 67.5313, 81.4719, 99.3918, 104.4479, 161.0049, 178.4108, 296.656, 453.3358, 525.0827, 670.0714, 763.4739, 779.938, 878.408, 893.9095, 985.7711, 1055.5354, 1112.1978, 1143.1897, 1145.9108, 1353.8341, 1388.268, 1396.5767, 1425.9807, 1440.1756, 1461.3315, 1466.1014, 1480.1362, 1575.5534, 1787.6075, 2876.1121, 3009.2685, 3026.5878, 3062.5928, 3071.1226, 3113.9292, 3143.2101, 3181.2549

S10.19 Ozonolysis of *Z*-2-butene (Alkene 18)

Compound: Z-MeCHCHMe + O_3 PRC1	**Energy (Hartree)** -382.229228168826
Reaction Coordinates: 6 1.594611 -1.581314 -0.370201 6 0.989111 -0.672755 0.651247 6 0.989117 0.672746 0.651251 6 1.594628 1.581305 -0.370192 1 0.866855 2.322125 -0.705141 1 1.963037 1.051473 -1.245483 1 2.431385 2.135662 0.064571	**Frequencies (cm^{-1}):** 16.2548, 56.2492, 82.7501, 94.2073, 102.5459, 114.1629, 128.3086, 277.87, 301.6874, 411.7046, 574.1599, 720.6377, 741.052, 868.7126, 976.6206, 998.751, 1030.3052, 1058.9184, 1066.0389, 1156.519, 1165.6025, 1176.5569,

1 0.551279 1.168773 1.510424 1 0.551269 -1.168783 1.510418 1 2.431358 -2.135689 0.064559 1 0.866828 -2.322120 -0.705160 1 1.963032 -1.051480 -1.245486 8 -1.608271 1.076845 -0.254240 8 -2.112165 0.000013 0.180794 8 -1.608294 -1.076839 -0.254221	1291.1732, 1396.1838, 1416.4702, 1443.1164, 1479.3426, 1482.1056, 1488.2765, 1492.2126, 1663.4207, 3018.9313, 3020.5414, 3066.2352, 3067.0328, 3108.8651, 3121.1368, 3133.9301, 3154.2931

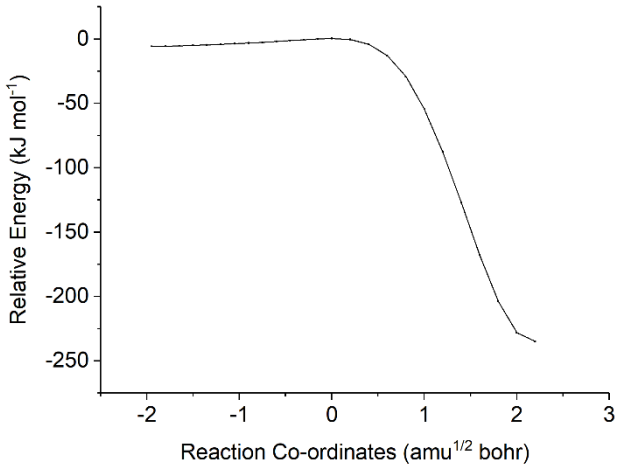
Compound: Z-MeCHCHMe + O_3 TS_{OZO} 1	**Energy (Hartree)** -382.225269220402
Reaction Coordinates: 6 1.460685 1.546710 -0.347977 6 0.775095 0.683188 0.660948 6 0.775100 -0.683186 0.660947 6 1.460697 -1.546701 -0.347978 1 2.509359 -1.696620 -0.071975 1 1.442045 -1.106098 -1.343229 1 0.994053 -2.528700 -0.400661 1 0.391178 -1.182477 1.540972 1 0.391168 1.182475 1.540974 1 2.509354 1.696613 -0.071989 1 1.442011 1.106119 -1.343233 1 0.994051 2.528714 -0.400639 8 -1.369485 -1.074479 -0.266424 8 -1.948857 -0.000005 0.132117 8 -1.369493 1.074473 -0.266425	**Frequencies (cm^{-1}):** -126.7195, 58.6512, 92.0451, 92.1884, 156.05, 168.8722, 192.9522, 282.759, 427.4912, 444.997, 579.3511, 733.5891, 751.9695, 880.9069, 956.2804, 1011.7671, 1027.6974, 1040.4947, 1063.9548, 1099.5493, 1118.7908, 1160.4635, 1273.9453, 1393.8061, 1414.0534, 1446.7595, 1473.8856, 1476.0358, 1485.7078, 1495.9745, 1594.0973, 3014.5466, 3014.8489, 3081.2648, 3082.4632, 3114.3126, 3118.4434, 3158.3962, 3177.8955
IRC:  	

Compound: Z-MeCHCHMe + O_3 POZ1	**Energy (Hartree)** -382.325132793566
Reaction Coordinates: 6 -1.392832 1.499076 -0.189052 6 -0.229835 0.785112 0.468761 6 -0.229817 -0.785116 0.468763 6 -1.392793 -1.499109 -0.189059 1 -1.517243 -1.188217 -1.224515 1 -2.315591 -1.297365 0.355138	**Frequencies (cm^{-1}):** 42.0681, 217.786, 240.8725, 272.6889, 324.4871, 355.1083, 456.5333, 489.9402, 690.333, 707.6178, 742.0599, 767.8912, 888.6334, 891.9836, 936.8086, 1038.7027, 1038.8919, 1075.434, 1115.7667, 1163.51, 1194.9491, 1328.465, 1341.8476,

