Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

"Effect of unsaturated substituents in the reaction of Criegee intermediates with water vapor"

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This supplementary material includes: the complete list of zero-point corrected energies, the distortion energy, the Mulliken charge distribution of central carbon and β carbon in $CH_2CHCHOO$, all the rate coefficients calculated in this work, variational effect for the lowest channel for each CI reaction with water monomer and water dimer, and the geometry parameters including reactant, van der Waals (vdW) complex, and TS.

In Table S1 we list the all the zero-point corrected energies for van der Waals (vdW) complex and transition state (TS) studied in this work. It is an extension of Table 1 of main text, where we only listed the lowest channel for each reaction.

Table S1 Complete list of zero-point corrected energies for van der Waals (vdW) complex and transition state (TS), in kcal mol^{-1}. Energies are from QCISD(T)/CBS//B3LYP/6-311+G(2d,2p) and zero-point correction using B3LYP/6-311+G(2d,2p).

***anti*-type CIs**	H_2O	vdW	TS	$(H_2O)_2$	vdW	TS
CH_2OO	1a	-6.30	3.92	2a	-10.13	-5.89
	1b	-6.30	3.05	2b	-10.32	-5.80
				2c	-9.84	-4.63
				2d	-10.02	-5.68
anti-CH_3CHOO	1a	-7.80	1.20	2a	-12.96	-6.74
	1b	-7.80	0.59	2b	-13.37	-7.01
				2c	-12.96	-5.79
				2d	-13.37	-6.49
anti_Syn-CH_3CH_2CHOO	1a	-8.04	0.63	2a	-13.31	-6.90
	1b	-8.04	0.25	2b	-13.72	-7.43
				2c	-13.31	-6.26
				2d	-13.72	-6.61
anti_Gauche-CH_3CH_2CHOO	1a	-7.86	1.14	2a	-12.26	-6.76
	1b	-7.86	0.46	2b	-12.74	-7.37
				2c	-12.33	-6.17
				2d	-12.74	-6.52
	1a'	-7.98	0.86	2a'	-12.96	-7.23
	1b'	-7.98	0.45	2b'	-13.37	-7.43
				2c'	-12.96	-6.21
				2d'	-13.37	-6.99
anti_Syn-$CH_2CHCHOO$_carbonyl insertion	1a	-6.45	4.16	2a	-10.67	-4.02
	1b	-6.45	3.15	2b	-10.75	-3.16
				2c	-10.67	-1.85
				2d	-10.75	-3.78
anti_Syn-$CH_2CHCHOO$_vinyl insertion	not found			2a	-10.60	7.84
				2b	-10.60	7.68
				2c	-10.60	8.34
				2d	-10.60	8.26
anti_Anti-$CH_2CHCHOO$_carbonyl insertion	1a	-6.77	5.22	2a	-11.90	-2.01
	1b	-6.77	4.18	2b	-11.90	-1.96
				2c	-11.90	-0.67
				2d	-11.90	-1.72
anti_Anti-$CH_2CHCHOO$_vinyl insertion	1a	-6.78	32.14	2a	-11.90	11.82
				2b	-11.90	11.57
anti-CHCCHOO	1a	-5.97	6.03	2a	-9.24	-2.35
	1b	-5.97	4.76	2b	-9.31	-1.62

				2c	-9.24	-0.31
				2d	-9.62	-2.09
***syn*-type CIs**	H_2O	vdW	TS	$(H_2O)_2$	vdW	TS
syn-CH_3CHOO	1a	-6.67	8.59	2a	-11.15	-2.46
	1b	-6.67	7.20	2b	-11.43	-2.42
				2c	-11.14	-0.87
				2d	-11.43	-2.77
$(CH_3)_2COO$	1a	-7.83	6.66	2a	-13.10	-2.45
	1b	-7.83	5.57	2b	-13.57	-2.66
				2c	-13.10	-1.07
				2d	-12.73	-1.89
syn_Anti-CH_3CH_2CHOO	1a	-6.75	8.45	2a	-11.79	-3.06
	1b	-6.75	6.70	2b	-11.95	-2.73
	1a'	-6.75	7.96	2c	-11.79	-1.15
	1b'	-6.75	6.73	2d	-11.95	-3.37
syn_Gauche-CH_3CH_2CHOO	1a	-6.38	9.94	2a	-11.33	-4.01
	1b	-6.38	8.58	2b	-11.61	-4.13
				2c	-11.33	-2.65
				2d	-11.61	-4.24
				2a'	-10.57	-1.19
				2b'	-10.90	-1.17
				2c'	-10.57	0.48
				2d'	-10.90	-1.36
syn_Syn-$CH_2CHCHOO$_carbonyl insertion	1a	-4.44	11.19	2a	-8.76	2.38
	1b	-4.44	10.78	2b	-9.13	2.10
				2c	-8.76	3.42
				2d	-9.13	2.61
syn_Syn-$CH_2CHCHOO$_vinyl insertion	1a	-4.44	9.61	2a	-7.48	3.88
	1b	-4.44	9.53	2b	-7.38	4.44
				2c	-7.48	4.92
				2d	-7.38	4.58
syn_Anti-$CH_2CHCHOO$_carbonyl insertion	1a	-5.88	8.21	2a	-10.02	0.73
	1b	-5.88	8.22	2b	-10.21	-0.75
				2c	-10.02	0.67
				2d	-10.31	0.64
syn_Anti-$CH_2CHCHOO$_vinyl insertion	1a	-5.89	26.51	2a	-9.33	8.88
				2b	-9.33	7.93
syn-CHCCHOO	1a	-4.68	9.18	2a	-8.71	0.75
	1b	-4.68	9.60	2b	-8.99	-0.27
				2c	-8.71	0.87
				2d	-8.80	1.19

The distortion energy versus reaction barrier is listed in Table S2 and plotted in Figure S1, see below.

Table S2 distortion energy versus reaction barrier for CIs react with (a) H_2O and (b) $(H_2O)_2$

CIs	channel	Reactant to TS energy	distortion-CI	distortion-water
CH_2OO	1a	1.31	12.14	6.19
	1b	0.33	11.77	5.65
	2a	-9.11	7.45	15.55

	2b	-8.89	7.84	16.54
	2c	-7.51	8.34	18.26
	2d	-8.87	7.39	16.47
anti-CH_3CHOO	1a	-0.70	11.83	10.05
	1b	-1.47	11.60	9.48
	2a	-9.00	8.27	22.04
	2b	-9.12	8.41	23.22
	2c	-7.68	8.73	25.04
	2d	-8.74	8.23	22.83
syn-CH_3CHOO	1a	6.53	18.87	7.96
	1b	5.18	18.34	7.92
	2a	-4.34	10.20	24.16
	2b	-4.32	10.59	24.40
	2c	-2.62	11.40	25.48
	2d	-4.65	9.67	25.64
$(CH_3)_2COO$	1a	5.27	18.77	11.87
	1b	4.17	18.18	11.95
	2a	-3.57	10.36	31.52
	2b	-3.72	10.49	32.21
	2c	-1.99	11.24	33.23
	2d	-3.87	9.85	33.20
anti_Anti-$CH_2CHCHOO$	1a	3.99	12.07	14.69
	1b	2.88	11.54	14.75
	2a	-3.05	9.03	29.28
	2b	-2.98	9.47	29.03
	2c	-1.51	9.70	30.56
	2d	-2.79	9.06	29.68
anti_Syn-$CH_2CHCHOO$	1a	2.86	10.66	14.09
	1b	1.59	10.86	12.02
	2a	-5.51	8.46	26.32
	2b	-4.37	8.64	28.84
	2c	-2.83	8.74	30.92
	2d	-5.29	8.48	26.98
syn_Anti-$CH_2CHCHOO$	1a	6.84	15.89	10.90
	1b	7.01	16.05	11.56
	2a	-0.10	9.85	30.57
	2b	-1.90	10.33	28.33
	2c	-0.33	10.79	29.41
	2d	-0.16	9.50	32.80
syn_Syn-$CH_2CHCHOO$	1a	10.06	19.56	10.15
	1b	9.70	20.19	9.90
	2a	1.57	12.37	29.26
	2b	1.24	11.77	29.82
	2c	2.69	12.55	30.54
	2d	1.88	11.84	31.67

anti-CHCCHOO	1a	4.43	11.94	11.62
	1b	3.01	11.71	10.54
	2a	-4.23	9.16	22.76
	2b	-3.25	9.20	24.36
	2c	-1.73	9.45	26.09
	2d	-3.99	9.13	23.22
syn-CHCCHOO	1a	7.51	16.38	8.73
	1b	8.03	16.56	8.97
	2a	-0.78	9.88	24.43
	2b	-1.91	10.22	23.82
	2c	-0.62	10.53	25.08
	2d	-0.21	9.75	26.31

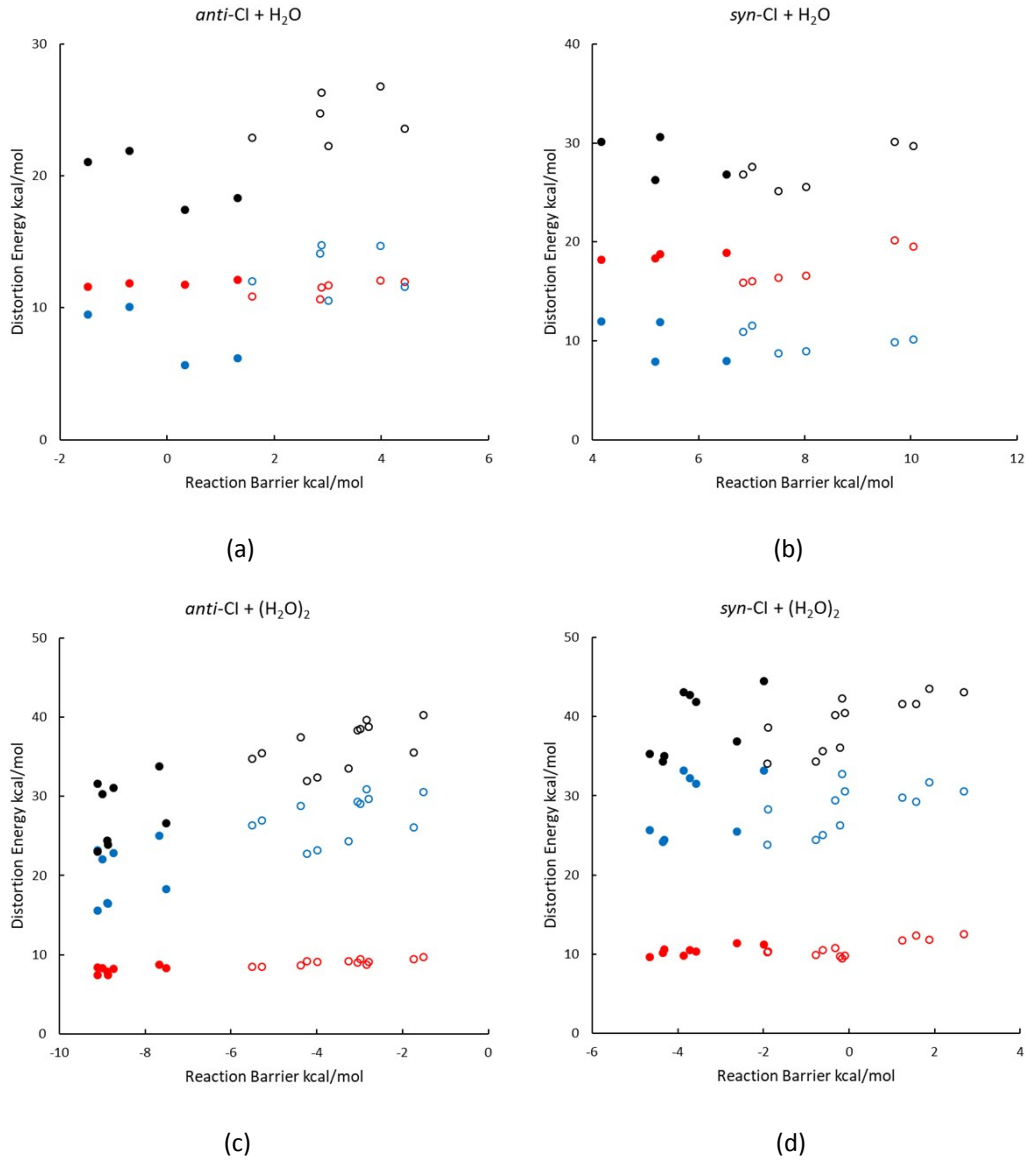

Figure S1 Distortion energy versus reaction barrier for the reaction of (a) *anti*-CI with H_2O, (b) *syn*-CI with H_2O, (c) *anti*-CI with $(H_2O)_2$, and (d) *syn*-CI with $(H_2O)_2$. Red circles are the CIs's contribution, blue

circles are the water's contribution, and black circles are the total distortion energy. Solid ones are for saturated CIs and empty ones are for unsaturated CIs, respectively.

To explain the different energy barrier between vinyl insertion and the carbonyl insertion reaction for $CH_2CHCHOO$, here we listed the Mulliken charge distribution of central carbon and β carbon in $CH_2CHCHOO$, along with energy barriers. One can clearly see that the carbonyl oxygen has a larger positive charge compared to the vinyl carbon.

Table S3 The Mulliken charge distribution of carbonyl carbon and vinyl-β carbon in $CH_2CHCHOO$.

mulliken charge distribution	Q (carbonyl C)	Q (vinyl-β C)
anti_Syn-$CH_2CHCHOO$	0.14	-0.238
anti_Anti-$CH_2CHCHOO$	0.113	-0.238
syn_Syn-$CH_2CHCHOO$	0.058	-0.214
syn_Anti-$CH_2CHCHOO$	0.111	-0.252

Here we list all the reaction rate coefficients studied in this work (by method 3 discussed in the main text). The unit is cm^3s^{-1}.

Table S4 The rate coefficients calculated in this work, in $cm^3\ s^{-1}$.

(a) CH_2OO

T(K)	CH_2OO			
	H_2O	$(H_2O)_2$	D_2O	$(D_2O)_2$
223.15	1.19E-16	2.04E-10	9.77E-17	1.49E-10
228.15	1.33E-16	1.42E-10	1.08E-16	1.02E-10
233.15	1.47E-16	9.98E-11	1.18E-16	7.08E-11
238.15	1.63E-16	7.13E-11	1.30E-16	4.99E-11
243.15	1.79E-16	5.16E-11	1.41E-16	3.56E-11
248.15	1.96E-16	3.78E-11	1.54E-16	2.58E-11
253.15	2.15E-16	2.80E-11	1.67E-16	1.89E-11
258.15	2.34E-16	2.10E-11	1.81E-16	1.40E-11
263.15	2.55E-16	1.59E-11	1.95E-16	1.04E-11
268.15	2.76E-16	1.21E-11	2.10E-16	7.90E-12
273.15	2.98E-16	9.38E-12	2.26E-16	6.04E-12
278.15	3.22E-16	7.30E-12	2.42E-16	4.65E-12
283.15	3.46E-16	5.73E-12	2.59E-16	3.62E-12
288.15	3.72E-16	4.54E-12	2.77E-16	2.84E-12
293.15	3.98E-16	3.62E-12	2.96E-16	2.24E-12
298.15	4.26E-16	2.91E-12	3.15E-16	1.79E-12
303.15	4.54E-16	2.35E-12	3.35E-16	1.43E-12

308.15	4.84E-16	1.92E-12	3.55E-16	1.16E-12
313.15	5.15E-16	1.57E-12	3.77E-16	9.42E-13
318.15	5.47E-16	1.30E-12	3.99E-16	7.71E-13
323.15	5.80E-16	1.08E-12	4.22E-16	6.35E-13

(b) CH_3CHOO and $(CH_3)_2COO$

T(K)	*anti*-CH_3CHOO		*syn*-CH_3CHOO		$(CH_3)_2COO$	
	H_2O	$(H_2O)_2$	H_2O	$(H_2O)_2$	H_2O	$(H_2O)_2$
223.15	3.08E-14	1.21E-09	6.13E-21	1.08E-13	3.78E-19	1.31E-13
228.15	2.99E-14	7.85E-10	8.29E-21	8.48E-14	4.57E-19	9.58E-14
233.15	2.91E-14	5.18E-10	1.11E-20	6.74E-14	5.51E-19	7.16E-14
238.15	2.84E-14	3.48E-10	1.46E-20	5.41E-14	6.60E-19	5.43E-14
243.15	2.78E-14	2.37E-10	1.91E-20	4.38E-14	7.86E-19	4.19E-14
248.15	2.72E-14	1.64E-10	2.47E-20	3.58E-14	9.33E-19	3.27E-14
253.15	2.67E-14	1.15E-10	3.17E-20	2.95E-14	1.10E-18	2.59E-14
258.15	2.63E-14	8.19E-11	4.03E-20	2.45E-14	1.29E-18	2.07E-14
263.15	2.59E-14	5.90E-11	5.08E-20	2.05E-14	1.51E-18	1.68E-14
268.15	2.55E-14	4.30E-11	6.35E-20	1.72E-14	1.76E-18	1.37E-14
273.15	2.51E-14	3.17E-11	7.88E-20	1.46E-14	2.04E-18	1.13E-14
278.15	2.48E-14	2.36E-11	9.71E-20	1.24E-14	2.36E-18	9.40E-15
283.15	2.45E-14	1.78E-11	1.19E-19	1.07E-14	2.71E-18	7.88E-15
288.15	2.43E-14	1.36E-11	1.45E-19	9.19E-15	3.11E-18	6.65E-15
293.15	2.41E-14	1.04E-11	1.75E-19	7.97E-15	3.55E-18	5.66E-15
298.15	2.38E-14	8.07E-12	2.10E-19	6.94E-15	4.04E-18	4.84E-15
303.15	2.37E-14	6.30E-12	2.51E-19	6.08E-15	4.58E-18	4.17E-15
308.15	2.35E-14	4.96E-12	2.98E-19	5.34E-15	5.18E-18	3.61E-15
313.15	2.33E-14	3.94E-12	3.53E-19	4.72E-15	5.84E-18	3.15E-15
318.15	2.32E-14	3.15E-12	4.15E-19	4.18E-15	6.56E-18	2.76E-15
323.15	2.31E-14	2.54E-12	4.87E-19	3.72E-15	7.35E-18	2.43E-15

(c) *anti*-CH_3CH_2CHOO

T(K)	*anti_Syn*-CH_3CH_2CHOO		*anti_Gauche*-CH_3CH_2CHOO	
	H_2O	$(H_2O)_2$	H_2O	$(H_2O)_2$
223.15	7.00E-14	2.19E-09	3.48E-14	1.73E-09
228.15	6.67E-14	1.38E-09	3.37E-14	1.10E-09
233.15	6.37E-14	8.94E-10	3.27E-14	7.18E-10
238.15	6.11E-14	5.88E-10	3.19E-14	4.76E-10
243.15	5.87E-14	3.93E-10	3.11E-14	3.20E-10
248.15	5.65E-14	2.67E-10	3.04E-14	2.19E-10
253.15	5.46E-14	1.85E-10	2.98E-14	1.52E-10
258.15	5.29E-14	1.29E-10	2.92E-14	1.07E-10
263.15	5.13E-14	9.19E-11	2.86E-14	7.63E-11
268.15	4.98E-14	6.61E-11	2.82E-14	5.51E-11
273.15	4.85E-14	4.81E-11	2.77E-14	4.03E-11
278.15	4.73E-14	3.54E-11	2.73E-14	2.98E-11

283.15	4.62E-14	2.64E-11	2.69E-14	2.22E-11
288.15	4.52E-14	1.99E-11	2.66E-14	1.68E-11
293.15	4.42E-14	1.51E-11	2.63E-14	1.28E-11
298.15	4.33E-14	1.16E-11	2.60E-14	9.83E-12
303.15	4.25E-14	8.96E-12	2.58E-14	7.62E-12
308.15	4.18E-14	6.99E-12	2.55E-14	5.96E-12
313.15	4.11E-14	5.51E-12	2.53E-14	4.70E-12
318.15	4.05E-14	4.37E-12	2.51E-14	3.73E-12
323.15	3.99E-14	3.49E-12	2.49E-14	2.99E-12

(d) *syn*-CH_3CH_2CHOO

T(K)	*syn_Anti*-CH_3CH_2CHOO		*syn_Gauche*-CH_3CH_2CHOO	
	H_2O	$(H_2O)_2$	H_2O	$(H_2O)_2$
223.15	1.39E-20	3.01E-13	7.89E-21	1.16E-12
228.15	1.83E-20	2.28E-13	1.05E-20	8.54E-13
233.15	2.38E-20	1.75E-13	1.38E-20	6.38E-13
238.15	3.07E-20	1.36E-13	1.79E-20	4.83E-13
243.15	3.92E-20	1.07E-13	2.30E-20	3.70E-13
248.15	4.96E-20	8.46E-14	2.94E-20	2.86E-13
253.15	6.22E-20	6.77E-14	3.71E-20	2.23E-13
258.15	7.74E-20	5.47E-14	4.66E-20	1.76E-13
263.15	9.56E-20	4.46E-14	5.80E-20	1.40E-13
268.15	1.17E-19	3.66E-14	7.16E-20	1.12E-13
273.15	1.43E-19	3.03E-14	8.77E-20	9.10E-14
278.15	1.73E-19	2.53E-14	1.07E-19	7.42E-14
283.15	2.08E-19	2.12E-14	1.29E-19	6.09E-14
288.15	2.48E-19	1.79E-14	1.56E-19	5.04E-14
293.15	2.95E-19	1.52E-14	1.86E-19	4.19E-14
298.15	3.49E-19	1.30E-14	2.22E-19	3.51E-14
303.15	4.11E-19	1.12E-14	2.63E-19	2.96E-14
308.15	4.82E-19	9.66E-15	3.09E-19	2.51E-14
313.15	5.62E-19	8.39E-15	3.63E-19	2.14E-14
318.15	6.52E-19	7.32E-15	4.24E-19	1.83E-14
323.15	7.55E-19	6.42E-15	4.93E-19	1.58E-14

(e) *anti_Anti*-$CH_2CHCHOO$

T(K)	*anti_Anti*-$CH_2CHCHOO$			
	H_2O	$(H_2O)_2$	H_2O (VI)	$(H_2O)_2$(VI)
223.15	3.14E-17	7.42E-14	1.63E-45	7.78E-28
228.15	3.36E-17	5.79E-14	7.74E-45	1.22E-27
233.15	3.62E-17	4.58E-14	3.44E-44	1.89E-27
238.15	3.90E-17	3.67E-14	1.43E-43	2.86E-27
243.15	4.21E-17	2.97E-14	5.65E-43	4.28E-27
248.15	4.55E-17	2.43E-14	2.10E-42	6.30E-27
253.15	4.92E-17	2.01E-14	7.44E-42	9.13E-27

258.15	5.32E-17	1.67E-14	2.51E-41	1.31E-26
263.15	5.75E-17	1.41E-14	8.08E-41	1.85E-26
268.15	6.22E-17	1.19E-14	2.49E-40	2.58E-26
273.15	6.72E-17	1.02E-14	7.37E-40	3.56E-26
278.15	7.25E-17	8.73E-15	2.10E-39	4.85E-26
283.15	7.82E-17	7.55E-15	5.77E-39	6.55E-26
288.15	8.43E-17	6.56E-15	1.53E-38	8.76E-26
293.15	9.07E-17	5.73E-15	3.92E-38	1.16E-25
298.15	9.76E-17	5.04E-15	9.76E-38	1.52E-25
303.15	1.05E-16	4.45E-15	2.36E-37	1.98E-25
308.15	1.13E-16	3.95E-15	5.53E-37	2.56E-25
313.15	1.21E-16	3.52E-15	1.26E-36	3.28E-25
318.15	1.29E-16	3.15E-15	2.81E-36	4.16E-25
323.15	1.38E-16	2.83E-15	6.11E-36	5.26E-25

(f) *anti_Syn*-$CH_2CHCHOO$

T(K)	*anti_Syn*-$CH_2CHCHOO$		
	H_2O	$(H_2O)_2$	$(H_2O)_2$(VI)
223.15	1.29E-16	1.91E-12	3.02E-24
228.15	1.37E-16	1.40E-12	4.09E-24
233.15	1.47E-16	1.05E-12	5.46E-24
238.15	1.57E-16	7.88E-13	7.19E-24
243.15	1.67E-16	6.01E-13	9.37E-24
248.15	1.79E-16	4.64E-13	1.21E-23
253.15	1.91E-16	3.62E-13	1.54E-23
258.15	2.03E-16	2.85E-13	1.94E-23
263.15	2.16E-16	2.26E-13	2.43E-23
268.15	2.30E-16	1.82E-13	3.01E-23
273.15	2.44E-16	1.47E-13	3.70E-23
278.15	2.60E-16	1.20E-13	4.52E-23
283.15	2.75E-16	9.84E-14	5.48E-23
288.15	2.92E-16	8.13E-14	6.59E-23
293.15	3.09E-16	6.77E-14	7.88E-23
298.15	3.26E-16	5.68E-14	9.37E-23
303.15	3.45E-16	4.79E-14	1.11E-22
308.15	3.64E-16	4.06E-14	1.30E-22
313.15	3.84E-16	3.47E-14	1.52E-22
318.15	4.04E-16	2.97E-14	1.77E-22
323.15	4.25E-16	2.56E-14	2.06E-22

(g) *syn_Anti*-$CH_2CHCHOO$

T(K)	*syn_Anti*-$CH_2CHCHOO$			
	H_2O	$(H_2O)_2$	H_2O(VI)	$(H_2O)_2$(VI)
223.15	2.04E-21	1.24E-15	7.13E-40	1.79E-23
228.15	2.78E-21	1.04E-15	2.47E-39	1.90E-23

233.15	3.77E-21	8.86E-16	8.16E-39	2.04E-23
238.15	5.04E-21	7.60E-16	2.56E-38	2.22E-23
243.15	6.69E-21	6.57E-16	7.68E-38	2.44E-23
248.15	8.80E-21	5.73E-16	2.20E-37	2.70E-23
253.15	1.15E-20	5.03E-16	6.08E-37	3.00E-23
258.15	1.48E-20	4.45E-16	1.62E-36	3.36E-23
263.15	1.89E-20	3.95E-16	4.14E-36	3.77E-23
268.15	2.41E-20	3.54E-16	1.02E-35	4.24E-23
273.15	3.04E-20	3.18E-16	2.45E-35	4.77E-23
278.15	3.80E-20	2.87E-16	5.70E-35	5.37E-23
283.15	4.73E-20	2.61E-16	1.29E-34	6.06E-23
288.15	5.84E-20	2.38E-16	2.83E-34	6.83E-23
293.15	7.17E-20	2.18E-16	6.05E-34	7.69E-23
298.15	8.75E-20	2.00E-16	1.26E-33	8.65E-23
303.15	1.06E-19	1.85E-16	2.57E-33	9.72E-23
308.15	1.28E-19	1.71E-16	5.13E-33	1.09E-22
313.15	1.54E-19	1.59E-16	1.00E-32	1.22E-22
318.15	1.84E-19	1.48E-16	1.91E-32	1.37E-22
323.15	2.18E-19	1.38E-16	3.58E-32	1.53E-22

(h) *syn_Syn*-$CH_2CHCHOO$

T(K)	*syn_Syn*-$CH_2CHCHOO$			
	H_2O	$(H_2O)_2$	H_2O(VI)	$(H_2O)_2$(VI)
223.15	4.83E-24	6.22E-18	4.19E-23	1.25E-20
228.15	7.71E-24	5.86E-18	6.41E-23	1.42E-20
233.15	1.21E-23	5.57E-18	9.65E-23	1.61E-20
238.15	1.87E-23	5.32E-18	1.43E-22	1.80E-20
243.15	2.83E-23	5.11E-18	2.08E-22	2.02E-20
248.15	4.23E-23	4.93E-18	2.98E-22	2.24E-20
253.15	6.23E-23	4.78E-18	4.22E-22	2.47E-20
258.15	9.05E-23	4.64E-18	5.90E-22	2.72E-20
263.15	1.30E-22	4.53E-18	8.14E-22	2.98E-20
268.15	1.84E-22	4.43E-18	1.11E-21	3.26E-20
273.15	2.57E-22	4.34E-18	1.50E-21	3.55E-20
278.15	3.56E-22	4.26E-18	2.00E-21	3.85E-20
283.15	4.88E-22	4.19E-18	2.64E-21	4.16E-20
288.15	6.62E-22	4.13E-18	3.46E-21	4.49E-20
293.15	8.89E-22	4.08E-18	4.48E-21	4.82E-20
298.15	1.18E-21	4.04E-18	5.77E-21	5.18E-20
303.15	1.56E-21	4.00E-18	7.37E-21	5.54E-20
308.15	2.04E-21	3.96E-18	9.33E-21	5.92E-20
313.15	2.65E-21	3.93E-18	1.17E-20	6.31E-20
318.15	3.42E-21	3.91E-18	1.47E-20	6.71E-20
323.15	4.37E-21	3.89E-18	1.82E-20	7.12E-20

(i) CHCCHOO

T(K)	*anti*-CHCCHOO		*syn*-CHCCHOO	
	H_2O	$(H_2O)_2$	H_2O	$(H_2O)_2$
223.15	3.34E-18	4.29E-14	1.04E-22	2.23E-16
228.15	3.89E-18	3.48E-14	1.53E-22	1.99E-16
233.15	4.51E-18	2.85E-14	2.23E-22	1.79E-16
238.15	5.21E-18	2.35E-14	3.19E-22	1.62E-16
243.15	5.99E-18	1.96E-14	4.51E-22	1.47E-16
248.15	6.86E-18	1.64E-14	6.29E-22	1.34E-16
253.15	7.83E-18	1.39E-14	8.68E-22	1.22E-16
258.15	8.91E-18	1.18E-14	1.18E-21	1.13E-16
263.15	1.01E-17	1.01E-14	1.60E-21	1.04E-16
268.15	1.14E-17	8.65E-15	2.13E-21	9.60E-17
273.15	1.28E-17	7.47E-15	2.82E-21	8.90E-17
278.15	1.44E-17	6.49E-15	3.69E-21	8.29E-17
283.15	1.61E-17	5.67E-15	4.79E-21	7.74E-17
288.15	1.79E-17	4.97E-15	6.17E-21	7.25E-17
293.15	2.00E-17	4.38E-15	7.88E-21	6.80E-17
298.15	2.21E-17	3.88E-15	9.99E-21	6.40E-17
303.15	2.45E-17	3.45E-15	1.26E-20	6.04E-17
308.15	2.70E-17	3.08E-15	1.57E-20	5.71E-17
313.15	2.97E-17	2.76E-15	1.95E-20	5.41E-17
318.15	3.26E-17	2.48E-15	2.41E-20	5.14E-17
323.15	3.57E-17	2.24E-15	2.95E-20	4.89E-17

Here we listed the variational effect of lowest channel for each CI reaction with water monomer and water dimer.

Table S5 variational effect of lowest channel for each CI reaction with water monomer and water dimer.

***anti*-type CIs**	223.15	243.15	263.15	283.15	298.15	313.15	323.15
$CH_2OO + H_2O$	0.77	0.79	0.81	0.83	0.84	0.86	0.86
$CH_2OO + (H_2O)_2$	0.68	0.72	0.75	0.78	0.81	0.83	0.84
anti-$CH_3CHOO + H_2O$	0.50	0.53	0.56	0.58	0.60	0.62	0.63
anti-$CH_3CHOO + (H_2O)2$	0.37	0.43	0.47	0.52	0.55	0.58	0.60
anti_Syn-$CH_3CH_2CHOO + H_2O$	0.51	0.55	0.58	0.61	0.63	0.65	0.66
anti_Syn-$CH_3CH_2CHOO + (H_2O)2$	0.37	0.43	0.47	0.52	0.56	0.59	0.61
anti_Gauche-$CH_3CH_2CHOO + H_2O$	0.52	0.56	0.59	0.62	0.64	0.66	0.68
anti_Gauche-$CH_3CH_2CHOO + (H_2O)2$	0.40	0.46	0.51	0.56	0.59	0.62	0.65
anti_Syn-$CH_2CHCHOO + H_2O$	0.44	0.48	0.51	0.54	0.56	0.58	0.59
anti_Syn-$CH_2CHCHOO + (H_2O)_2$	0.38	0.44	0.49	0.55	0.58	0.61	0.63
anti_Anti-$CH_2CHCHOO + H_2O$	0.42	0.46	0.48	0.51	0.53	0.54	0.55
anti_Anti-$CH_2CHCHOO + (H_2O)_2$	0.47	0.52	0.57	0.61	0.64	0.67	0.69
anti-$CHCCHOO + H_2O$	0.46	0.49	0.52	0.55	0.56	0.58	0.59
anti-$CHCCHOO + (H_2O)_2$	0.45	0.51	0.56	0.60	0.63	0.66	0.68