1 -1.223872 -2.575232 -0.171270 1 -0.108523 -1.126847 1.500178 1 -0.108540 1.126847 1.500174 1 -2.315621 1.297313 0.355154 1 -1.223936 2.575203 -0.171267 1 -1.517285 1.188180 -1.224506 8 0.953256 -1.113052 -0.270391 8 1.818804 0.000023 0.006348 8 0.953225 1.113071 -0.270402	1374.6588, 1396.2842, 1418.8497, 1425.166, 1477.6269, 1495.4667, 1496.0745, 1511.8998, 3007.2687, 3029.4442, 3042.5818, 3047.0352, 3103.932, 3106.9928, 3117.9326, 3125.302

Compound: Z-MeCHCHMe + O_3 PRC 2	**Energy (Hartree)** -382.231445320259
Reaction Coordinates: 6 -1.710958 1.584226 -0.379563 6 -1.072263 0.670414 0.619644 6 -1.072322 -0.670316 0.619695 6 -1.711114 -1.584150 -0.379431 1 -0.988692 -2.310762 -0.756827 1 -2.136706 -1.056951 -1.230670 1 -2.512753 -2.160579 0.091186 1 -0.583786 -1.163590 1.451924 1 -0.583684 1.163709 1.451836 1 -2.512515 2.160805 0.091010 1 -0.988452 2.310711 -0.757046 1 -2.136631 1.056994 -1.230740 8 1.849154 -1.077159 0.127274 8 2.031893 -0.000018 -0.503902 8 1.849349 1.077005 0.127534	**Frequencies (cm^{-1}):** 6.413, 41.3805, 47.2305, 70.6879, 99.9927, 120.8342, 127.4886, 228.7989, 290.0326, 411.0696, 572.9587, 712.183, 742.3021, 866.9998, 976.4639, 1002.2744, 1028.0497, 1061.2945, 1065.6396, 1162.3368, 1169.9433, 1193.5159, 1294.8591, 1395.7512, 1416.9709, 1442.2763, 1480.5241, 1483.9126, 1490.2773, 1493.2641, 1679.781, 3017.2871, 3019.0741, 3058.9747, 3059.3398, 3103.344, 3115.1089, 3140.9575, 3160.6417

Compound: Z-MeCHCHMe + O_3 TS_{OZO} 2	**Energy (Hartree)** -382.222466209398
Reaction Coordinates: 6 1.387324 1.529584 -0.400625 6 0.775662 0.685788 0.674014 6 0.775681 -0.685766 0.674016 6 1.387375 -1.529550 -0.400614 1 2.478075 -1.540950 -0.302784 1 1.161084 -1.149252 -1.397051 1 1.038530 -2.557876 -0.340926 1 0.494581 -1.183917 1.590545 1 0.494552 1.183934 1.590542 1 2.478025 1.540995 -0.302820 1 1.161014 1.149287 -1.397059 1 1.038467 2.557904 -0.340926 8 -1.451206 -1.073518 0.130315 8 -1.635120 -0.000017 -0.558186 8 -1.451246 1.073478 0.130337	**Frequencies (cm^{-1}):** -179.9205, 43.8862, 124.2775, 137.72, 168.9872, 173.3792, 182.0554, 276.102, 463.5741, 471.5026, 586.5898, 738.3545, 757.4602, 882.7404, 957.6907, 1013.7444, 1023.7251, 1036.9449, 1066.0898, 1084.4722, 1108.6346, 1156.9499, 1262.4221, 1394.0517, 1415.8244, 1441.2058, 1476.8589, 1478.9441, 1483.9517, 1494.4465, 1573.8758, 3007.8466, 3009.2464, 3070.5035, 3071.2607, 3116.4031, 3118.3456, 3178.0145, 3195.2417
IRC:	

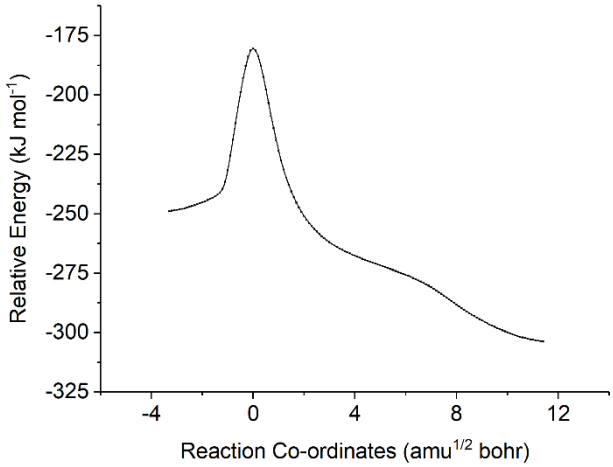


Compound: Z-MeCHCHMe + O_3 POZ 2	**Energy (Hartree)** -382.324192708349
Reaction Coordinates: 6 1.470219 1.296843 -0.298783 6 0.785023 0.254289 0.567603 6 -0.784924 0.254580 0.567607 6 -1.469738 1.297365 -0.298800 1 -1.180615 1.197178 -1.343262 1 -1.227382 2.306792 0.035484 1 -2.549075 1.170177 -0.227928 1 -1.152923 0.312605 1.592608 1 1.153048 0.312155 1.592603 1 1.228241 2.306351 0.035533 1 2.549509 1.169251 -0.227924 1 1.181049 1.196793 -1.343245 8 -1.112008 -1.078196 0.143258 8 -0.000273 -1.416927 -0.703932 8 1.111615 -1.078598 0.143220	**Frequencies (cm^{-1}):** 38.0005, 223.0042, 262.0402, 279.9635, 296.2165, 393.5632, 465.8663, 510.717, 698.1451, 704.8326, 760.4771, 764.8873, 879.3777, 900.4635, 932.0543, 1026.3986, 1043.613, 1047.2818, 1088.068, 1153.8241, 1160.3873, 1304.9292, 1310.2585, 1374.0934, 1382.1807, 1412.317, 1416.8266, 1478.9981, 1491.6342, 1499.5966, 1509.4278, 3039.3843, 3045.313, 3052.3473, 3068.0879, 3100.7529, 3106.1756, 3117.9367, 3125.8741

Compound: Z-MeCHCHMe + O_3 TS_{ANTI}	**Energy (Hartree)** -382.296039569149
Reaction Coordinates: 6 -0.741319 -1.747586 -0.608345 6 -0.734657 -0.709330 0.503511 6 0.849341 0.284438 0.409615 6 2.086490 -0.511244 0.135651 1 2.087797 -0.906204 -0.878105 1 2.157592 -1.340297 0.838180 1 2.971787 0.113809 0.268115 1 0.759626 0.775905 1.373132 1 -0.483689 -1.104330 1.503252 1 -0.741813 -1.264419 -1.584138 1 0.104154 -2.432462 -0.539282 1 -1.657173 -2.334566 -0.525864 8 0.464558 1.067467 -0.610475 8 -0.585439 1.796425 -0.262622	**Frequencies (cm^{-1}):** -450.9137, 116.6802, 167.919, 191.7874, 227.3382, 280.7835, 340.4079, 366.0788, 482.1771, 519.0225, 582.5343, 624.7029, 844.0629, 913.3318, 960.6072, 1004.8262, 1032.13, 1116.4549, 1117.7743, 1147.9238, 1180.4388, 1261.693, 1310.7033, 1386.1431, 1397.3511, 1421.6919, 1437.8482, 1478.149, 1482.1633, 1493.9688, 1499.6401, 2902.6942, 3035.189, 3038.3987, 3094.1163, 3099.0198, 3117.0922, 3121.6752, 3135.561

8 -1.623795 0.210470 0.485862	

IRC:

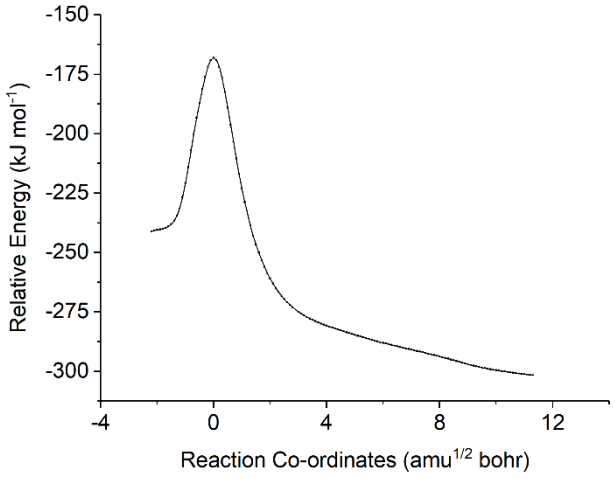


Compound: Z-MeCHCHMe + O_3 C_{ANTI}	**Energy (Hartree)** -382.336899685096
Reaction Coordinates: 6 2.343775 0.721478 0.120516 6 2.169715 -0.758425 0.028389 1 3.097053 -1.356608 0.135989 8 1.118323 -1.331528 -0.149821 1 1.399571 1.256080 0.007787 1 2.805386 0.961770 1.083103 1 3.059259 1.039533 -0.643935 6 -1.455772 -0.146320 -0.358444 6 -2.141036 -1.342437 0.166753 1 -2.517854 -1.169482 1.171743 1 -1.438274 -2.178122 0.172056 1 -2.968033 -1.617249 -0.493195 1 -1.008267 -0.100555 -1.344954 8 -1.387401 0.884997 0.347305 8 -0.722038 1.986387 -0.176469	**Frequencies (cm^{-1}):** 42.9772, 75.8743, 80.8582, 103.8231, 118.0927, 133.2153, 179.3389, 199.657, 270.7004, 325.2615, 532.6896, 550.0271, 781.9405, 865.21, 876.4563, 896.8721, 960.332, 1074.5883, 1145.2725, 1152.4784, 1162.7796, 1349.0463, 1389.7674, 1409.4093, 1425.1553, 1459.1251, 1466.4471, 1468.0809, 1480.0693, 1592.9126, 1781.7088, 2882.7063, 2999.1247, 3026.4688, 3060.1949, 3076.741, 3094.4859, 3135.6023, 3170.0262

Compound: Z-MeCHCHMe + O_3 TS_{SYN}	**Energy (Hartree)** -382.292399119526
Reaction Coordinates: 6 2.174760 0.183728 0.008248 6 0.909299 -0.602714 0.362039 6 -0.401201 0.707424 0.605689 6 -0.369631 1.641351 -0.570465 1 -0.242545 1.107566 -1.506342 1 0.425467 2.372500 -0.447937 1 -1.323311 2.174340 -0.605298	**Frequencies (cm^{-1}):** -465.7696, 104.6257, 190.1491, 226.6786, 263.2551, 304.7061, 309.9565, 361.0558, 483.5747, 527.3944, 574.4322, 702.2875, 862.2176, 907.7514, 951.0997, 1000.5877, 1023.4662, 1078.6887, 1103.5071, 1152.076, 1198.078,

1 -0.244369 1.142285 1.589103 1 0.937517 -1.012702 1.385146 1 2.379704 0.970858 0.734485 1 3.009493 -0.517832 0.027093 1 2.110787 0.605837 -0.991453 8 -1.420990 -0.168444 0.685470 8 -1.592712 -0.781138 -0.470976 8 0.397188 -1.353117 -0.541728	1212.5444, 1344.5156, 1388.517, 1396.7728, 1424.2704, 1436.318, 1470.2561, 1487.4215, 1494.1252, 1502.7881, 2914.2447, 3035.4291, 3037.0332, 3095.3983, 3112.3989, 3125.0849, 3132.9402, 3159.3922