***syn*-type CIs**	223.15	243.15	263.15	283.15	298.15	313.15	323.15
syn-$CH_3CHOO + H_2O$	0.63	0.66	0.68	0.71	0.72	0.74	0.75
syn-$CH_3CHOO + (H_2O)_2$	0.30	0.35	0.39	0.44	0.47	0.50	0.52
$(CH_3)_2COO + H_2O$	0.43	0.46	0.49	0.52	0.54	0.55	0.57
$(CH_3)_2COO + (H_2O)_2$	0.55	0.60	0.64	0.68	0.71	0.73	0.75
syn_Anti-$CH_3CH_2CHOO + H_2O$	0.61	0.64	0.66	0.69	0.71	0.72	0.73
syn_Anti-$CH_3CH_2CHOO + (H_2O)_2$	0.37	0.42	0.47	0.52	0.55	0.58	0.60
syn_Gauche-$CH_3CH_2CHOO + H_2O$	0.69	0.72	0.75	0.77	0.79	0.80	0.81
syn_Gauche-$CH_3CH_2CHOO + (H_2O)_2$	0.34	0.40	0.45	0.49	0.52	0.55	0.57
syn_Anti-$CH_2CHCHOO + H_2O$	0.47	0.50	0.53	0.56	0.58	0.59	0.60
syn_Anti-$CH_2CHCHOO + (H_2O)_2$	0.38	0.43	0.49	0.54	0.57	0.61	0.63
syn_Syn-$CH_2CHCHOO + H_2O$	0.49	0.53	0.56	0.58	0.60	0.62	0.63
syn_Syn-$CH_2CHCHOO + H_2O$ VI	0.83	0.85	0.87	0.88	0.89	0.90	0.91
syn_Syn-$CH_2CHCHOO + (H_2O)_2$	0.52	0.57	0.62	0.66	0.69	0.72	0.74
syn_Syn-$CH_2CHCHOO + (H_2O)_2$ VI	0.65	0.69	0.73	0.76	0.78	0.81	0.82
syn-$CHCCHOO + H_2O$	0.57	0.60	0.63	0.65	0.67	0.69	0.70
syn-$CHCCHOO + (H_2O)_2$	0.43	0.48	0.54	0.59	0.62	0.65	0.67

Below are the optimized geometries studied in this work for the Criegee Intermediates, vdW complex, transition states, obtained by B3LYP/6-311+G(2d,2p):

$(CH_3)_2COO$

C	0.4915324045	0.2547705759	-0.0707839595
O	-0.5232267129	-0.4531589839	-0.3365505655
O	-1.7499466841	0.178684224	-0.3752151478
C	1.793503328	-0.4620343155	-0.0385245882
H	2.4809212902	-0.0260609355	-0.7673730953
H	2.2595925393	-0.3510771651	0.9434559432
H	1.6584511697	-1.5181041133	-0.2566239081
C	0.3280527869	1.6974890144	0.1821469195
H	-0.1604109552	2.1561724214	-0.6817109205
H	-0.3785926866	1.8357770679	1.004804961
H	1.2787893203	2.1776861495	0.3963674251

$(CH_3)_2COO$ 1a TS

C	0.9965631246	0.2715181363	0.1060298781
O	-0.0832568631	-0.3676318641	-0.2221930876
O	-1.2392257251	0.441689734	0.1375611824
O	0.3772596216	1.9059634737	-0.8612792224
H	-0.5779257766	1.4671801616	-0.4699875852
H	0.5414082641	2.7154943912	-0.3682567999
C	1.1597981892	0.8705369882	1.4703950614
H	1.5362576476	0.0757558512	2.1219363302

H	1.8995541182	1.6675355391	1.4630367136
H	0.2108783164	1.2205900168	1.8586238795
C	2.2117115939	-0.198972864	-0.6238088042
H	2.9323215921	0.6118152673	-0.7014521803
H	2.6761681887	-1.0120989875	-0.0614561647
H	1.9471667085	-0.5513548438	-1.6159602009

$(CH_3)_2COO$ 1a vdW

C	0.6203545273	-0.6538724674	0.2437443888
O	-0.4755600587	-0.8757416332	-0.3441288326
O	-1.5891805513	-0.1360891022	0.0632509265
O	-0.6459746903	2.274834087	-0.8333574772
H	-1.1659633457	1.4803478974	-0.5822009361
H	-1.1554689441	2.7273437865	-1.508648706
C	0.7134495065	0.3293782298	1.3366308559
H	1.6716571868	0.2612555591	1.8442378106
H	0.578415832	1.3332992866	0.9209001092
H	-0.122106558	0.1783306238	2.0222794346
C	1.7768607207	-1.4460399549	-0.2494868096
H	2.559234255	-0.7676075213	-0.5972905418
H	2.2021130958	-2.0311463171	0.5686979073
H	1.481716024	-2.1068674741	-1.0596561298

$(CH_3)_2COO$ 1b TS

C	0.9979375092	0.2393833138	0.0887668924
O	-0.0798590155	-0.4051488882	-0.2438580313
O	-1.2377653765	0.405598612	0.1010435681
O	0.3866484401	1.947906143	-0.7695342829
H	-0.5678332937	1.4602552752	-0.4302558469
H	0.4140122857	1.8332411405	-1.7259315923
C	1.1520828885	0.8727944525	1.4355054226
H	1.5301147571	0.0969706984	2.1083038578
H	1.8775063414	1.6799877281	1.3973328971
H	0.2022145173	1.2344904726	1.8087792714
C	2.2243816892	-0.2440185793	-0.6165279563
H	2.9104445095	0.5873969808	-0.7649003595
H	2.7295797588	-0.9844219186	0.0070849933
H	1.9730319889	-0.6964174308	-1.5719228336

$(CH_3)_2COO$ 1b vdW

C	0.6215014885	-0.6487223022	0.2548323994
O	-0.4673662885	-0.8811436805	-0.3419901933
O	-1.5889604813	-0.1446028495	0.0488138939
O	-0.6502277088	2.2646225257	-0.8570171171

H	-1.1682936313	1.4691979476	-0.6048609099
H	-1.1555541001	2.7091447134	-1.5406931206
C	0.6984917553	0.3433269354	1.3410001307
H	1.6520365845	0.2843950305	1.8584425343
H	0.5620421325	1.3432865734	0.9162814366
H	-0.1429050522	0.1928697423	2.0195995459
C	1.7871081326	-1.4381911148	-0.2209960266
H	2.5691231749	-0.7580948287	-0.5663479508
H	2.2075226131	-2.0146728058	0.6057661249
H	1.5035413808	-2.1068038868	-1.0289097475

$(CH_3)_2COO$ 2a TS

C	1.3129881236	-0.3206357374	-0.3192678942
O	1.7211912985	0.89979091	-0.1423474213
O	2.8580348126	1.2796844156	-0.9627732529
O	0.1965995431	-0.2483529805	-1.8851795815
H	-0.6269847655	0.1784949404	-1.6234245309
H	0.7438062508	0.5078827102	-2.4826487533
O	1.5159676473	1.4953937631	-2.9647187529
H	2.2426476968	1.480344905	-2.0628464866
H	1.988208283	1.276822319	-3.7711741144
C	2.2506477647	-1.367787709	-0.8319195617
H	3.034422949	-1.4964240516	-0.0824369514
H	1.7219225935	-2.3055774783	-0.9734300046
H	2.7273206338	-1.0575285817	-1.7533011861
C	0.2887403944	-0.7104915887	0.708557576
H	-0.3141443455	-1.5404746327	0.3512177394
H	0.8135934506	-1.0251630123	1.6123464894
H	-0.3454563306	0.136040809	0.962372687

$(CH_3)_2COO$ 2a vdW

C	0.1055415344	-0.568471731	1.0561267501
O	0.4202363544	0.6454218313	0.9177470469
O	1.5115484148	0.9300202266	0.078535658
O	-1.6291083991	-0.5685521202	-1.4495962519
H	-2.4904353281	-0.5038421616	-1.8675454561
H	-1.1233086457	0.2092088893	-1.7685971526
O	-0.0016835371	1.5888292095	-2.061387353
H	0.6340390017	1.4614838634	-1.311952601
H	0.5308380361	1.600692485	-2.8599619636
C	0.87924232	-1.630774616	0.3904091929
H	1.9421324994	-1.4712421096	0.5767753479
H	0.5538160604	-2.6145120784	0.7157943027
H	0.7378590979	-1.5322611425	-0.687884393

C	-1.0773595181	-0.8294626826	1.9113585183
H	-1.8430994195	-1.3001975004	1.2913615545
H	-0.8172387035	-1.5271073838	2.7094848947
H	-1.4676637681	0.0924430211	2.3328239051

$(CH_3)_2COO$ 2b TS

C	1.9781981764	-1.4222186	-0.6663815198
O	2.6876606283	-0.347688947	-0.509226418
O	4.0223916212	-0.4241636834	-1.0800688039
O	3.2287400945	-0.0423560054	-3.3280304413
H	3.1216608091	0.8866803468	-3.5454820632
H	3.7147401556	-0.1405798088	-2.2812303427
O	1.2588600168	-1.1651078561	-2.4385514101
H	2.0941995671	-0.6180595571	-2.9356578098
H	1.1495030036	-1.9990457822	-2.9077013679
C	2.6526065051	-2.7486436171	-0.8381568064
H	3.1670036912	-2.9747208134	0.0987668407
H	1.9172114352	-3.5268773616	-1.0289078925
H	3.4014912113	-2.7154715915	-1.6202181659
C	0.6916224586	-1.3478318694	0.1012494354
H	-0.0344030904	-2.0498308085	-0.2981612109
H	0.8963332647	-1.6058963166	1.1422936304
H	0.2860324517	-0.3411717287	0.0600313459

$(CH_3)_2COO$ 2b vdW

C	-0.2680407181	-0.440065934	1.0815482317
O	0.3649330532	0.6428116273	0.9444789565
O	1.659242508	0.5578794013	0.3979314355
O	0.9282315591	1.1045831906	-2.1340213159
H	0.9722595051	2.0491749337	-2.2998800612
H	1.3064514385	0.9708754274	-1.2270543742
O	-1.4803221804	-0.1866411578	-1.6841801483
H	-0.6844510065	0.3245543469	-1.9446571595
H	-1.8253386021	-0.5559949359	-2.4999084365
C	0.3531856019	-1.7250037743	0.7157383715
H	1.3215473765	-1.8067930301	1.2129454812
H	-0.296283885	-2.5595418238	0.962334355
H	0.5656793717	-1.7134070893	-0.3546411319
C	-1.6469041078	-0.3135963279	1.6106531337
H	-2.3346940993	-0.6148584258	0.8171017173
H	-1.7898023423	-0.9862571393	2.457625983
H	-1.8628994727	0.710340711	1.9020199625

$(CH_3)_2COO$ 2c TS

C	1.3409126528	-0.3749608014	-0.3461004904
O	1.7843052653	0.8386303675	-0.2253917598
O	2.9109071211	1.1506173784	-1.0888008953
O	0.2185678297	-0.2441012398	-1.8971524226
H	0.2821829951	-1.0360767074	-2.4405986609
H	0.6918392597	0.5957533368	-2.4626090906
O	1.3881671136	1.6455998306	-2.8981000705
H	2.2149439646	1.5090681279	-2.0985896784
H	1.7649316066	1.5482099923	-3.7753543731
C	2.2673457079	-1.472581975	-0.7740834548
H	2.9929816037	-1.616357978	0.0298364222
H	1.7196192857	-2.4014439547	-0.9160797386
H	2.8191171854	-1.197978363	-1.664888929
C	0.2791724762	-0.6720015216	0.6716822548
H	-0.3173869495	-1.5260080932	0.3646166083
H	0.7656025015	-0.9036294264	1.62126934
H	-0.3642476193	0.1926860267	0.8056929388

$(CH_3)_2COO$ 2c vdW

C	0.1098422639	-0.5654948743	1.0651192022
O	0.4094200595	0.6526680478	0.9307630094
O	1.4965772895	0.9536410263	0.0918703461
O	-1.6263301515	-0.5783386078	-1.4395163903
H	-2.4886619594	-0.5228432133	-1.8567178571
H	-1.1303952898	0.2067197925	-1.7561229786
O	-0.026098574	1.6010999115	-2.0448121777
H	0.6116468355	1.4790241397	-1.2962190663
H	0.5057047294	1.6223100135	-2.843671851
C	0.8961718751	-1.6158395903	0.3952371679
H	1.9571321091	-1.4438299717	0.5815019906
H	0.5831411012	-2.6046461705	0.717402147
H	0.7528715854	-1.5153427828	-0.6826201948
C	-1.0691774479	-0.8440499251	1.9201701284
H	-1.8294511737	-1.322060934	1.2990144321
H	-0.7999273397	-1.5411892535	2.7157062624
H	-1.4705659126	0.0714943922	2.3450778296

$(CH_3)_2COO$ 2d TS

C	1.9355471667	-1.3575519782	-0.6546995511
O	2.5965704227	-0.2602786918	-0.4343656394
O	3.9452124701	-0.2491240159	-0.9727306606
O	3.3051024305	-0.281309283	-3.3005131251
H	3.3194763996	0.5744410882	-3.7346139794
H	3.6998375416	-0.1832037296	-2.2052503437

O	1.1971381903	-1.1423531753	-2.4241587179
H	2.0819375349	-0.7180997619	-2.9345714826
H	0.5565516508	-0.4260377828	-2.3538218481
C	2.6581802883	-2.6388787221	-0.9269651914
H	3.2443487406	-2.8753409144	-0.0365554351
H	1.9437020612	-3.4341303341	-1.117941194
H	3.34688041	-2.5445343525	-1.7578938016
C	0.6609954714	-1.3998821526	0.1390933508
H	-0.0514299037	-2.0787958975	-0.3202552638
H	0.8956112181	-1.7638885644	1.1410891115
H	0.2289159069	-0.4059137321	0.2326247715

$(CH_3)_2COO$ 2d vdW

C	-0.2689468862	-0.4376000324	1.0711537934
O	0.3733574537	0.6390637166	0.9286487403
O	1.6667899363	0.5402238144	0.3823631671
O	0.9401052279	1.0807130563	-2.1521701869
H	0.9922687132	2.0240577663	-2.3227015662
H	1.3173103494	0.9482239776	-1.2446024067
O	-1.4794663056	-0.1873635564	-1.6956399297
H	-0.6792407072	0.3156260902	-1.9587371349
H	-1.8277964268	-0.5577497368	-2.509489676
C	0.3410662876	-1.7296635419	0.7116253883
H	1.3087692779	-1.817375685	1.2091054111
H	-0.3155631071	-2.557315763	0.9624315497
H	0.5534674906	-1.7252023126	-0.3588260006
C	-1.6465734262	-0.2965786739	1.59980213
H	-2.337081409	-0.5957963826	0.8078391771
H	-1.7951461846	-0.9637781137	2.4501119048
H	-1.853645284	0.730619377	1.8861256391

anti_Syn-CH_3CH_2CHOO

C	-0.2187769326	-0.0248791388	0.4160223645
H	-0.3297541114	-0.7348054864	1.2312419724
O	-1.2451050969	0.2217735135	-0.2599881973
O	-2.4200258482	-0.4115001345	0.0703622564
C	1.065813798	0.6403599543	0.0875746717
H	1.4081163572	1.1482369985	0.9971682101
H	1.8056187413	-0.1514188002	-0.0804885898
C	1.0219576401	1.6066521737	-1.0939506894
H	0.3163315773	2.41629088	-0.9157766961
H	2.0072817148	2.0407537886	-1.2540336175
H	0.7192558704	1.0989051112	-2.008135345

anti_Syn-CH_3CH_2CHOO 1a TS

C	1.0523334642	0.2151668184	-0.0204812717
H	1.1439339269	0.6593017126	0.9644210557
O	-0.0092738396	-0.4648049317	-0.2535761608
O	-1.1136326945	0.241508725	0.3830117173
O	0.2480993921	1.909995145	-0.6857776476
H	-0.6015860863	1.3830839919	-0.200201874
H	0.4795813957	2.6527219447	-0.1187724836
C	2.2743218379	-0.084926275	-0.8155404553
H	2.8954129612	0.8116871606	-0.7887260287
H	2.8272817004	-0.8458123388	-0.251614828
C	2.0174790783	-0.5416051201	-2.25011007
H	2.9638403232	-0.7118357408	-2.7613111098
H	1.4445736482	-1.4660799358	-2.2753766489
H	1.4604718924	0.216708844	-2.7971281944

anti_Syn-CH_3CH_2CHOO 1a vdW

C	0.5142539859	-0.1046291004	0.3520160591
H	0.5440883151	0.6412985161	1.1396473386
O	-0.5979475949	-0.5951872999	0.0577788742
O	-1.7176377248	-0.1341405102	0.7532474244
O	-0.9312926821	2.4674339181	0.498383502
H	-1.4344769462	1.6344648712	0.6361242918
H	-1.5112071351	3.0464842405	-0.0007140229
C	1.7264325824	-0.5358325044	-0.3803784097
H	2.1776314001	0.3770403836	-0.7872610363
H	2.4441488649	-0.8841932324	0.3717956356
C	1.5099160005	-1.5822879328	-1.4699740371
H	2.4591637449	-1.8231455304	-1.9449119724
H	1.0907166247	-2.4995789696	-1.0599820345
H	0.8273065647	-1.2181978495	-2.2357956128

anti_Syn-CH_3CH_2CHOO 1b TS

C	1.0276530173	0.2237217411	-0.0634619157
H	1.1160151549	0.6684089521	0.9205535559
O	-0.0266767788	-0.4673372093	-0.3050066797
O	-1.1362512915	0.2160015237	0.3481773459
O	0.2364244699	1.9797217047	-0.5552374747
H	-0.6128069681	1.402883104	-0.1362091452
H	0.0909617182	2.0179289991	-1.5072011756
C	2.2614715425	-0.063191114	-0.846496085
H	2.8522743296	0.8540805635	-0.8454601877
H	2.8353576871	-0.7827515477	-0.2508299746
C	2.0390247146	-0.5904026101	-2.2625412647