IRC



Compound: Z-MeCHCHMe + O_3 CPr_{SYN}	**Energy (Hartree)** -382.341847196068
Reaction Coordinates: 6 -2.575388 -0.475137 -0.224658 6 -1.656799 0.539062 0.382613 1 -1.558708 0.485092 1.481750 8 -1.055700 1.384963 -0.240999 1 -2.640652 -0.350326 -1.303167 1 -2.200388 -1.470587 0.020789 1 -3.567732 -0.382682 0.224597 6 1.704683 -0.009558 -0.693935 6 2.140169 0.870844 0.392701 1 1.266121 1.406451 0.775659 1 2.887025 1.579181 0.045049 1 2.513051 0.262837 1.220399 1 1.979315 0.121918 -1.734281 8 0.973295 -1.018077 -0.513133 8 0.538153 -1.267281 0.770243	**Frequencies (cm^{-1}):** 44.5356, 61.3265, 85.2874, 89.2671, 100.2886, 127.2994, 171.6681, 196.4532, 300.2958, 455.0499, 513.2373, 669.8265, 764.9019, 779.3715, 884.3228, 892.1279, 981.2246, 1058.843, 1116.8874, 1127.3066, 1135.3539, 1353.0833, 1374.0802, 1395.2676, 1427.7885, 1441.5812, 1461.2162, 1467.253, 1472.0736, 1572.9701, 1778.6069, 2923.9538, 3021.7811, 3025.2706, 3068.0434, 3084.0704, 3131.4128, 3138.9098, 3173.2592

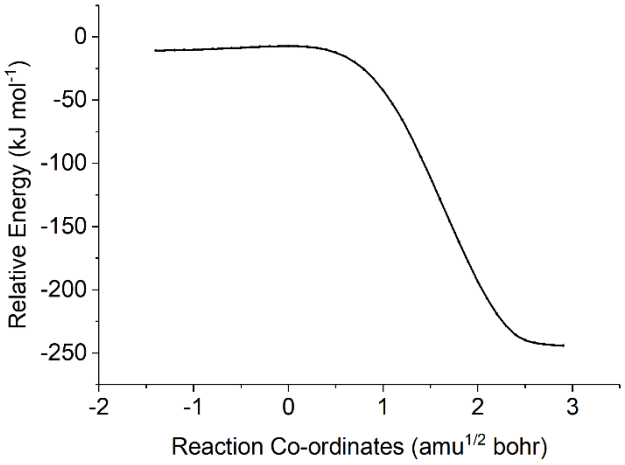
Compound: Z-MeCHCHMe + O_3 TS_{POZ} 1	**Energy (Hartree)** -382.321485722886
Reaction Coordinates: 6 0.182724 1.775886 -0.581804 1 0.216392 1.291005 -1.555960 6 -0.711469 -0.427476 0.455564 6 -2.140921 -0.148666 0.038491 1 -2.184398 0.354061 -0.925402	**Frequencies (cm^{-1}):** -134.2804, 163.7151, 205.7858, 226.8465, 259.4079, 333.162, 408.2272, 516.3173, 673.3651, 710.3546, 779.2753, 804.8931, 853.5614, 888.3796, 962.0843,

1 -2.625930 0.477676 0.787747 1 -2.699210 -1.080915 -0.032187 1 -0.683507 -0.965346 1.408878 1 0.203425 1.229747 1.520810 1 -0.735938 2.359624 -0.510990 1 1.025735 2.461374 -0.507721 6 0.262300 0.754210 0.539789 8 -0.101772 -1.220853 -0.559332 8 1.505872 0.057283 0.561212 8 1.336854 -1.067799 -0.364058	1005.0111, 1039.3048, 1087.6986, 1113.4352, 1164.2126, 1180.9661, 1282.1568, 1339.0451, 1369.728, 1387.8416, 1415.3228, 1418.4199, 1483.0492, 1492.0999, 1499.5139, 1507.2902, 3005.7406, 3040.9999, 3046.1081, 3058.5875, 3103.8353, 3108.2972, 3121.6559, 3125.1516
IRC Energy too low for IRC to take place	

S10.20 Ozonolysis of 2-methylpropene (Alkene 19)

Compound: $(CH_3)_2CCH_2$ + O3 PRC	**Energy (Hartree)** -382.236083327848
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.824158 -0.601839 1.158834 6 -1.319940 0.285715 0.056344 6 -0.596484 1.385252 0.304018 6 -1.725130 -0.100766 -1.336310 1 -0.270135 2.038674 -0.492606 1 -0.335408 1.675152 1.313372 1 -1.388262 -1.112792 -1.571671 1 -1.314691 0.578560 -2.080906 1 -2.814789 -0.101504 -1.431201 1 -2.917807 -0.602590 1.176838 1 -1.514282 -1.637045 1.000280 1 -1.467942 -0.279619 2.136015 8 2.237554 0.768557 -0.080777 8 2.080016 -0.423044 0.301886 8 1.284628 -1.141640 -0.364538	13.2204, 44.2658, 61.6635, 66.7373, 108.93, 160.9186, 204.0624, 233.4983, 382.3804, 438.6805, 447.2956, 705.214, 742.4158, 814.159, 935.0968, 961.2337, 989.6545, 1014.287, 1085.9076, 1104.8397, 1169.5686, 1195.7772, 1301.4263, 1410.1072, 1414.8522, 1439.8801, 1470.9504, 1480.9185, 1489.411, 1503.1939, 1671.4078, 3013.1628, 3018.4672, 3058.355, 3061.3415, 3104.211, 3110.2042, 3138.3913, 3221.9192

Compound: $(CH_3)_2CCH_2$ + O_3 TS_{ozo}	**Energy (Hartree)** -382.225921208913
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.435640 -0.838117 1.086069 6 -0.976739 0.241742 0.146859 6 -0.197860 1.276256 0.598455 6 -1.650320 0.314019 -1.191081 1 -0.043102 2.156252 -0.006361 1 0.103465 1.335294 1.633905 1 -1.626613 -0.650809 -1.697239 1 -1.183015 1.055588 -1.835653 1 -2.702774 0.585158 -1.061880 1 -2.427837 -0.589263 1.476145 1 -1.518134 -1.799148 0.580955 1 -0.763404 -0.946041 1.936181 8 1.898487 0.685989 0.069088 8 1.737168 -0.592289 0.076333 8 0.829941 -0.982503 -0.753904	-200.6631, 61.9624, 130.0607, 170.9458, 185.1998, 195.7286, 212.0207, 390.6483, 429.2649, 450.2241, 474.3117, 741.9401, 775.7663, 808.4966, 949.5694, 954.9689, 986.7612, 1020.5955, 1067.2692, 1080.8425, 1087.3552, 1122.3664, 1308.4295, 1409.1944, 1409.6658, 1426.1079, 1472.0263, 1480.6726, 1487.4262, 1503.5581, 1582.3866, 3011.6863, 3017.2626, 3076.1051, 3078.4167, 3114.0848, 3118.9519, 3156.4788, 3246.2811
IRC	

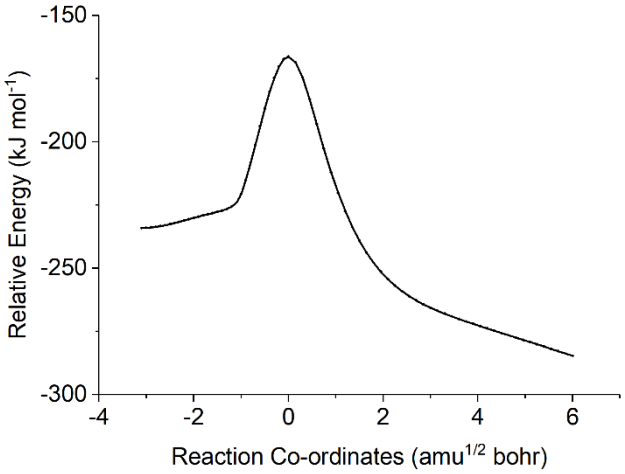


Compound: $(CH_3)_2CCH_2$ + O3 POZ	**Energy (Hartree)** -382.327176695013
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.293510 1.195388 0.644156 6 0.602622 -0.015200 0.027727 6 -0.462424 -0.624090 0.994698 6 1.585534 -1.040703 -0.519289 1 -0.294166 -1.679424 1.202030 1 -0.512860 -0.056636 1.926309 1 2.199791 -0.598452 -1.303423 1 1.055890 -1.896432 -0.935451 1 2.249191 -1.386277 0.273928 1 1.831727 0.911070 1.550333 1 2.007626 1.624466 -0.058060 1 0.559666 1.956642 0.905660 8 -1.692465 -0.541174 0.287162 8 -1.492573 0.654548 -0.497622 8 -0.216502 0.390709 -1.095174	80.0602, 222.7854, 258.4457, 285.5419, 335.1301, 379.6914, 404.4257, 489.6463, 606.3722, 701.6879, 745.0957, 806.7591, 880.0871, 924.237, 934.6973, 962.0069, 981.4057, 1010.6615, 1042.6659, 1184.2543, 1209.9053, 1243.3396, 1290.8022, 1354.3792, 1404.1802, 1421.3895, 1480.4039, 1488.7181, 1497.9931, 1504.6803, 1512.8664, 3030.0927, 3033.6991, 3039.9606, 3094.5957, 3103.0264, 3106.5376, 3113.4511, 3114.5155

Compound: $(CH_3)_2CCH_2$ + O_3 TS_{AO}	**Energy (Hartree)** -382.297810552684
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.930711 0.436070 -0.595089 6 -0.646102 -0.052458 0.015149 6 0.621471 1.316250 0.071448 6 -0.694106 -0.578627 1.427775 1 0.215141 1.778140 0.983666 1 0.401271 1.870563 -0.851894 1 -1.313597 0.073392 2.040732 1 0.298352 -0.656845 1.858313 1 -1.146215 -1.573775 1.414010 1 -2.261384 1.341634 -0.088006 1 -1.800566 0.652787 -1.653481 1 -2.716400 -0.313618 -0.482312 8 1.746576 0.722655 0.172754 8 1.220571 -1.175188 -0.384344	-451.3844, 161.9753, 177.7789, 194.0767, 244.9575, 301.2076, 326.3375, 377.7665, 397.314, 527.9858, 565.0285, 641.4867, 787.8394, 880.9253, 959.7992, 990.7402, 997.4451, 1031.5578, 1139.43, 1178.3834, 1222.2873, 1285.0709, 1292.5411, 1367.7344, 1404.2913, 1419.738, 1469.6832, 1480.3633, 1492.504, 1502.8754, 1534.2718, 2921.1346, 2983.4244, 3032.4621, 3037.4782, 3097.404, 3105.2941, 3126.0785, 3157.7927