H	2.9971145246	-0.772071568	-2.7469404141
H	1.4766964831	-1.5216041313	-2.2567288016
H	1.4883203966	0.1278715923	-2.8693517833

anti_Syn-CH_3CH_2CHOO 1b vdW

C	0.5131599978	-0.1025993892	0.354061561
H	0.5321297022	0.6382528971	1.1468032135
O	-0.5930927761	-0.6007251296	0.0502675312
O	-1.7206070004	-0.1540112015	0.7424411609
O	-0.9553647872	2.4558868679	0.509375006
H	-1.4520934851	1.6177118992	0.6387104494
H	-1.5374552508	3.033259851	0.0108677364
C	1.7331071928	-0.518427657	-0.3743139931
H	2.1786715048	0.4010055948	-0.7725422906
H	2.4495806575	-0.8656397514	0.3795741125
C	1.5317555791	-1.5593698959	-1.472068001
H	2.485697141	-1.7888546944	-1.9432175984
H	1.1182101601	-2.4829665765	-1.0705786079
H	0.8503273643	-1.1960358146	-2.2392992798

anti_Syn-CH_3CH_2CHOO 2a TS

C	1.1821729219	-0.1547359122	-0.2315171895
H	1.9513671866	-0.8362723535	-0.5743639221
O	1.5406270232	1.0708755456	-0.0863999955
O	2.7582076737	1.3794564953	-0.8288338686
O	0.2940759848	-0.3065797479	-1.88751114
H	-0.5694743995	0.1121355166	-1.7961498489
H	0.8852452471	0.3638908615	-2.5084386619
O	1.7156393203	1.3246556385	-3.0366112906
H	2.2725984484	1.4387537249	-2.0827581317
H	2.3214478486	1.0013842171	-3.7078115908
C	0.150635941	-0.6611113776	0.7335782241
H	-0.2557102107	-1.58786477	0.330681168
H	0.7111870915	-0.9336632893	1.6335831654
C	-0.9563155347	0.3297417365	1.0947906833
H	-1.6219104607	-0.1115213929	1.8350448921
H	-0.5454875603	1.2484088532	1.5075130449
H	-1.5635435213	0.5962022543	0.2287594619

anti_Syn-CH_3CH_2CHOO 2a vdW

C	0.2538330573	-0.5985074726	0.7707143034
H	0.8992058412	-1.2825330078	0.2298413638
O	0.557658727	0.611963054	0.7546951089
O	1.7162381787	0.9701065097	0.0359856668

O	-0.8210697027	-1.1301925364	-1.7607167823
H	-1.6499729896	-1.1306666964	-2.2447540874
H	-0.2882870044	-0.4018379486	-2.1505247376
O	0.7633651888	0.9864839758	-2.4799999547
H	1.1734536691	1.0857320976	-1.5818000749
H	1.4942650104	0.8593662126	-3.0895057733
C	-0.9270723291	-1.0579434822	1.5321349383
H	-1.5082791935	-1.6646529221	0.8321991366
H	-0.5552421545	-1.7650248203	2.2843323854
C	-1.7738889912	0.0387415566	2.1712007482
H	-2.6143729888	-0.4057538939	2.7011932898
H	-1.1956958468	0.6273425246	2.8814668569
H	-2.1664874718	0.7178668493	1.4163476123

anti_Syn-CH_3CH_2CHOO 2b TS

C	1.8709941962	-1.2036221723	-0.685457022
H	2.4505466761	-2.1197030322	-0.7144229593
O	2.5540886955	-0.1230742436	-0.5710708144
O	3.9404681442	-0.3147201974	-0.9880786576
O	3.4174834778	-0.1893128695	-3.3585524334
H	3.3265715038	0.7118539039	-3.6774325977
H	3.7732289434	-0.1644930759	-2.3014642759
O	1.3960798846	-1.2834499473	-2.5228137729
H	2.2418200664	-0.7743836503	-2.9999401654
H	1.4145801544	-2.196885244	-2.8298078845
C	0.5200901595	-1.2059783432	-0.0381767207
H	-0.0396795005	-2.0512002297	-0.4376799074
H	0.7053770148	-1.4285298344	1.0184423374
C	-0.268894624	0.094565147	-0.1797363194
H	-1.2268943147	0.004591715	0.3304824707
H	0.2708597991	0.9328821512	0.2557237907
H	-0.4583382766	0.3162259229	-1.2281770683

anti_Syn-CH_3CH_2CHOO 2b vdW

C	-0.1065646627	-0.5365773475	0.8852698006
H	0.4548304519	-1.4398916993	0.6720700031
O	0.5074997075	0.5473798325	0.8094268899
O	1.8712700803	0.4808130039	0.4493823443
O	1.6121273841	0.3737044041	-2.2146362857
H	1.621836655	1.2588736552	-2.5859998401
H	1.8110892772	0.4794442176	-1.2475922209
O	-0.6840949359	-1.0584088764	-1.8019665837
H	0.0973805256	-0.533069252	-2.0846357976
H	-0.711929821	-1.8126883889	-2.395257245

C	-1.5326477014	-0.5571069987	1.2732611303
H	-2.0419112229	-1.0980574384	0.4700225201
H	-1.608159106	-1.2053247366	2.1547395611
C	-2.173561237	0.8047821895	1.5234506383
H	-3.2177006996	0.6744119001	1.8019692266
H	-1.670866691	1.3423490847	2.3258733252
H	-2.134884004	1.4234004501	0.6287585337

anti_Syn-CH_3CH_2CHOO 2c TS

C	1.2368379244	-0.2672842063	-0.187822047
H	1.9945066568	-0.9910828709	-0.4677649679
O	1.6401549199	0.9492876018	-0.1070768158
O	2.8479929325	1.168164276	-0.895339585
O	0.3281560864	-0.3745783156	-1.8428715181
H	0.5276263248	-1.2200739199	-2.2593737066
H	0.8191008127	0.409491534	-2.43953671
O	1.5319932917	1.4632516501	-2.9166382416
H	2.241851172	1.4283947668	-2.0483400523
H	2.0208364632	1.3014758837	-3.7267640563
C	0.1540050546	-0.6668401678	0.767570657
H	-0.2664324379	-1.6098627365	0.4191653533
H	0.6645336829	-0.88474761	1.7120605277
C	-0.9389310402	0.3797786082	0.9789153493
H	-1.675181534	0.0082921303	1.6903736366
H	-0.5261962271	1.3077657376	1.3687923427
H	-1.4465710826	0.5992466385	0.041773834

anti_Syn-CH_3CH_2CHOO 2c vdW

C	0.2843465606	-0.5389793738	0.7796245229
H	0.9839547741	-1.1956192224	0.2733510821
O	0.5091402939	0.6877379426	0.7302515309
O	1.6567502263	1.0986806129	0.0222724295
O	-0.700657072	-1.2182262198	-1.7530883518
H	-1.5174945434	-1.2880770323	-2.2523581838
H	-0.2083079474	-0.4689148655	-2.156118095
O	0.7575535324	0.9745367548	-2.5104038656
H	1.1414904573	1.1282589554	-1.6083240863
H	1.507729865	0.876826103	-3.1016389542
C	-0.8798457081	-1.0510890325	1.5331365319
H	-1.4056601731	-1.7160222767	0.8423467089
H	-0.478637904	-1.7086012265	2.3146304638
C	-1.8092932105	0.0069486436	2.1204227119
H	-2.6299975626	-0.4750959857	2.6485883839
H	-1.2855243096	0.6539431161	2.8220640763

H	-2.2293482789	0.6351341068	1.3367870943

anti_Syn-CH_3CH_2CHOO 2d TS

C	1.839612035	-1.0913836472	-0.7489241332
H	2.4542766579	-1.9782176552	-0.8484486781
O	2.4718217177	0.0139645088	-0.5696249472
O	3.8765191849	-0.0843501916	-0.9554654081
O	3.5497590323	-0.4217052147	-3.3469154876
H	3.6156312435	0.3872643266	-3.8595155254
H	3.7926774629	-0.1958609289	-2.2859154266
O	1.3584812518	-1.1944010165	-2.5678190532
H	2.2722203641	-0.8420882977	-3.0404603697
H	0.692295281	-0.5140781422	-2.7163689469
C	0.5095918068	-1.2131009896	-0.0648476324
H	-0.0215811713	-2.0496740777	-0.5164449997
H	0.7442915722	-1.51117118	0.9620649046
C	-0.3447462762	0.0546978565	-0.0515930871
H	-1.2581368933	-0.1196072437	0.514988896
H	0.1875235464	0.8863991938	0.4046948787
H	-0.6404068158	0.3574326993	-1.057114984

anti_Syn-CH_3CH_2CHOO 2d vdW

C	-0.1201217605	-0.5590260514	0.8776844103
H	0.4254152362	-1.4700792482	0.6563993286
O	0.5148643214	0.5139188768	0.8196162521
O	1.8794347633	0.4259839809	0.4672673914
O	1.6355755028	0.357773278	-2.1994727152
H	1.6644614702	1.2472592084	-2.5593478886
H	1.8302382064	0.447372897	-1.2299267054
O	-0.6900075043	-1.0355103675	-1.8195925976
H	0.1031047669	-0.5215896686	-2.0906013343
H	-0.72829682	-1.7815012104	-2.4226992897
C	-1.5488244496	-0.5573347511	1.2564683303
H	-2.0630321627	-1.0782138548	0.4431759536
H	-1.6423301645	-1.2151725312	2.1290498746
C	-2.1654084205	0.8132151889	1.5201425764
H	-3.213615994	0.6992150098	1.7904406765
H	-1.6578245563	1.3308486541	2.3325318837
H	-2.1092084348	1.4423295893	0.6337368532

anti_Gauche-CH_3CH_2CHOO

C	0.2911152969	0.2879212462	0.1124792497
H	-0.0387328856	1.0205866495	0.8446128257
O	-0.5814155921	-0.1572525847	-0.6724959562

O	-1.8665321437	0.3080924985	-0.5626142463
C	1.6840766093	-0.2087484216	0.0130500057
H	2.3315160357	0.6462528268	-0.2083070448
H	1.7529834481	-0.8982592366	-0.8271550762
C	2.1594615328	-0.8741634984	1.3177458353
H	1.5665736448	-1.7592158122	1.5434935186
H	3.2013135271	-1.1759417801	1.2214929021
H	2.0850185266	-0.1899928876	2.1629979864

anti_Gauche-CH_3CH_2CHOO 1a TS

C	1.0463148438	0.2649114554	0.0086686544
H	1.1200450124	0.7663054313	0.9679257455
O	0.036083425	-0.5020048978	-0.1711286773
O	-1.1086312594	0.1467104374	0.4576254101
O	0.1035471875	1.8670890188	-0.7194313316
H	-0.6910206538	1.3042137543	-0.1988286869
H	0.2751774273	2.6550141926	-0.1935160491
C	2.2651638775	0.0082493053	-0.8063417023
H	2.714272477	-0.9046181495	-0.3988783611
H	1.9591449993	-0.2186274518	-1.8264426235
C	3.2767261067	1.1542995017	-0.7615326746
H	3.574160781	1.3848852083	0.2622351293
H	4.1752383829	0.8829395787	-1.3129403579
H	2.8625063927	2.0543006153	-1.2115834752

anti_Gauche-CH_3CH_2CHOO 1a vdW

C	0.3466658993	-0.380500324	0.4163355071
H	0.1938354007	0.4927816901	1.0431062507
O	-0.6681441702	-1.0079854563	0.0362128114
O	-1.9160129591	-0.5415412305	0.4415240299
O	-1.2803055106	2.0693789159	-0.0555731835
H	-1.7350744141	1.2157707302	0.1174226883
H	-1.8246007422	2.5338170408	-0.6949111254
C	1.6845175224	-0.8321309009	-0.0268690881
H	2.2661935218	-1.0688172094	0.87008787
H	1.5806275192	-1.7466274194	-0.6086479331
C	2.4156057963	0.2633453772	-0.8271446815
H	2.505775486	1.1826744506	-0.2500884237
H	3.4169153751	-0.0784877104	-1.0835581497
H	1.8821632754	0.4939630461	-1.7473085724

anti_Gauche-CH_3CH_2CHOO 1b TS

C	1.0361492811	0.2655466071	-0.0200181607
H	1.0953911455	0.8107739655	0.9152326109

O	0.0400010636	-0.5264689309	-0.177184551
O	-1.1152273214	0.1214034117	0.434407851
O	0.0943316548	1.9023701825	-0.669678288
H	-0.6920877362	1.3094226014	-0.1812162055
H	-0.0632407749	1.8204870031	-1.6172791917
C	2.2723569667	-0.0034289 -0.8072122092	
H	2.7189144753	-0.9005616305	-0.3634005855
H	1.9960917954	-0.2720792234	-1.82673196
C	3.2756053226	1.1511120785	-0.7717540822
H	3.5703781816	1.3863840118	0.2509574866
H	4.1744735277	0.8831675311	-1.3243506623
H	2.8542424181	2.051432292	-1.2138630525

anti_Gauche-CH_3CH_2CHOO 1b vdW

C	0.3463223829	-0.3672268614	0.427937861
H	0.1708784496	0.5163643496	1.0339964267
O	-0.6530509248	-1.0178994309	0.0459068364
O	-1.9138059278	-0.5623598564	0.4227447094
O	-1.3098630951	2.0471805168	-0.1191910606
H	-1.7543484209	1.1904551281	0.0647744852
H	-1.851282557	2.4899430221	-0.7761075964
C	1.6973948555	-0.807359497	0.0142526366
H	2.2688349796	-1.0165366548	0.9245276318
H	1.616111977	-1.7351569639	-0.5497942841
C	2.4240561667	0.2824351568	-0.7977264928
H	2.4916197467	1.2147559454	-0.2387060781
H	3.4341719813	-0.0492349286	-1.0319907033
H	1.9012833862	0.4858050743	-1.7303553717

anti_Gauche-CH_3CH_2CHOO 2a TS

C	1.1607950619	-0.2032543098	-0.2797087365
H	1.8832110522	-0.8922289185	-0.7028179128
O	1.5817270554	0.9897089834	-0.0579675209
O	2.7947773483	1.294729305	-0.8105371794
O	0.2048291234	-0.1700341369	-1.9106650005
H	-0.610412371	0.3180355509	-1.7440888447
H	0.8242606581	0.4931749708	-2.5014524611
O	1.7061783815	1.4408245855	-2.9974000068
H	2.2833726522	1.4640632572	-2.0576467393
H	2.2810052566	1.1279778448	-3.6999952312
C	0.1325876192	-0.7149683871	0.6869133871
H	-0.6561497691	0.0308970429	0.7978286462
H	0.6458393184	-0.7529078466	1.6522567199
C	-0.4311312982	-2.0926430943	0.3417760181