8 0.060364 -0.784928 -0.880502	

IRC



Compound: $(CH_3)_2CCH_2$ + O3 C_{AO}	**Energy (Hartree)** -382.341486411877
Reaction Coordinates:	**Frequencies (cm^{-1}):**
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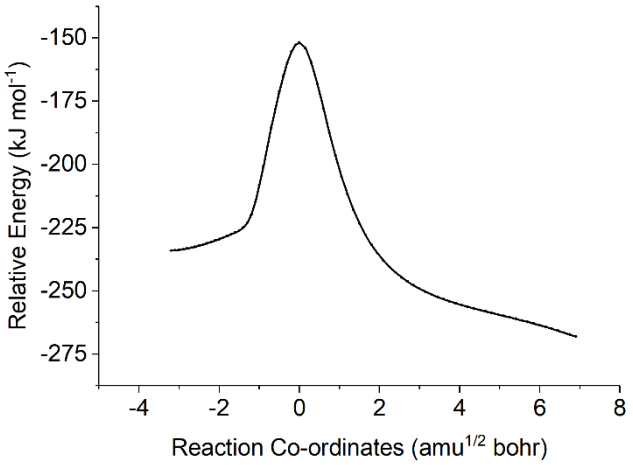
Compound: $(CH_3)_2CCH_2$ + O_3 TS_{FO}	**Energy (Hartree)** -382.292467755139
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.186010 1.459163 0.013213 6 0.730152 0.008980 0.203404 6 -0.582798 -0.257857 -1.111567 6 1.754319 -1.054703 -0.230514 1 -0.622491 -1.339814 -1.096221 1 -0.297127 0.240825 -2.030129 1 2.043274 -0.951734 -1.277036 1 1.359786 -2.052457 -0.051484 1 2.650458 -0.927795 0.379048 1 1.601803 1.638325 -0.978985 1 0.356888 2.141148 0.189547	-448.4063, 105.6065, 197.3812, 223.1851, 256.7873, 295.2322, 297.1893, 406.6525, 487.1599, 493.27, 552.0641, 606.1783, 769.8578, 888.663, 914.2972, 981.6376, 1000.5277, 1056.9223, 1066.2426, 1160.2609, 1182.0942, 1222.9942, 1267.5665, 1379.3347, 1397.6846, 1412.6804, 1473.0153, 1481.7119, 1486.9202, 1493.1104, 1504.0795, 3028.8231, 3033.7111,

1 1.962247 1.675933 0.749201 8 -1.600834 0.353308 -0.515223 8 -1.909782 -0.273767 0.606306 8 0.062999 -0.249282 1.267522	3088.3762, 3093.6254, 3104.4006, 3122.7197, 3124.3114, 3221.8747

IRC



Compound: $(CH_3)_2CCH_2$ + O3 C_{FO}	**Energy (Hartree)** -382.334939529468
Reaction Coordinates: 6 -3.027434 -0.206214 -0.032585 6 -1.523681 -0.059575 0.009154 6 -0.973876 1.342228 -0.040487 1 -1.506913 1.984490 0.663305 1 0.096331 1.364295 0.160651 1 -1.156900 1.756174 -1.036238 8 -0.806720 -1.040626 0.077180 1 -3.455815 0.202623 0.885706 1 -3.447739 0.369470 -0.858970 1 -3.304803 -1.252663 -0.125160 6 1.868621 -1.133264 0.148599 1 1.808896 -2.040853 -0.434867 1 1.576975 -1.054498 1.186321 8 2.330170 -0.136076 -0.443598 8 2.392574 1.053191 0.247814	**Frequencies (cm^{-1}):** 31.9742, 54.7165, 81.1514, 84.3169, 99.2779, 112.666, 155.0764, 205.748, 395.907, 498.6377, 518.5888, 547.041, 680.6712, 791.9739, 860.1657, 890.2118, 906.0155, 994.0329, 1092.057, 1124.4266, 1234.7156, 1246.5682, 1388.5228, 1401.6351, 1414.0699, 1462.2137, 1465.6447, 1477.1367, 1495.2706, 1568.4278, 1752.3072, 3015.2894, 3031.9002, 3073.2498, 3085.3958, 3110.8754, 3134.6449, 3139.0544, 3278.2398

S11 Example MESMER Input File for O_3 + 1-Propene:

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>

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xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">

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timestamp="20190613_164702" />

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1464.08 1508.28 1579.47 1689.46 2956.35 3020.80 3031.27 3081.66 3140.65
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      </property>
      <property title="basis">
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      </property>
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        <scalar>B3LYP</scalar>
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      <property title="Energy" dictRef="me:ZPE">
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zeroPointVibEnergyAdded="true">0.00</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">204.95 425.86 592.52 924.20 947.72 950.30 1027.49 1075.02
1192.56 1330.73 1409.89 1452.59 1479.59 1494.42 1708.03 3014.16 3054.98 3090.02
3122.29 3128.63 3208.66</array>
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</property>

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<atom id="a3" elementType="C" x3="0.246523" y3="1.167424" z3="0.181761" />
<atom id="a4" elementType="H" x3="-0.151447" y3="1.870719" z3="-0.548496" />

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  <atom id="a6" elementType="O" x3="1.410517" y3="0.590862" z3="-0.404377" />
  <atom id="a7" elementType="O" x3="1.391085" y3="-0.754568" z3="0.128139" />
  <atom id="a8" elementType="O" x3="0.032978" y3="-1.138922" z3="-0.110778" />
  <atom id="a9" elementType="H" x3="-0.811837" y3="-0.188223" z3="1.515612" />
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  </property>
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<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

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</property>

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</property>

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<property dictRef="me:frequenciesScaleFactor" default="true">