H	0.3656412126	-2.8316886676	0.2533361815
H	-1.1063158755	-2.4265605177	1.1282290067
H	-0.9787634259	-2.0806056619	-0.5978043262

anti_Gauche-CH_3CH_2CHOO 2a vdW

C	0.3112185181	-0.4143050931	0.946569667
H	0.8832616394	-1.0642437317	0.292535438
O	0.5814797218	0.8057533444	0.9277978844
O	1.6375617641	1.2137977768	0.0963637373
O	-0.6731701763	-0.8523483691	-1.7156474993
H	-1.4387836786	-1.046387968	-2.2608941297
H	-0.3129498696	-0.0045758351	-2.0564970358
O	0.4373204635	1.5963286341	-2.2856565034
H	0.9184283684	1.5819719401	-1.4195516242
H	1.11686664	1.6757269543	-2.9593771911
C	-0.7190514412	-0.9053395353	1.8899774664
H	-1.2077616839	-0.0510748232	2.3566512319
H	-0.1749353447	-1.4368695496	2.681145933
C	-1.7326956461	-1.864685047	1.2491467811
H	-1.2338926976	-2.7075943786	0.7734001349
H	-2.4021118867	-2.2501713326	2.0164070848
H	-2.3196196907	-1.3540889864	0.4904306249

anti_Gauche-CH_3CH_2CHOO 2b TS

C	1.8535397403	-1.2461721664	-0.7259448443
H	2.422982198	-2.1670902979	-0.7977791408
O	2.5445433285	-0.1788351973	-0.5541103581
O	3.933110672	-0.3622846872	-0.9699870281
O	3.417383271	-0.0698462966	-3.3319737575
H	3.328225401	0.8523270751	-3.584405228
H	3.7729189043	-0.1185976055	-2.2844541159
O	1.3936258095	-1.2246189328	-2.5681092781
H	2.2336627346	-0.681791892	-3.0035727416
H	1.4234816017	-2.1135553866	-2.9395450399
C	0.5007806392	-1.2470442631	-0.0828717106
H	0.0029292612	-0.3082300111	-0.3221591488
H	0.695846306	-1.2353101305	0.9939259249
C	-0.3691086082	-2.4498747171	-0.4422311299
H	0.1459922548	-3.3904227408	-0.2404418645
H	-1.2807402671	-2.4425556437	0.1531507846
H	-0.6572262468	-2.4306041065	-1.4913143233

anti_Gauche-CH_3CH_2CHOO 2b vdW

C	-0.0532410043	-0.3591457019	0.9902917105

H	0.4731861734	-1.2630382285	0.7013674325
O	0.5726120678	0.7178746894	0.901364569
O	1.9088894334	0.63844001	0.4578521507
O	1.541343395	1.018379671	-2.1668550913
H	1.4904019586	1.9525284274	-2.3816748404
H	1.7842461558	0.9676978825	-1.2061723259
O	-0.6490672324	-0.5647725678	-1.7309620394
H	0.0803310512	0.0340177069	-2.0071018103
H	-0.6163110908	-1.3007059486	-2.3470650654
C	-1.418394498	-0.3557533133	1.5656478945
H	-1.8059845709	0.6622363143	1.5486011563
H	-1.2960869745	-0.6285122117	2.6224556781
C	-2.3757435006	-1.3472318508	0.8939324865
H	-1.9795217152	-2.3623675431	0.927648563
H	-3.3306540967	-1.3436508275	1.4167824284
H	-2.5356105518	-1.0779905083	-0.1461658967

anti_Gauche-CH_3CH_2CHOO 2c TS

C	1.2144118163	-0.3012609377	-0.28733665
H	1.9456494074	-1.0353802011	-0.6103143997
O	1.6565730733	0.8953803129	-0.1422956603
O	2.8704007218	1.1176589152	-0.9218344164
O	0.2991059682	-0.2824907486	-1.9394555137
H	0.4734588539	-1.0985532662	-2.4210367359
H	0.8030229671	0.5250014889	-2.482009255
O	1.5454269648	1.5936471562	-2.9071362231
H	2.2593927862	1.4810552724	-2.0597331394
H	2.0214547974	1.4719200895	-3.7317745766
C	0.1217553302	-0.6972109044	0.658254405
H	-0.6304802852	0.0905179257	0.6647754677
H	0.5855664072	-0.6994326517	1.6493314499
C	-0.4993173434	-2.0622313235	0.3690584168
H	0.2591140538	-2.8456403982	0.3245297409
H	-1.1984890868	-2.3295020614	1.1598435639
H	-1.0473684323	-2.0560766679	-0.5709774743

anti_Gauche-CH_3CH_2CHOO 2c vdW

C	0.3235056334	-0.4543520547	0.9264248691
H	0.941072058	-1.1801431203	0.4076561346
O	0.6355730071	0.7489203599	0.8061941898
O	1.7723473567	1.032975446	0.0264733072
O	-0.8448575751	-0.6822249301	-1.6281481814
H	-0.7857895652	-1.3142870302	-2.3482390986
H	-0.4473595504	0.1467989897	-1.9725009164

O	0.4184858373	1.7035274521	-2.1978645677
H	1.0116019434	1.5849943658	-1.4126135366
H	0.9928250584	1.8870098533	-2.9444079913
C	-0.8026615681	-0.8226202861	1.8151403849
H	-1.380407694	0.0728770205	2.0408494909
H	-0.3477752275	-1.1530836464	2.7582595863
C	-1.682435828	-1.9479443439	1.2551576517
H	-1.0950077901	-2.8438704303	1.0532843192
H	-2.4494296529	-2.2070676106	1.9830531827
H	-2.1568244429	-1.6373760348	0.3284831757

anti_Gauche-CH_3CH_2CHOO 2d TS

C	1.7925619787	-1.1398021997	-0.7556371064
H	2.3880340733	-2.0245977748	-0.9522563771
O	2.4473538067	-0.0648244397	-0.4960417964
O	3.8441688077	-0.1521610826	-0.9136084293
O	3.4857751168	-0.3233003931	-3.322602668
H	3.585012808	0.5121816188	-3.7848305529
H	3.7435337632	-0.1745161149	-2.2580667374
O	1.2647477824	-1.0508980624	-2.5687815952
H	2.1850734604	-0.710688956	-3.0255440642
H	0.6482172561	-0.3112280929	-2.6206054414
C	0.4753480192	-1.2811198702	-0.0498720926
H	-0.0976744569	-0.3604753171	-0.1723301715
H	0.7293121811	-1.3358522365	1.012865507
C	-0.3325867304	-2.5122623328	-0.4576303387
H	0.244363521	-3.4257739931	-0.3113432274
H	-1.2312312247	-2.5869745235	0.1529417947
H	-0.6294661625	-2.4703552296	-1.5029227032

anti_Gauche-CH_3CH_2CHOO 2d vdW

C	-0.0111305055	-0.4511660373	0.9318271422
H	0.4431717055	-1.3574556458	0.5446919819
O	0.6748973892	0.5916310416	0.892923749
O	1.9797115269	0.4715553654	0.3716838994
O	1.5048984726	1.0839401309	-2.1911437302
H	1.5011106003	2.0338264803	-2.3292669348
H	1.7921841643	0.9414916342	-1.2521783939
O	-0.7545844639	-0.4004200635	-1.7602447285
H	-0.0043386443	0.175752059	-2.0285392162
H	-0.7984508765	-1.0845459699	-2.432778229
C	-1.342806454	-0.4157955562	1.5799623859
H	-1.667035888	0.6208666613	1.6637867149
H	-1.1846383901	-0.7800756744	2.6039166898

C	-2.392219704	-1.2925879292	0.8866258587
H	-2.0583714208	-2.328261825	0.8191420771
H	-3.3175858146	-1.2764218606	1.4599280636
H	-2.5872056971	-0.9309988109	-0.1189023299

anti_Gauche-CH_3CH_2CHOO 1a' TS

C	1.0220788733	0.2240776654	-0.0096597125
H	1.0604659436	0.6374454133	0.9925900998
O	-0.0269995977	-0.4438138734	-0.3224076711
O	-1.1638956629	0.2456253031	0.2720860641
O	0.2677317276	1.937787345	-0.6682739068
H	-0.6109181239	1.4076180007	-0.2516549965
H	0.4663539192	2.6646087096	-0.0688974316
C	2.2795195805	-0.0830617391	-0.7425681114
H	2.8541136854	0.8409932417	-0.8076981128
H	2.02961399	-0.3923338349	-1.7557715431
C	3.0986187536	-1.1654141118	-0.0173563734
H	2.5514783072	-2.1053796514	0.0305261472
H	4.0308960687	-1.3406978638	-0.551896779
H	3.3476655352	-0.8637696044	1.0003173271

anti_Gauche-CH_3CH_2CHOO 1a' vdW

C	0.2896198358	-0.207561791	0.0431886189
H	0.3850235844	0.6517624199	0.6996791192
O	-0.8624242106	-0.643962551	-0.1809326482
O	-1.937491528	0.0169668328	0.4081962982
O	-0.9245921273	2.4859403043	-0.1786016214
H	-1.4983564172	1.7244152784	0.0584195756
H	-1.4424603457	3.0313879598	-0.774483766
C	1.4506886149	-0.8699165958	-0.5918921833
H	1.9217604428	-0.1285116588	-1.2460521514
H	1.0993344725	-1.6884856399	-1.2181125617
C	2.4790563471	-1.3537751158	0.446352687
H	2.0535951256	-2.1206018871	1.0919145333
H	3.3436035101	-1.7772259698	-0.0618940792
H	2.8262756955	-0.5329905861	1.073463179

anti_Gauche-CH_3CH_2CHOO 1b' TS

C	0.9975886879	0.2283345945	-0.0440396272
H	1.0386272868	0.6426048595	0.9568226677
O	-0.0528655888	-0.4368240005	-0.3634836569
O	-1.1863541224	0.2445178411	0.2477420332
O	0.2676191937	2.007907068	-0.5344487846
H	-0.6120577086	1.4440134755	-0.1805733836

H	0.1845728367	2.0603213184	-1.4935088501
C	2.2602986299	-0.0768550513	-0.770477177
H	2.8266490641	0.8521392908	-0.8408914791
H	2.02411526	-0.4108465389	-1.7800261251
C	3.0873675039	-1.1383431326	-0.0228197065
H	2.5502404594	-2.0832944347	0.0380421065
H	4.0249237317	-1.3117540166	-0.5486070082
H	3.3254797656	-0.8144682732	0.9902569907

anti_Gauche-CH_3CH_2CHOO 1b' vdW

C	0.2901930255	-0.206830951	0.0425867769
H	0.3750826433	0.6397166613	0.7168791901
O	-0.8575415633	-0.6437172528	-0.2017835676
O	-1.9414714411	0.0007114405	0.3893813363
O	-0.9339867173	2.4852269857	-0.1381610727
H	-1.506630121	1.7166619858	0.0779214256
H	-1.4483235386	3.0401279438	-0.7283464321
C	1.4605864861	-0.8514013012	-0.5936756895
H	1.9348255819	-0.095126951	-1.2282317739
H	1.1192711697	-1.658913314	-1.2394968789
C	2.4806653351	-1.3512720854	0.4451601898
H	2.052236447	-2.1325939342	1.0710798609
H	3.3521928207	-1.760794288	-0.0625785091
H	2.8178278721	-0.5415809395	1.0918731441

anti_Gauche-CH_3CH_2CHOO 2a' TS

C	1.2077584714	-0.1817080744	-0.1995925349
H	1.982076024	-0.8440856098	-0.5695784023
O	1.5433959285	1.0499880848	-0.0536918327
O	2.7316976968	1.3942523234	-0.8269308049
O	0.2619196681	-0.3359634549	-1.8190195198
H	-0.6026439514	0.0690527509	-1.6818112493
H	0.8132933025	0.3470398859	-2.4520699092
O	1.6144381126	1.3365298764	-3.0054442061
H	2.1982756718	1.45557383	-2.0792116957
H	2.2047472435	1.0345361902	-3.6999387634
C	0.2099011163	-0.6996334802	0.7926103585
H	-0.2478208892	-1.5972914818	0.3805671999
H	-0.5703632233	0.0491552255	0.9350665238
C	0.8927766191	-1.0121311965	2.1328893898
H	1.3359941402	-0.1165139469	2.5639156307
H	0.162123212	-1.407763154	2.8369587425
H	1.6793618571	-1.7573377686	2.0125810732

anti_Gauche-CH_3CH_2CHOO 2a' vdW

C	0.1511513434	-0.2413895385	0.7192165648
H	0.7099792244	-0.9563500922	0.1242609648
O	0.4790458118	0.9611308008	0.6331252445
O	1.5411828784	1.275851821	-0.2329754593
O	-1.1680174512	-0.949260629	-1.6639325055
H	-2.0404758924	-0.9681790363	-2.0637690467
H	-0.6747017045	-0.2454959249	-2.1405730693
O	0.3452325919	1.1168891341	-2.6423474174
H	0.8374732394	1.2764984084	-1.7963487687
H	1.0165016067	0.9523916936	-3.3088661304
C	-0.9367611882	-0.6376229049	1.638108223
H	-1.7042213885	-1.1047026014	1.0163832802
H	-1.3631561748	0.25310015	2.0964860958
C	-0.448634266	-1.6400461971	2.7001067853
H	0.3054037556	-1.1952275913	3.3479158191
H	-1.2873990112	-1.9527385022	3.3196362543
H	-0.0223413748	-2.5304619902	2.2386041655

anti_Gauche-CH_3CH_2CHOO 2b' TS

C	1.876973375	-1.2312734072	-0.6525987062
H	2.4713356904	-2.137215087	-0.7112120187
O	2.5448858242	-0.1411550262	-0.5394457717
O	3.9228686268	-0.29948414	-0.996545082
O	3.3217430099	-0.1483208215	-3.3543553844
H	3.2111612827	0.7569876489	-3.6548567476
H	3.7106982945	-0.1325503139	-2.3201353849
O	1.3375613505	-1.2831215883	-2.4648333667
H	2.1543392346	-0.7594076446	-2.9598690214
H	1.3481864547	-2.1881922301	-2.7966339728
C	0.5483998336	-1.2479231116	0.0373851714
H	-0.0524739017	-2.0481395276	-0.3917571662
H	0.0401594648	-0.3069850079	-0.1679802817
C	0.7230163499	-1.4571517915	1.5492882161
H	1.2973519593	-0.6458725968	1.9925092986
H	-0.2526069006	-1.4907781211	2.0322024074
H	1.2360890512	-2.3944202337	1.767238811

anti_Gauche-CH_3CH_2CHOO 2b' vdW

C	-0.0651716434	-0.1719305783	0.7837287777
H	0.3951403562	-1.1071019802	0.4822536131
O	0.6126669948	0.8688016019	0.6478872292
O	1.9027422563	0.7227029341	0.101485857
O	1.2829998967	0.5386764611	-2.5018739547

H	1.2871790704	1.4114979906	-2.9016433484
H	1.6124458919	0.6614855843	-1.5738510947
O	-1.019347085	-0.7708180013	-1.8041128378
H	-0.2498191973	-0.2921146992	-2.1846457578
H	-1.1579691279	-1.5285284502	-2.3770632347
C	-1.4287677061	-0.0880065715	1.3470106572
H	-2.101584083	-0.3677670108	0.5310931979
H	-1.6421386317	0.9444268682	1.6194430761
C	-1.6235391106	-1.0426094975	2.5370918724
H	-0.9765875513	-0.7755098375	3.371650548
H	-2.6556747814	-0.994722925	2.8796244498
H	-1.4117305486	-2.0743148889	2.2567579495

anti_Gauche-CH_3CH_2CHOO 2c' TS

C	1.2862759149	-0.3001545932	-0.2021911918
H	2.0588385389	-0.9991884336	-0.5061762766
O	1.6590062622	0.9254318318	-0.1089291583
O	2.8478095614	1.1908161063	-0.9122229171
O	0.3367774137	-0.402872629	-1.8222151986
H	0.5251888154	-1.240672791	-2.2594501708
H	0.7962867616	0.3886211867	-2.4211236585
O	1.4860792119	1.4679341302	-2.9140359812
H	2.2057895112	1.4482614923	-2.067854873
H	1.9671591223	1.321365513	-3.7316884126
C	0.234022405	-0.7252595651	0.7750521875
H	-0.2279276291	-1.6400936004	0.4071387538
H	-0.5364989615	0.0435495029	0.8073186078
C	0.841281133	-0.9507394669	2.1678333391
H	1.2781244648	-0.0329599075	2.5567593923
H	0.0672478572	-1.2819955635	2.8587293162
H	1.6193966172	-1.7146262132	2.1469642418

anti_Gauche-CH_3CH_2CHOO 2c' vdW

C	0.1379842783	-0.2499336335	0.7126726055
H	0.6771915765	-0.976180838	0.113298014
O	0.4935582246	0.9448079025	0.6281649505
O	1.5588113993	1.2369028528	-0.2420254772
O	-1.2082619573	-0.920348891	-1.6661657344
H	-2.0827370629	-0.9177673309	-2.0620160835
H	-0.7007739738	-0.2270536654	-2.1432708393
O	0.3484978033	1.1124154256	-2.6462457893
H	0.8481897527	1.2581961546	-1.8021213405
H	1.0126875178	0.9340295377	-3.316275042
C	-0.954706256	-0.6230558893	1.6355612389

H	-1.7357253196	-1.0703689051	1.0161899198
H	-1.3580245898	0.276170805	2.0982016887
C	-0.4853519896	-1.6394813677	2.6927024004
H	0.2818464558	-1.2141793029	3.3381620844
H	-1.3283750637	-1.9341147845	3.3152960076
H	-0.0821427955	-2.5383900699	2.2269383964

anti_Gauche-CH_3CH_2CHOO 2d' TS

C	1.8191897731	-1.1013749264	-0.6694278329
H	2.4548200858	-1.9721836802	-0.7845393653
O	2.4256708179	0.0216611787	-0.5148755636
O	3.8188574044	-0.0364859505	-0.9468414462
O	3.406879158	-0.3723734342	-3.3315310263
H	3.4319300356	0.44118052	-3.8404987975
H	3.6871641352	-0.146238456	-2.2887962534
O	1.2696024146	-1.2192848772	-2.4650625147
H	2.145313249	-0.8370691759	-2.9720327581
H	0.5750472826	-0.560029344	-2.5770926524
C	0.5144244681	-1.2355897526	0.057032464
H	-0.0552280938	-2.0376981668	-0.4087068328
H	-0.0493607155	-0.3077763196	-0.049566165
C	0.7542789472	-1.5395452903	1.5438068962
H	1.3065505534	-0.7339136463	2.0237641111
H	-0.1997373014	-1.656003868	2.0560394038
H	1.3186277857	-2.4632478108	1.6729333329

anti_Gauche-CH_3CH_2CHOO 2d' vdW

C	-0.0634208434	-0.1877393135	0.7750893374
H	0.4100177634	-1.1180180711	0.4788507817
O	0.6019403778	0.8609858054	0.6390273075
O	1.8963257395	0.7293519515	0.0991856415
O	1.2912987958	0.5291577799	-2.5064412287
H	1.2864201973	1.4006661964	-2.9090573386
H	1.6147713792	0.6590947605	-1.5772883944
O	-0.9977138097	-0.8069041455	-1.8152352085
H	-0.2324515879	-0.3198040055	-2.1937106906
H	-1.124106831	-1.5681332631	-2.3863466462
C	-1.4306206652	-0.1191422973	1.3316709473
H	-2.0959932403	-0.4099682112	0.513521496
H	-1.6582243524	0.9114021023	1.5997013581
C	-1.6190384663	-1.0722712035	2.5239542656
H	-0.9794580514	-0.7943690599	3.3606645412
H	-2.6533075886	-1.036255422	2.8614687671
H	-1.3929678167	-2.1021326032	2.2480130636

syn_Anti-CH_3CH_2CHOO

C	0.4590277461	0.7016376474	-0.0000045665
H	0.7752487291	1.7390946601	-0.0000100892
O	-0.7956550381	0.571062864	-0.0000039028
O	-1.2946539029	-0.7042639881	0.0000029089
C	1.3737903168	-0.4493578945	0.0000015794
H	1.0986870578	-1.0748339813	0.8579745518
H	1.0986869593	-1.0748432256	-0.8579646223
C	2.8523785335	-0.0668466875	-0.0000005605
H	3.4738323765	-0.960419438	0.0000042299
H	3.115014563	0.5174157603	-0.8823621822
H	3.1150146588	0.5174252832	0.8823547285

syn_Gauche-CH_3CH_2CHOO 1a TS

C	0.8346387447	0.2719532693	0.1867524321
H	1.7051310712	-0.1747984924	-0.2910111377
O	-0.2450323545	-0.3634862649	-0.1024791282
O	-1.3722868507	0.5370337599	0.1322275901
O	0.3822053716	1.7625094903	-1.0197100577
H	-0.5926874149	1.4718108114	-0.6333074881
H	0.5863458254	2.627978897	-0.6522599059
C	1.0604496693	1.0042691691	1.4729630063
H	0.1817496107	1.5868419774	1.7303081543
H	1.1233528651	0.1988139344	2.2164329747
C	2.3502143425	1.8226551406	1.5047408351
H	2.5170869256	2.221215736	2.5039735528
H	3.2181045159	1.2165328858	1.2410265979
H	2.3175586781	2.6664456862	0.8157105744

syn_Gauche-CH_3CH_2CHOO 1a vdW

C	0.5077751128	-0.9368769955	0.2211171116
H	1.2875740036	-1.683267757	0.100958272
O	-0.5846375554	-1.3082297664	-0.2803408539
O	-1.6567712395	-0.4330731247	-0.1955864506
O	-0.6337042594	1.5815280489	-1.7861406135
H	-1.1767101079	0.913049231	-1.3205568341
H	-1.0798318407	1.7592285574	-2.6168674652
C	0.7109204885	0.3490389134	0.9010875072
H	0.5891502376	1.1329446945	0.1421992409
H	-0.1464619305	0.4943994847	1.5671922195
C	2.0563886089	0.4557715779	1.6180269303
H	2.1512662994	1.4320611483	2.0892399376
H	2.1595583503	-0.2995171244	2.3974723964

H	2.8893888323	0.344115112	0.9234056019

syn_Gauche-CH_3CH_2CHOO 1b TS

C	0.8387108993	0.2348478676	0.192277714
H	1.7172977501	-0.2217006076	-0.2634193038
O	-0.2382482828	-0.4027837041	-0.1102783992
O	-1.3677398268	0.4975997217	0.10161906
O	0.3999058772	1.8217039863	-0.9208232835
H	-0.5768720132	1.4738487333	-0.5809051849
H	0.46739958	1.5621493516	-1.8466002849
C	1.050986799	1.0005379365	1.4575305221
H	0.1771177304	1.6037559248	1.6791184031
H	1.0952779	0.2179988585	2.2269367899
C	2.3411321755	1.8173436106	1.4662090346
H	2.4955628309	2.2629403561	2.4475990432
H	3.2125471335	1.1977853516	1.2458181194
H	2.2946854469	2.616832613	0.73029577

syn_Gauche-CH_3CH_2CHOO 1b vdW

C	0.5125540805	-0.9319308002	0.2300069757
H	1.2973747683	-1.6743702825	0.1183654731
O	-0.5755492698	-1.3136029832	-0.273069965
O	-1.6533420853	-0.4444547241	-0.1989264306
O	-0.636232574	1.5648267748	-1.799996749
H	-1.17700639	0.896413453	-1.3317289837
H	-1.0800979166	1.7337627302	-2.6337584651
C	0.7051087974	0.3600957091	0.9014214755
H	0.5815949842	1.1377263104	0.1363838009
H	-0.1558105254	0.5050062671	1.5630472559
C	2.0470133153	0.4802735329	1.6228977866
H	2.1340320515	1.460511721	2.0873820416
H	2.1516702485	-0.2687070473	2.4082099958
H	2.8834595156	0.3687103386	0.9324147883

syn_Anti-CH_3CH_2CHOO 2a TS

C	1.3668941883	-0.2951262821	-0.4346505338
H	0.6158218617	-0.5742432161	0.2992528352
O	1.8323359155	0.8800375119	-0.1715729743
O	2.9449690164	1.2627353774	-1.0295308082
O	0.1424237023	-0.0868115195	-1.8520091584
H	-0.6267311449	0.3643565749	-1.4853676487
H	0.6758529024	0.6665660925	-2.4434133967
O	1.4799999767	1.6533072742	-2.9371061922
H	2.2434952388	1.5657098065	-2.1203451126

H	1.8945636933	1.462213301	-3.7815264701
C	2.2136373119	-1.3882274323	-1.0083883012
H	2.5637736823	-1.0967336486	-1.9946273789
H	3.1068696585	-1.4122740257	-0.3771922332
C	1.5119865625	-2.7441588267	-1.0318085382
H	2.1904283069	-3.5118663732	-1.4011365615
H	1.1881073368	-3.0459624926	-0.0342216516
H	0.6392417907	-2.7226591215	-1.6818718756

syn_Anti-CH_3CH_2CHOO 2a vdW

C	-0.010446393	-0.3543119791	1.1105352044
H	-0.8584480118	-0.5239874211	1.7652974097
O	0.3758574132	0.8393496078	1.1238310236
O	1.454982089	1.1578756865	0.2902369885
O	-1.8887032511	-0.091295518	-1.0083932918
H	-2.8072290691	0.1851957529	-1.0458879914
H	-1.3735431274	0.663342556	-1.3632921153
O	-0.1882993662	1.9895751601	-1.718594836
H	0.5097910743	1.8179851729	-1.0416263839
H	0.2645118127	2.0437057093	-2.5631816446
C	0.6358818967	-1.4191467282	0.3303431286
H	0.6715573438	-1.0762116407	-0.7066987827
H	1.6880500146	-1.4365076053	0.6396328159
C	-0.0479821791	-2.7767313717	0.4670668097
H	0.4868626285	-3.5267361128	-0.1127905425
H	-0.0698427714	-3.1154142756	1.5036659734
H	-1.0699691036	-2.7303429928	0.0943342342

syn_Anti-CH_3CH_2CHOO 2b TS

C	2.0289791099	-1.3309849479	-0.7107613131
H	1.0773736359	-1.2828281479	-0.1913732919
O	2.7113766745	-0.2588450611	-0.4918363245
O	4.0484403189	-0.3075423192	-1.0714294151
O	3.2019456649	0.1419046428	-3.3072250914
H	3.0934021971	1.0794798411	-3.4846449772
H	3.704564953	0.0205878782	-2.3149276041
O	1.2537360725	-1.0277798984	-2.3977334675
H	2.0580146453	-0.4652537215	-2.8940978794
H	1.1287767305	-1.8453338394	-2.8917167158
C	2.6826455134	-2.6709897554	-0.8641216149
H	3.326906757	-2.7659406513	0.0152553638
H	3.3593840246	-2.6522788822	-1.7140115065
C	1.6928420494	-3.833216171	-0.930602677
H	1.0699343544	-3.7995143733	-1.8257338751

H	2.228465033	-4.7809689203	-0.9478715565
H	1.0269392657	-3.8454996731	-0.0667510538

syn_Anti-CH_3CH_2CHOO 2b vdW

C	-0.3821435612	-0.1841159241	1.0779768519
H	-1.3904491598	-0.0785597403	1.4637471844
O	0.2373594076	0.9060921216	1.0466471958
O	1.540473863	0.8700353052	0.5339857184
O	0.7830654684	1.5872690817	-1.9767309821
H	0.8271812647	2.538933343	-2.0962627491
H	1.1884676722	1.407740209	-1.094100982
O	-1.6199114484	0.2948455224	-1.4173186133
H	-0.8447164473	0.8086863822	-1.7262368332
H	-2.0579359285	-0.0179100383	-2.2118928955
C	0.2000000493	-1.4673619528	0.6612260757
H	1.1161851192	-1.6020520102	1.2484957971
H	0.5623599773	-1.3296385843	-0.3612262288
C	-0.7640616915	-2.6443549404	0.7837784936
H	-1.6413584192	-2.4942721719	0.155864441
H	-0.2771152687	-3.5641223039	0.4649929352
H	-1.0978668971	-2.7872122989	1.8121345909

syn_Anti-CH_3CH_2CHOO 2c TS

C	1.3806002198	-0.3150783062	-0.4907435623
H	0.6096649803	-0.5270849015	0.2433435657
O	1.8811204771	0.8557683949	-0.2818553209
O	2.9852516564	1.1685045135	-1.1814539786
O	0.1635662962	-0.0467438263	-1.8804650783
H	0.1213710967	-0.8108151657	-2.4650148138
H	0.6354333174	0.7806487801	-2.4345821458
O	1.3748746481	1.8310661119	-2.8823249819
H	2.2159796609	1.6332750944	-2.1714393396
H	1.7024626241	1.7639440412	-3.7820040677
C	2.2188792292	-1.4605658719	-0.9755127417
H	2.6515049477	-1.2127250772	-1.9408366729
H	3.0641032043	-1.4963772522	-0.2816450375
C	1.4835269318	-2.8001041366	-0.9884854384
H	2.1687973498	-3.601943489	-1.2587278394
H	1.0650383253	-3.0387832187	-0.0099424057
H	0.6641280349	-2.8203806907	-1.7088231411

syn_Anti-CH_3CH_2CHOO 2c vdW

C	-0.0081646273	-0.3573580879	1.1206567325
H	-0.8520543393	-0.5323014725	1.7793339892

O	0.3735847589	0.8377489956	1.1355569821
O	1.4470782791	1.1629786869	0.2972935201
O	-1.8985090886	-0.0952303104	-0.9876133867
H	-2.8182850516	0.1777900167	-1.0194726389
H	-1.3881453286	0.6624799607	-1.3428966016
O	-0.2099274055	1.9943760164	-1.700358097
H	0.4923621758	1.8234420517	-1.0275797324
H	0.2382347197	2.0528222153	-2.5471341509
C	0.6381706594	-1.4173145082	0.3338552248
H	0.6670826623	-1.0711087663	-0.7023101594
H	1.6920055584	-1.4315307566	0.6375812477
C	-0.0397188221	-2.7779482088	0.4700217723
H	0.4949740231	-3.5241174128	-0.1149018625
H	-0.0548403201	-3.119843933	1.5056861119
H	-1.0638158535	-2.7343974866	0.1027790487

syn_Anti-CH_3CH_2CHOO 2d TS

C	1.9951220917	-1.295228178	-0.6401119667
H	1.0594016014	-1.328598961	-0.0893756092
O	2.6374866807	-0.2085473892	-0.3647985885
O	3.9756807185	-0.1677817411	-0.935933317
O	3.2452920328	-0.1180963784	-3.2523701172
H	3.2543839328	0.756054679	-3.6488063152
H	3.6778575455	-0.0612410306	-2.2094291501
O	1.1699709176	-1.0215805154	-2.3174147506
H	2.0182868633	-0.5757679377	-2.8464581892
H	0.5317772818	-0.3136082387	-2.1749342331
C	2.6854858597	-2.5935831836	-0.9180967577
H	3.3994342708	-2.7122694259	-0.0975695151
H	3.2889230624	-2.5024523398	-1.8173524646
C	1.7255914936	-3.7785575279	-0.9986632647
H	1.035182502	-3.6673056621	-1.8326881853
H	2.2832259537	-4.7027762324	-1.1425572377
H	1.1419781917	-3.886680937	-0.082714338

syn_Anti-CH_3CH_2CHOO 2d vdW

C	-0.2939097227	-0.1761045362	1.0731779809
H	-1.2660794732	-0.0309030826	1.5319186507
O	0.3794048745	0.8812263147	1.0282601859
O	1.6402162463	0.7941910432	0.4241000617
O	0.750748681	1.6275039733	-2.0061752618
H	0.8373818565	2.5789043268	-2.1022531844
H	1.2059275338	1.3998721698	-1.1596453656
O	-1.6735886292	0.4436134544	-1.3143727591

H	-0.8951862979	0.9262760275	-1.6629649534
H	-2.1815458636	0.1787927303	-2.084359216
C	0.188563784	-1.4739629418	0.5811667668
H	1.1345843456	-1.6738953879	1.0983651225
H	0.4863173594	-1.3232022988	-0.4601280053
C	-0.8263383565	-2.6030403295	0.7389787655
H	-1.7356009044	-2.3884747655	0.1789310721
H	-0.4124834112	-3.5362411317	0.3613899902
H	-1.0955150225	-2.760578566	1.7840031494

syn_Gauche-CH_3CH_2CHOO

C	-0.2629084038	0.6813921044	-0.0125437943
H	-0.019853914	1.7100875609	-0.2533627237
O	-1.4714169073	0.5414980602	0.3235101314
O	-1.9130552055	-0.7132568716	0.6479168881
C	0.6963201785	-0.4367523012	-0.0701975644
H	0.5280377362	-1.0493308257	0.8185729236
H	1.7075725763	-0.0315961875	-0.050349641
C	0.4920566328	-1.3186856471	-1.3242362579
H	1.1980964482	-2.1471985736	-1.2992354914
H	-0.5172798591	-1.7208216348	-1.3395966515
H	0.6656578378	-0.7515532739	-2.2380165389

syn_Gauche-CH_3CH_2CHOO 1a TS

C	0.8010967264	0.2406027833	0.2196452692
H	1.7070196921	-0.2502100662	-0.1323159976
O	-0.2471519005	-0.3720874014	-0.2019326748
O	-1.3661553838	0.5643737479	-0.2133553472
O	0.5849140898	1.7154858626	-1.0966258076
H	-0.440323793	1.45674063	-0.8722246527
H	0.7472727669	2.5837336675	-0.7152476239
C	0.9671882072	0.9936304544	1.5060155526
H	1.8459025157	1.6318098578	1.3843338792
H	1.2947929962	0.2031783482	2.1967240485
C	-0.196209964	1.7566344277	2.1328180671
H	-1.0608765338	1.1156071196	2.2704338114
H	0.1194718569	2.1447233653	3.1023213511
H	-0.5111202762	2.5962222031	1.5172581248

syn_Gauche-CH_3CH_2CHOO 1a vdW

C	0.5279346172	-1.0433896317	0.422425232
H	1.0998032502	-1.9509029973	0.5887264076
O	-0.4101070813	-1.2309703193	-0.3947623644
O	-1.2327150798	-0.159340796	-0.7025734205