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</propertyList>

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  <me:DistributionCalcMethod default="true" name="Boltzmann" />
  <me:energyTransferModel name="ExponentialDown" default="true" />
  <me:deltaEDown units="cm-1">300.0</me:deltaEDown>
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    <atom id="a3" elementType="C" x3="-0.319630" y3="1.177145" z3="0.070401" />
    <atom id="a4" elementType="H" x3="-0.487873" y3="1.944716" z3="0.823288" />
    <atom id="a5" elementType="H" x3="-0.031970" y3="1.631370" z3="-0.880474" />
    <atom id="a6" elementType="O" x3="-1.539167" y3="0.459373" z3="-0.060512" />
    <atom id="a7" elementType="O" x3="-1.069230" y3="-0.827669" z3="-0.500997" />
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    <atom id="a9" elementType="H" x3="1.003755" y3="0.228290" z3="1.548449" />
    <atom id="a10" elementType="H" x3="2.474743" y3="0.992813" z3="-0.375366" />
    <atom id="a11" elementType="H" x3="1.641410" y3="-0.162621" z3="-1.426001" />
    <atom id="a12" elementType="H" x3="2.619423" y3="-0.740974" z3="-0.066630" />
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    <bond atomRefs2="a8 a2" order="1" />
    <bond atomRefs2="a2 a9" order="1" />
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    </property>
    <property title="basis">
     <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
    </property>
    <property title="method">
     <scalar>B3LYP</scalar>
    </property>
    <property title="File Format">
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    </property>
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zeroPointVibEnergyAdded="true">-235.70</scalar>
    </property>
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835.09 904.91 934.15 954.79 1002.13 1062.49 1110.89 1165.63 1241.22 1308.39 1345.08
1380.99 1411.28 1486.88 1496.36 1506.91 3029.38 3033.44 3063.31 3095.20 3110.69
3116.89</array>
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     <array units="cm-1">0.217 0.117 0.092</array>
    </property>
    <property title="Symmetry Number" dictRef="me:symmetryNumber">
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    <me:DistributionCalcMethod default="true" name="Boltzmann" />
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      <atom id="a3" elementType="C" x3="0.971533" y3="1.353841" z3="-0.316182" />
      <atom id="a4" elementType="H" x3="0.531213" y3="1.938242" z3="-1.112426" />
      <atom id="a5" elementType="H" x3="1.068868" y3="1.835740" z3="0.648039" />
      <atom id="a6" elementType="H" x3="1.323959" y3="-0.317086" z3="-1.516737" />
      <atom id="a7" elementType="H" x3="2.105661" y3="-0.251830" z3="1.477924" />
      <atom id="a8" elementType="H" x3="1.478727" y3="-1.680958" z3="0.645647" />
      <atom id="a9" elementType="H" x3="3.055910" y3="-1.045358" z3="0.210847" />
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z3="0.752210" />
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      <bond atomRefs2="a12 a11" order="1" />
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      <bond atomRefs2="a1 a7" order="1" />
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        <scalar>Gaussian 09, Revision D.01</scalar>
      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
      <property title="method">
        <scalar>B3LYP</scalar>
      </property>
      <property title="File Format">
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      </property>
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        <scalar units="kJ/mol" convention="computational"
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741.88 925.19 952.25 956.03 1008.94 1069.60 1163.20 1192.11 1196.83 1325.78 1407.21
1449.56 1477.89 1493.02 1667.02 3019.25 3064.56 3098.95 3134.08 3139.23
3220.60</array>
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      <property title="Symmetry Number" dictRef="me:symmetryNumber">
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        <scalar>5.0</scalar>
      </property>
      <property dictRef="me:epsilon" default="true">
        <scalar>50.0</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor" default="true">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod xsi:type="QMRotors" />
    <me:DistributionCalcMethod default="true" name="Boltzmann" />
    <me:energyTransferModel name="ExponentialDown" default="true" />
    <me:deltaEDown units="cm-1">300.0</me:deltaEDown>
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    <atom id="a5" elementType="H" x3="0.511754" y3="1.915285" z3="1.063783" />
    <atom id="a6" elementType="H" x3="1.389971" y3="-0.298113" z3="1.496664" />
    <atom id="a7" elementType="H" x3="3.146442" y3="-0.982935" z3="-0.233810" />
    <atom id="a8" elementType="H" x3="1.600609" y3="-1.696077" z3="-0.641658" />
    <atom id="a9" elementType="H" x3="2.155223" y3="-0.253003" z3="-1.505010" />
    <atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.736533" y3="0.801348"
z3="-0.451900" />
    <atom id="a11" elementType="O" x3="-1.633209" y3="-0.454117" z3="-0.385960" />
    <atom id="a12" elementType="O" spinMultiplicity="2" x3="-1.279821" y3="-0.945198"
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    <bond atomRefs2="a2 a6" order="1" />
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    </property>
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zeroPointVibEnergyAdded="true">-14.82</scalar>
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    <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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742.72 924.13 951.24 959.39 1011.05 1069.60 1168.06 1194.72 1197.61 1326.27 1408.37
1451.06 1477.70 1494.37 1672.39 3015.97 3057.21 3094.56 3136.03 3141.22
3226.57</array>
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    <property dictRef="me:epsilon" default="true">
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    <me:DistributionCalcMethod default="true" name="Boltzmann" />
    <me:energyTransferModel name="ExponentialDown" default="true" />
    <me:deltaEDown units="cm-1">300.0</me:deltaEDown>
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     <atom id="a2" elementType="C" x3="0.704892" y3="-0.095474" z3="0.369695" />
     <atom id="a3" elementType="C" x3="-0.497599" y3="1.290475" z3="-0.095848" />
     <atom id="a4" elementType="H" x3="-0.181191" y3="1.950361" z3="0.727608" />
     <atom id="a5" elementType="H" x3="-0.106096" y3="1.573175" z3="-1.084563" />
     <atom id="a6" elementType="H" x3="0.465767" y3="-0.120182" z3="1.427646" />
     <atom id="a7" elementType="H" x3="2.797103" y3="-0.533157" z3="0.389879" />
     <atom id="a8" elementType="H" x3="2.404011" y3="1.180431" z3="0.278889" />
     <atom id="a9" elementType="H" x3="2.204504" y3="0.138218" z3="-1.140033" />
     <atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.642531" y3="0.750919"
z3="-0.019875" />
     <atom id="a11" elementType="O" spinMultiplicity="2" x3="-1.134302" y3="-1.261881"
z3="0.114900" />
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</bondArray>

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<scalar>Gaussian 09, Revision D.01</scalar>

</property>

<property title="basis">

<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

<scalar>g03</scalar>

</property>

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</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

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      <property dictRef="me:frequenciesScaleFactor" default="true">
        <scalar>1</scalar>
      </property>
    </propertyList>
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      <atom id="a6" elementType="H" x3="-1.203517" y3="-0.031654" z3="1.537554" />
      <atom id="a7" elementType="H" x3="-2.730821" y3="-0.335153" z3="-0.601855" />
      <atom id="a8" elementType="H" x3="-2.213169" y3="1.328091" z3="-0.307063" />
      <atom id="a9" elementType="H" x3="-1.396042" y3="0.333887" z3="-1.538607" />
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z3="-0.367051" />
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z3="0.273239" />
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</property>

<property title="basis">

<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

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</property>

<property title="File Format">

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</property>

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</property>

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848.66 897.37 947.79 1017.56 1051.81 1112.74 1170.13 1222.41 1267.65 1317.82 1398.67
1451.48 1477.75 1481.97 1499.91 2891.63 3032.51 3092.50 3106.45 3118.82
3224.46</array>

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      <atom id="a3" elementType="C" x3="0.400100" y3="1.129165" z3="0.043748" />
      <atom id="a4" elementType="H" x3="0.272014" y3="2.028118" z3="-0.546933" />
      <atom id="a5" elementType="H" x3="0.150824" y3="1.152906" z3="1.097425" />
      <atom id="a6" elementType="H" x3="-0.899090" y3="0.060505" z3="-1.547828" />
      <atom id="a7" elementType="H" x3="-1.950961" y3="0.042396" z3="1.377925" />
      <atom id="a8" elementType="H" x3="-2.938163" y3="-0.371555" z3="-0.025995" />
      <atom id="a9" elementType="H" x3="-2.345793" y3="1.281110" z3="0.155790" />
      <atom id="a10" elementType="O" x3="1.515835" y3="0.486568" z3="-0.264913" />
      <atom id="a11" elementType="O" spinMultiplicity="2" x3="1.626155" y3="-0.617773"
z3="0.450336" />
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      <bond atomRefs2="a3 a5" order="1" />
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      </property>
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      </property>
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        <scalar>B3LYP</scalar>
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873.65 884.71 988.54 989.69 1062.21 1090.56 1182.05 1229.85 1265.85 1351.31 1392.08
1451.36 1479.27 1483.45 1501.20 2912.54 3029.00 3091.75 3104.88 3115.75
3224.03</array>
      </property>
      <property title="ImaginaryFrequency" dictRef="me:imFreqs">
        <scalar units="cm-1">447.29</scalar>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
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      </property>
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      <property dictRef="me:frequenciesScaleFactor" default="true">
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      <atom id="a3" elementType="C" x3="-0.481983" y3="1.364071" z3="0.249512" />
      <atom id="a4" elementType="H" x3="0.044756" y3="1.912973" z3="1.015219" />
      <atom id="a5" elementType="H" x3="-0.647546" y3="1.872572" z3="-0.689368" />
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      <bond atomRefs2="a1 a9" order="1" />
      <bond atomRefs2="a1 a2" order="1" />
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      <bond atomRefs2="a2 a6" order="1" />
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      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
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<property title="File Format">

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</property>

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743.36 919.21 949.34 962.03 990.92 1054.68 1085.52 1117.27 1199.16 1300.89 1407.93
1445.11 1476.59 1492.81 1591.48 3019.96 3076.47 3109.70 3154.11 3165.25
3245.18</array>

</property>

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<property dictRef="me:frequenciesScaleFactor" default="true">

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<me:DOSCMethod xsi:type="QMRotors" />

</molecule>

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      <atom id="a7" elementType="H" x3="-1.872560" y3="-1.626643" z3="-0.255180" />
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      <atom id="a9" elementType="H" x3="-2.980842" y3="-0.273298" z3="-0.426744" />
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zeroPointVibEnergyAdded="true">15.96</scalar>
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742.19 916.13 952.95 955.96 989.43 1054.69 1079.77 1111.36 1196.19 1295.66 1406.63
1442.81 1479.03 1493.33 1586.14 3015.07 3074.40 3111.87 3155.43 3174.47
3251.32</array>
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<atom id="a3" elementType="C" x3="0.296814" y3="1.113797" z3="0.488690" />
<atom id="a4" elementType="H" x3="-0.100018" y3="2.072517" z3="0.158989" />
<atom id="a5" elementType="H" x3="0.825170" y3="1.214993" z3="1.439952" />
<atom id="a6" elementType="H" x3="-1.218772" y3="-0.047703" z3="1.526952" />
<atom id="a7" elementType="H" x3="-1.277398" y3="0.095444" z3="-1.546414" />
<atom id="a8" elementType="H" x3="-2.363395" y3="-0.889421" z3="-0.556673" />
<atom id="a9" elementType="C" x3="-0.743890" y3="-0.000174" z3="0.545489" />
<atom id="a10" elementType="O" x3="1.159387" y3="0.666047" z3="-0.541085" />
<atom id="a11" elementType="O" x3="0.106131" y3="-1.146123" z3="0.506226" />
<atom id="a12" elementType="O" x3="1.217267" y3="-0.786482" z3="-0.378590" />
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</property>

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</property>

<property title="method">

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</property>

<property title="File Format">

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<property dictRef="me:frequenciesScaleFactor" default="true">

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    <atom id="a7" elementType="H" x3="2.136289" y3="-0.003363" z3="1.195784" />
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</bondArray>

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<property title="method">

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</property>

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<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

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<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

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1429.40 1471.58 1495.34 1539.20 2919.34 2983.64 3034.73 3105.23 3132.48
3154.73</array>

</property>

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        <molecule ref="O3" role="excessReactant" />
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    </reactantList>
    <productList>
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    <n>0</n>
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</reaction>
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    <me:MarquardtTolerance>0.1</me:MarquardtTolerance>
    </me:calcMethod>-->
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:printGrainedSpeciesProfile />
    <me:eigenvalues>3</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not
shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
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  </me:control>
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    <dc:source>R1_f.xml</dc:source>
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    <dc:date>20190613_180524</dc:date>
    <dc:contributor>c1675612</dc:contributor>
  </metadataList>
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