O	0.6283554848	1.3981563885	-2.0399565813
H	-0.1548326813	0.903465609	-1.726631594
H	0.4612391412	1.6033872279	-2.9622535342
C	0.8168931471	0.2347176528	1.0969219326
H	0.8006646248	1.023672973	0.3427959755
H	1.8176802352	0.1750400591	1.5228153453
C	-0.2210925874	0.5545499551	2.1995194894
H	-0.2122659602	-0.2006116849	2.9846912801
H	0.0277330001	1.5143611163	2.6485243661
H	-1.2183151105	0.6150784474	1.7729564657

syn_Gauche-CH_3CH_2CHOO 1b TS

C	0.7983252892	0.2149544508	0.2086477098
H	1.707671769	-0.2770861597	-0.136525256
O	-0.2468277569	-0.4034252596	-0.2181739244
O	-1.3707388412	0.524666642	-0.2273900951
O	0.5559559235	1.7967819106	-0.9969936105
H	-0.4605253792	1.4722684966	-0.806752794
H	0.7603821167	1.514152968	-1.8952642072
C	0.9664274504	0.9861578535	1.4803986709
H	1.8346916501	1.6301428302	1.3313165323
H	1.3016929871	0.2077374011	2.1818005229
C	-0.1935423029	1.7628402344	2.0955615748
H	-1.0611221305	1.1294304256	2.2508718748
H	0.1283366051	2.1663299082	3.0567877769
H	-0.4940073805	2.5920132984	1.4609842248

syn_Gauche-CH_3CH_2CHOO 1b vdW

C	0.5446592158	-1.0344646132	0.4248373415
H	1.130719091	-1.9325548174	0.5928793715
O	-0.3913191769	-1.2387658434	-0.3907052663
O	-1.2307975169	-0.1808475376	-0.7003927917
O	0.6043423068	1.4016814908	-2.0442077935
H	-0.1707171783	0.8957626691	-1.7286065321
H	0.4329849505	1.6018053796	-2.9668487451
C	0.8145637098	0.2497846993	1.0955506338
H	0.7852258069	1.0363532249	0.3393303812
H	1.8166537559	0.2067731587	1.5203881977
C	-0.2269620299	0.556472469	2.1985443673
H	-0.2055125666	-0.1963373971	2.9857285725
H	0.0074835302	1.5212338256	2.6446697062
H	-1.2255018984	0.6003882917	1.7730305572

syn_Gauche-CH_3CH_2CHOO 1a' TS

C	0.832604517	0.2378067297	0.2093670995
H	1.6910019194	-0.2433033037	-0.255644797
O	-0.2713514668	-0.3210402349	-0.1436670127
O	-1.3533353895	0.6293918624	0.0944219942
O	0.5126412566	1.8140305204	-0.9231231253
H	-0.4894696552	1.5642644115	-0.5924946859
H	0.7588753332	2.6341231586	-0.4837339189
C	1.0515172113	0.9012795928	1.53355451
H	1.9124741314	1.565193265	1.4520485318
H	0.1734688725	1.4783936303	1.8045023754
C	1.3287153682	-0.1836071862	2.5911949742
H	1.5358054984	0.2881866925	3.5506878515
H	0.4654585608	-0.8358717706	2.7097647674
H	2.1908138426	-0.7972153678	2.3268754358

syn_Gauche-CH_3CH_2CHOO 1a' vdW

C	0.2077903406	-1.0635607572	0.1091495096
H	0.8156002111	-1.9592598989	0.0201887072
O	-0.7193978581	-1.0339980929	-0.7406606461
O	-1.5602524327	0.0684604473	-0.7306552452
O	0.3046389088	1.9793102478	-1.4419701376
H	-0.4827517725	1.4108470179	-1.3180627375
H	0.1926298599	2.4126538813	-2.29072309
C	0.4415588101	-0.0188820843	1.1147372701
H	0.7306002558	0.8888918818	0.5691652017
H	-0.5346646457	0.2330487169	1.5430463513
C	1.4803371592	-0.4047633469	2.1672171293
H	1.6172226855	0.4121962528	2.8729253851
H	1.1733680417	-1.2840202219	2.7340660232
H	2.4499554363	-0.6132310437	1.7141862788

syn_Gauche-CH_3CH_2CHOO 1b' TS

C	0.8283948923	0.19441097	0.1972143196
H	1.6871147646	-0.3019870289	-0.2536242428
O	-0.2781625399	-0.3639861666	-0.1557286968
O	-1.3561447343	0.5922635377	0.0691502834
O	0.5216051691	1.8509172729	-0.8433939787
H	-0.4814622165	1.5592262428	-0.5477728237
H	0.5952645503	1.6310543383	-1.77913586
C	1.051387428	0.89040593	1.5001801981
H	1.9078981107	1.552790446	1.3888191426
H	0.180308629	1.4845276711	1.7536994629
C	1.3243813188	-0.1673138496	2.5855401673
H	1.5353627116	0.3309658284	3.5306763068

H	0.4595343596	-0.8134601803	2.7263564606
H	2.1841975567	-0.7921400118	2.3393162608

syn_Gauche-CH_3CH_2CHOO 1b' vdW

C	0.2129849603	-1.0609025965	0.1217865417
H	0.82567018	-1.9543802243	0.0447271394
O	-0.7118108187	-1.0457481449	-0.7310041638
O	-1.5583692248	0.0523713361	-0.73591078
O	0.2987466274	1.9647355104	-1.4633234011
H	-0.4860653184	1.3936245774	-1.33530087
H	0.1870331303	2.3878843211	-2.3172434937
C	0.4383671355	-0.0037425868	1.1161822798
H	0.7243410618	0.8993066587	0.5612334462
H	-0.5404132365	0.2479311032	1.5387691417
C	1.4759879908	-0.3723222824	2.1759796694
H	1.6065547072	0.4532477215	2.8728091171
H	1.1718769811	-1.246710461	2.7518287106
H	2.4480128238	-0.5808479324	1.7281626626

syn_Gauche-CH_3CH_2CHOO 2a TS

C	1.4277680884	-0.2822448272	-0.3692971567
H	0.7037813754	-0.5578331003	0.3926216942
O	1.8352057651	0.9287655659	-0.1733248307
O	2.910157756	1.3348240344	-1.0701577488
O	0.193434382	-0.2243308368	-1.7767373442
H	-0.5928229044	0.2119988333	-1.4281707373
H	0.6714876339	0.5091219719	-2.422940282
O	1.4142791028	1.5222924724	-2.9943663321
H	2.1742285295	1.5336897453	-2.1867961628
H	1.8428255487	1.3043507913	-3.8252399476
C	2.3225252872	-1.3649114106	-0.8879706739
H	1.7106440884	-2.2471485916	-1.0665823416
H	2.7611295875	-1.0499934046	-1.8297400969
C	3.4309110093	-1.6577562389	0.1351933611
H	4.0600397398	-2.4681126288	-0.2306259098
H	4.0511768572	-0.7769894309	0.2846134372
H	3.0202361533	-1.9648149448	1.0980730719

syn_Gauche-CH_3CH_2CHOO 2a vdW

C	-0.2794641617	-0.3526134007	1.0642609307
H	-1.122415551	-0.4739580317	1.7352382987
O	0.0547041024	0.8506005511	0.9390218037
O	1.1297065901	1.1363484237	0.0845866996
O	-2.0948054603	-0.4473849366	-1.0491317995

H	-3.0230209069	-0.2040496003	-1.0797506559
H	-1.6196023936	0.2780141577	-1.5063704099
O	-0.51636031	1.6186169742	-2.0279706932
H	0.1770976275	1.572859676	-1.325717839
H	-0.0519379227	1.5837026061	-2.8672246912
C	0.4260095781	-1.4871582917	0.4440642528
H	-0.2533417548	-2.3362936589	0.4149965398
H	0.6893388107	-1.2013857458	-0.5723846657
C	1.7124367551	-1.8313995329	1.2310447086
H	2.2136006881	-2.6656102939	0.7430247805
H	2.3873177354	-0.9792812091	1.2451272278
H	1.4884915736	-2.1255936874	2.2560585122

syn_Gauche-CH_3CH_2CHOO 2b TS

C	2.0828443591	-1.4181766697	-0.7309183397
H	1.1489306825	-1.3341624785	-0.1848861683
O	2.7950763495	-0.3564221964	-0.5526303473
O	4.1094671794	-0.4337707384	-1.1823862732
O	3.1784330028	0.0454646724	-3.3860115602
H	3.0589387571	0.9850773103	-3.5445789795
H	3.7165586629	-0.0842239273	-2.4287060654
O	1.2837751039	-1.1651890696	-2.4041859401
H	2.0507321412	-0.5876164599	-2.9251723984
H	1.193383042	-2.0010923045	-2.8749875712
C	2.696376292	-2.7795503558	-0.8652749754
H	1.9045168037	-3.4892229632	-1.1091903761
H	3.4273106673	-2.7670100736	-1.6683186293
C	3.3775616929	-3.1755628082	0.4547006559
H	3.7914217933	-4.179019235	0.3657150928
H	4.186550466	-2.4848341058	0.6803778548
H	2.6734940042	-3.1767995967	1.2876440204

syn_Gauche-CH_3CH_2CHOO 2b vdW

C	-0.6374475824	-0.1764979883	0.956506209
H	-1.6362713788	-0.0155448456	1.3459758934
O	0.0045724522	0.8954163865	0.8445452305
O	1.3079262081	0.8146291982	0.3293468074
O	0.5233253102	1.3342839801	-2.2151332144
H	0.5735013604	2.2712002967	-2.4188578473
H	0.941040527	1.22761317	-1.325645968
O	-1.8786793451	0.1353780926	-1.4875232061
H	-1.1020916868	0.6050072653	-1.8586374545
H	-2.243708303	-0.3748554997	-2.2140605464
C	-0.0891640701	-1.5113087954	0.6597654022

H	-0.9212805092	-2.1958068007	0.5066575456
H	0.4939942705	-1.4348679208	-0.2562971732
C	0.8232254007	-2.0023086395	1.8084921993
H	1.2182460717	-2.9838888673	1.5523338566
H	1.6555351692	-1.3173355547	1.9482932309
H	0.2740081053	-2.0931444774	2.745164035

syn_Gauche-CH_3CH_2CHOO 2c TS

C	1.4656094531	-0.3179858024	-0.4321224859
H	0.7190188096	-0.5177497175	0.3297958585
O	1.9077003315	0.8894032619	-0.3069098615
O	2.970267104	1.2100791935	-1.2544299127
O	0.2380978592	-0.2301625877	-1.8226906147
H	0.2878422268	-1.0251875515	-2.3642486775
H	0.6230367355	0.6026595323	-2.4205826098
O	1.27191543	1.6956531915	-2.9384840718
H	2.1364452604	1.588145878	-2.254511458
H	1.580151992	1.6195510553	-3.8443064674
C	2.3541866583	-1.4524966564	-0.8498339452
H	1.7368953289	-2.3427809481	-0.9796728828
H	2.8324646681	-1.2046113121	-1.7928368519
C	3.4231282528	-1.699161892	0.2264639301
H	4.0457480513	-2.5450449 -0.0617365857	
H	4.0566394967	-0.8216702772	0.3329561712
H	2.9753333418	-1.9278854677	1.1942254652

syn_Gauche-CH_3CH_2CHOO 2c vdW

C	-0.287275349	-0.3591690211	1.0785389723
H	-1.1321104763	-0.4968307283	1.7439755117
O	0.0286246523	0.8497126254	0.9606846068
O	1.1039574055	1.1562450316	0.1139026105
O	-2.0885356871	-0.4727765374	-1.0459454013
H	-3.0202748023	-0.2439293744	-1.0809415941
H	-1.6221626881	0.2620991365	-1.4971021226
O	-0.5371612607	1.6222844568	-2.0061289084
H	0.1528323441	1.584200332	-1.3000155742
H	-0.067369461	1.5985747575	-2.8427816511
C	0.4395869058	-1.4796237108	0.4574252977
H	-0.2261217316	-2.3391964344	0.4205355778
H	0.7043027183	-1.1850887169	-0.5561582288
C	1.7266683702	-1.8071947806	1.2504294486
H	2.2437497889	-2.631172689	0.7616314102
H	2.3879461229	-0.9446402194	1.2723240556
H	1.5014131481	-2.1095731274	2.2727709895

syn_Gauche-CH_3CH_2CHOO 2d TS

C	1.9998346363	-1.3891072928	-0.6958113613
H	1.0610407615	-1.4171432416	-0.1499331162
O	2.6299600535	-0.2900501135	-0.4349394123
O	3.971641988	-0.2347325863	-1.0008616734
O	3.2710292775	-0.2527877647	-3.3339781887
H	3.266387113	0.6133389523	-3.7478287477
H	3.6833113905	-0.161717389	-2.3000116532
O	1.2041531899	-1.1745308059	-2.3817809305
H	2.0414323411	-0.7354559383	-2.9190272704
H	0.5565909595	-0.4695892743	-2.2674553956
C	2.6985427405	-2.6922585967	-0.9295594377
H	1.9493816299	-3.4196876688	-1.2367701594
H	3.4202206381	-2.5803930727	-1.7330377008
C	3.4077547287	-3.139769909	0.3583321395
H	3.8858804731	-4.1042448766	0.1930483237
H	4.1707523561	-2.4184001479	0.6414254754
H	2.7071167229	-3.2536742743	1.1867701086

syn_Gauche-CH_3CH_2CHOO 2d vdW

C	-0.5809551351	-0.119426534	0.9517447127
H	-1.5452850268	0.1072270478	1.3921278763
O	0.1321445678	0.904582472	0.8228254611
O	1.3996717873	0.7378204652	0.2429522444
O	0.5338328835	1.3568536621	-2.2524690268
H	0.6430440773	2.2909676216	-2.4456981769
H	0.9849114369	1.2047692092	-1.3861832121
O	-1.9121218666	0.3239871234	-1.4236677237
H	-1.121829801	0.7420411399	-1.8262032267
H	-2.3483064807	-0.1457469196	-2.1381843539
C	-0.1474240196	-1.4853779134	0.6102524362
H	-1.0341100888	-2.1046534027	0.4890806495
H	0.3949754878	-1.4359671336	-0.3323230115
C	0.780589425	-2.0612210036	1.7058371115
H	1.0894288256	-3.0644550691	1.417223622
H	1.6668620866	-1.4412574304	1.8137159878
H	0.2719318406	-2.1278143348	2.6671266302

syn_Gauche-CH_3CH_2CHOO 2a' TS

C	1.4076607702	-0.2718148762	-0.438119072
H	0.6446173224	-0.6147737297	0.2551101564
O	1.7475623939	0.9347530367	-0.1288705258
O	2.8465363291	1.4546605852	-0.9289285592

O	0.2489133377	-0.142161553	-1.9047405681
H	-0.5881060119	0.1682435035	-1.5404481562
H	0.6795391915	0.7177707069	-2.4198518054
O	1.3456612792	1.8564636782	-2.8177203684
H	2.1094209649	1.7882650039	-2.0185361349
H	1.7819437618	1.7957348024	-3.6706993201
C	2.3715674059	-1.328552867	-0.9112427525
H	1.8642868691	-2.2841328905	-0.7733884373
H	3.1840556834	-1.2847498211	-0.1791536003
C	2.9568971467	-1.2632970386	-2.3232500683
H	3.5401555314	-0.3590811393	-2.4597671511
H	3.6063026534	-2.1259301817	-2.4736673056
H	2.1719273715	-1.3045142199	-3.0754433312

syn_Gauche-CH_3CH_2CHOO 2a' vdW

C	-0.0329891935	-0.646457152	1.2782446477
H	-0.94046894	-0.9863567298	1.7641969461
O	0.0262007501	0.6051819687	1.2173421399
O	1.1246484693	1.1703770464	0.5676963173
O	-2.0655531149	-0.3647486601	-1.013035252
H	-3.0004088579	-0.161889762	-1.0912604953
H	-1.5999220252	0.4561831074	-1.2686215355
O	-0.5298558708	1.9491636289	-1.4750207154
H	0.1564555562	1.8256928997	-0.7791876896
H	-0.0579308759	2.1372429453	-2.2892450866
C	1.0093745045	-1.5566419993	0.7717036727
H	0.8990914301	-2.5118806794	1.2844815672
H	1.9737464113	-1.1109492341	1.0231446113
C	0.9381850686	-1.7675257726	-0.7600832542
H	1.1222839868	-0.8304531734	-1.2766575851
H	1.7042812665	-2.4858012328	-1.0474084413
H	-0.0361185653	-2.1427892009	-1.0622438473

syn_Gauche-CH_3CH_2CHOO 2b' TS

C	2.0716932156	-1.4089280947	-0.8005806257
H	1.1028670193	-1.4114839157	-0.3124546468
O	2.6798348822	-0.3055564772	-0.5251964984
O	4.0311259975	-0.2318467569	-1.0654657952
O	3.1742926548	0.310320145	-3.2869026429
H	2.9816156176	1.2453794788	-3.3914303389
H	3.6744029643	0.1637962506	-2.3127516053
O	1.3381338603	-1.1146531006	-2.4938745485
H	2.0798688236	-0.4455066456	-2.9333308492
H	1.3307545894	-1.9169067893	-3.0273716058

C	2.7560418215	-2.7499282517	-0.8988281378
H	1.964740465	-3.501284698	-0.8566819181
H	3.3054446716	-2.8236678813	0.0452646074
C	3.7094521426	-3.0606918715	-2.0554041896
H	4.5378808901	-2.3620253469	-2.0722540428
H	4.0942800087	-4.073029496	-1.9310813793
H	3.2112673761	-3.023485549	-3.0243767833

syn_Gauche-CH_3CH_2CHOO 2b' vdW

C	-0.5270013621	-0.4551245467	1.2262899939
H	-1.5875052989	-0.5169266224	1.4426315988
O	-0.1411233913	0.7322423456	1.105131942
O	1.1991187032	0.9435198095	0.7675400645
O	0.4877908054	1.6592546961	-1.7640538508
H	0.4471553841	2.6118505467	-1.8770387979
H	0.8690423563	1.5119663481	-0.866178726
O	-1.8556125212	0.1414032046	-1.3803960903
H	-1.1033957015	0.723270254	-1.6100935328
H	-2.2668018967	-0.088640872	-2.2165268473
C	0.3539732482	-1.6307447992	1.109146667
H	-0.115891202	-2.4576825592	1.6412945037
H	1.2995826351	-1.3702742708	1.5880531337
C	0.6319430132	-2.0370821445	-0.3582404854
H	1.1429487244	-1.236395544	-0.8841998681
H	1.2669887925	-2.9214749952	-0.3587902294
H	-0.2923762887	-2.2634528507	-0.8836144755

syn_Gauche-CH_3CH_2CHOO 2c' TS

C	1.4225800825	-0.2741436942	-0.487655229
H	0.653363416	-0.5614661493	0.2217506022
O	1.8048408025	0.9301419859	-0.225165375
O	2.8845308216	1.40093118	-1.0831267961
O	0.2301113669	-0.0896480222	-1.8941611933
H	0.3134916329	-0.8163852466	-2.5206377593
H	0.5953241708	0.8156352194	-2.3873453303
O	1.2115893752	1.9866018092	-2.7651314053
H	2.060215302	1.8468916111	-2.0711753787
H	1.5475366111	2.0232082029	-3.6634981081
C	2.353527979	-1.3850220395	-0.9103721556
H	1.793291353	-2.3154147649	-0.7959834715
H	3.1183933308	-1.3872637834	-0.1272940896
C	3.0409941776	-1.3541086588	-2.2771878849
H	3.6510723035	-0.4639340093	-2.3794065044
H	3.6712263784	-2.2381351843	-2.3761392442

H	2.3260098961	-1.379368456	-3.1007906768

syn_Gauche-CH_3CH_2CHOO 2c' vdW

C	-0.0169821364	-0.6544517066	1.2782427474
H	-0.9167086564	-1.0070891946	1.7695064103
O	0.027794786	0.598081375	1.2237624859
O	1.1146544359	1.1790146721	0.5685336096
O	-2.0708294653	-0.383052266	-0.9952365116
H	-3.0084784653	-0.1902182073	-1.0649182911
H	-1.6164120394	0.4443957771	-1.2499928029
O	-0.5646910151	1.9503100396	-1.4566725973
H	0.1284932231	1.8307456565	-0.7669964422
H	-0.1014130931	2.1480421962	-2.2735716485
C	1.0313529931	-1.5501859948	0.7584385511
H	0.9358152477	-2.509354614	1.2668213922
H	1.9926897737	-1.0951152682	1.0046491514
C	0.9502443567	-1.753570441	-0.7738693875
H	1.1197617937	-0.8117220309	-1.2867361683
H	1.7219578522	-2.4616812475	-1.071218177
H	-0.022213591	-2.1380537454	-1.0703313215

syn_Gauche-CH_3CH_2CHOO 2d' TS

C	2.0271593813	-1.4053867739	-0.7781674482
H	1.0499967269	-1.4654044873	-0.3073591113
O	2.5826283181	-0.2836156301	-0.4586439258
O	3.9514866245	-0.1558632359	-0.9364165445
O	3.2701721756	0.1523392221	-3.256997553
H	3.1375682437	1.0732093616	-3.4939961681
H	3.6797427044	0.1060597433	-2.2225744213
O	1.3457047078	-1.1851695913	-2.5144444338
H	2.1255110112	-0.5578526909	-2.94842811
H	0.5733228307	-0.6195772136	-2.4037598765
C	2.7696697178	-2.7094530542	-0.9060464908
H	2.0158017788	-3.4941161063	-0.8307439967
H	3.3755038814	-2.7515063156	0.0046006011
C	3.6606506884	-2.9756796159	-2.1218089163
H	4.4709910604	-2.257740441	-2.181132194
H	4.0839637386	-3.9760144192	-2.0294958509
H	3.0881884105	-2.9393737519	-3.0456435597

syn_Gauche-CH_3CH_2CHOO 2d' vdW

C	-0.5471185278	-0.4474035136	1.2151630152
H	-1.6113796698	-0.5012602041	1.4145098911
O	-0.1512722715	0.7368812653	1.0960109216

O	1.1956611259	0.9378769899	0.7794277248
O	0.530263041	1.6490356987	-1.7659131243
H	0.4979350401	2.6014602923	-1.8829517329
H	0.8959306299	1.5024972842	-0.8614581394
O	-1.8292951747	0.148411774	-1.4148355569
H	-1.0695320953	0.7243580391	-1.634392814
H	-2.2284395731	-0.081959509	-2.2566933462
C	0.3276291336	-1.6293552999	1.1165346395
H	-0.1563920437	-2.4511353686	1.6439631504
H	1.2671124966	-1.3734886154	1.609765461
C	0.6265415791	-2.0429818938	-0.3446860077
H	1.1514171096	-1.2477054629	-0.8651665928
H	1.2554923701	-2.9316258555	-0.3317680059
H	-0.2906711699	-2.2650676206	-0.8841544836

anti_Anti-$CH_2CHCHOO$

C	-0.1507529385	0.2141898063	-0.0816585002
O	1.112237684	0.1107412427	-0.0258760898
C	-0.9533103002	-0.8956854614	0.3199684923
H	-0.4282474189	-1.7803652791	0.6560651155
O	1.8591351457	1.1798400133	-0.4130435737
H	-0.5532344467	1.1567954662	-0.4376071654
C	-2.2930551519	-0.8496598996	0.2845258895
H	-2.8918388895	-1.6943548705	0.5903704333
H	-2.8199776841	0.0335429821	-0.0510326017

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 1a TS

C	1.6878856649	-0.1267684901	-0.0227343931
H	2.6186663862	-0.5437533078	0.3424495594
O	1.3923542416	1.0808346884	0.3295553724
O	2.6206216634	1.8477110181	0.2696021285
C	0.5806291768	-0.9993862408	-0.3665030649
H	-0.3497259657	-0.5169235373	-0.6328931593
C	0.7134269892	-2.3247365381	-0.3560071091
H	1.6515712233	-2.7976325466	-0.0956915292
H	-0.1098885762	-2.9762724046	-0.6104544665
O	2.6198802864	0.4760215491	-1.679095435
H	3.4233539253	-0.0372834961	-1.8111905685
H	2.8462609849	1.2891343058	-0.9071483348

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 1a vdW

C	-0.3305670441	-0.2708870124	0.2194342757
H	0.4006773923	-0.4259748804	-0.5694204287

O	-0.3652218463	0.8574642767	0.7955407428
O	0.5315207599	1.8269026025	0.4106508252
C	-1.2658857097	-1.2689236321	0.6348648592
H	-1.9551053625	-1.0038182957	1.4258372116
C	-1.2808806679	-2.4811180461	0.0633022158
H	-0.5887480283	-2.7396456256	-0.7268401328
H	-1.9844223941	-3.2396018821	0.3729615809
O	1.881319015	0.6793811596	-1.725866226
H	2.1382002392	1.238477833	-2.4621748469
H	1.5261286465	1.2728765027	-1.0323010767

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 1b TS

C	1.6668511481	-0.10295989	-0.0332203174
H	2.6181124034	-0.5057538872	0.289108131
O	1.3680506003	1.1081746837	0.3141658276
O	2.5818090201	1.8888512337	0.198867791
C	0.5541215261	-0.99057769	-0.3157134448
H	-0.4138273476	-0.5270736569	-0.4538766059
C	0.7248587615	-2.3091830164	-0.4054382413
H	1.6996214	-2.7611665573	-0.2782801134
H	-0.1018054662	-2.9714181698	-0.6183772808
O	2.6847237917	0.4065897971	-1.6698574777
H	2.0581329322	0.7025260384	-2.3398162593
H	2.8360432304	1.2769011148	-0.9408230091

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 1b vdW

C	-0.3272829838	-0.2714521666	0.2259355497
H	0.3971877042	-0.4268279513	-0.5690882985
O	-0.369415672	0.8629849784	0.7894542994
O	0.5112260457	1.8386428537	0.3836716098
C	-1.2458159342	-1.2758164984	0.6630054749
H	-1.9295838121	-1.0099080417	1.4584273807
C	-1.2522563011	-2.4946305379	0.105533635
H	-0.5656469663	-2.7539175305	-0.689165627
H	-1.9431080335	-3.257905636	0.4315591213
O	1.8516224661	0.6828447688	-1.7543068101
H	2.0936659197	1.2364458359	-2.4997384323
H	1.4967825672	1.2799959256	-1.0637069028

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2a TS

C	1.8655290955	-0.2847360489	-0.3915051196
H	2.7678061594	-0.6799920932	0.0559344588
O	1.5448188049	0.9276263886	-0.080433023
O	2.6904359412	1.6830640001	0.3923068775

C	0.721159099	-1.1687197737	-0.6390915344
H	-0.2189934855	-0.676108567	-0.8516904636
C	0.8204267745	-2.4923824618	-0.5674888814
H	1.761340097	-2.9793031115	-0.3478675648
H	-0.0379644741	-3.128813687	-0.7270018058
O	3.6312039389	2.0192629487	-1.8202705701
H	4.5885796096	2.0930071904	-1.8030655221
H	3.2457201737	1.9830007607	-0.7544141669
O	2.7301997311	-0.2259394799	-2.074613208
H	2.0415117278	-0.2166257442	-2.7490539121
H	3.2061668069	0.7820896787	-2.0650045645

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2a vdW

C	-0.7016421808	-0.2214543742	0.4654798015
H	-0.3857270017	-0.0297678662	-0.5561878747
O	-0.6066631306	0.70215351	1.3241720732
O	-0.099372003	1.9233295952	0.9028373979
C	-1.203773982	-1.4959220404	0.8735077396
H	-1.5344830026	-1.6063875279	1.8977139943
C	-1.2366294035	-2.5088945008	-0.0045357815
H	-0.8774689628	-2.3763435981	-1.0166173978
H	-1.6043636472	-3.4844454122	0.2782165842
O	1.9853983348	1.4553506798	-0.7583275388
H	2.800964498	1.4784590106	-0.2530973102
H	1.2588881788	1.7017047693	-0.1327511035
O	0.8736789292	-0.5630745061	-2.2760226449
H	0.8299015649	-0.3087389577	-3.2007232275
H	1.4166538085	0.1250092186	-1.8398027118

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2b TS

C	1.7979126422	-0.2297897679	-0.285068279
H	2.6718387271	-0.5670797534	0.2593820462
O	1.4685882065	1.0058540074	-0.1228797515
O	2.5899325507	1.7967715338	0.3609679676
C	0.6865255179	-1.1526516972	-0.5246089267
H	-0.1779601754	-0.7388029143	-1.0252716061
C	0.7310024333	-2.417023499	-0.1176597611
H	1.5972640592	-2.8206354128	0.3907237083
H	-0.1016856792	-3.0874243145	-0.2734818845
O	3.7426036618	1.9066893727	-1.7685321072
H	3.4107633047	2.6010729428	-2.3430363347
H	3.2338686633	1.98593683	-0.7610645131
O	2.6417545439	-0.2496053424	-1.9905853304
H	3.2905793702	-0.9604469231	-2.0392572815

H	3.1832221739	0.7244619379	-2.0056789463

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2b vdW

C	-0.4872474548	-0.2980306184	0.6580231306
H	0.431938154	-0.4928883855	0.1126059363
O	-0.6269631996	0.8072556798	1.2565605917
O	0.4185508922	1.7168587724	1.181340108
C	-1.554170619	-1.2480803905	0.7024314844
H	-2.4262293387	-1.0039250807	1.2944377999
C	-1.4549948879	-2.3910453449	0.0082061251
H	-0.5806557515	-2.5988037619	-0.5944900751
H	-2.24870323	-3.1237193106	0.0178352483
O	1.3805126328	1.7058637136	-1.3483309658
H	0.9551374561	2.4052368768	-1.8492031316
H	1.0576624972	1.789801826	-0.4163565823
O	1.4369085208	-1.0205453725	-1.7688642892
H	2.3311755849	-1.3181562492	-1.9515891516
H	1.4756957434	-0.0425243544	-1.7920982288

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2c TS

C	1.8293136317	-0.2503576123	-0.2833006459
H	2.6901335963	-0.6107269432	0.2673906095
O	1.5277212667	0.992313407	-0.1186004793
O	2.6719043071	1.7584471982	0.3473824186
C	0.694859386	-1.1441972295	-0.5274984986
H	-0.1532136553	-0.7084288315	-1.037512108
C	0.7014797778	-2.4076934109	-0.1157186874
H	1.5519709749	-2.8329834824	0.4016336494
H	-0.147752724	-3.0558139933	-0.2764116979
O	3.62775045	1.9467119968	-1.8737388596
H	4.5820010347	2.0512502827	-1.8606849776
H	3.2378107111	1.987271779	-0.8075562228
O	2.680495155	-0.2901644457	-1.97663136
H	3.3292584699	-1.0015271353	-2.0068951237
H	3.2082046181	0.6935924205	-2.0253910167

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2c vdW

C	-0.7519567869	-0.1421009019	0.4188522091
H	-0.3695719569	-0.1011848808	-0.5972478523
O	-0.7113692805	0.8990205092	1.1356810355
O	-0.1751067088	2.0483080484	0.5720323886
C	-1.2823126233	-1.346020508	0.9775935384
H	-1.6794559967	-1.3063508503	1.9832141855
C	-1.2598334475	-2.4779073987	0.2589282502

H	-0.8350476663	-2.4937249924	-0.7361506976
H	-1.6472750136	-3.4037035232	0.6585124336
O	2.0127570759	1.3558010426	-0.8626798343
H	2.793619571	1.4596115736	-0.3145770887
H	1.2474341208	1.6863822753	-0.3289653891
O	0.9983749876	-0.8732452232	-2.1337843451
H	1.015615481	-0.7587560689	-3.0868159047
H	1.5131222442	-0.1241111016	-1.769912929

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2d TS

C	1.7663272857	-0.1818583557	-0.2837093665
H	2.6419665633	-0.4858124677	0.2745913082
O	1.4038704277	1.0535720155	-0.1674919042
O	2.4951807357	1.8942429282	0.29388659
C	0.6573133278	-1.1227640662	-0.4783001623
H	-0.2779080072	-0.6894643306	-0.8091985577
C	0.7780508577	-2.4218515441	-0.2238287575
H	1.7131769135	-2.848755243	0.1135966379
H	-0.0562688933	-3.0973536719	-0.3461115878
O	3.7791782944	1.8544304329	-1.7621492303
H	3.5155382882	2.5353950147	-2.3854512107
H	3.2055746373	1.9961418044	-0.7959162012
O	2.7380267841	-0.3397591002	-1.8976622116
H	2.0900526735	-0.4137466131	-2.6069409244
H	3.2342631117	0.6540551967	-1.974848422

anti_Anti-$CH_2CHCHOO$ carbonyl insertion 2d vdW

C	-0.5073042065	-0.2829961182	0.6489977119
H	0.4306621803	-0.4875054599	0.1403257625
O	-0.6722085663	0.8373080055	1.2121591331
O	0.3710819829	1.750262957	1.1474023988
C	-1.5707663184	-1.2373336336	0.6833539729
H	-2.4634324428	-0.9820255827	1.2388130326
C	-1.4429739121	-2.398115876	0.0242581133
H	-0.5478336865	-2.6173183145	-0.542795307
H	-2.2331983146	-3.1346034634	0.0271371682
O	1.418013001	1.6760515893	-1.347222868
H	1.0066128008	2.3592610495	-1.8809967024
H	1.0634740643	1.7834203498	-0.4292750374
O	1.5010384308	-1.060394275	-1.6911705033
H	2.4023190937	-1.3579378604	-1.8355144478
H	1.5361228933	-0.0831633675	-1.7397324273

anti_Anti-$CH_2CHCHOO$ vinyl insertion 1a TS

C	-0.1614616388	-0.0711587987	-0.1191555148
O	1.138568079	0.085478394	-0.2403628314
C	-0.7022700746	-1.0040646696	0.7412136607
H	-0.0670012852	-1.7485660566	1.1964676708
O	1.3448178595	1.5112970593	-0.0528411979
H	-0.7632672674	0.7260274846	-0.5354995441
C	-1.7265327721	-0.4067349648	1.4445945849
H	-2.0065188899	-0.7707345807	2.4216333381
H	-2.3678442414	0.3345154217	1.0001565793
O	-0.4071282644	1.3430294523	1.8754282953
H	0.7659799804	1.6273627081	0.8070036017
H	-0.4779180152	2.0579732504	2.5199214772

anti_Anti-$CH_2CHCHOO$ vinyl insertion 1a vdW

C	-0.1844114037	-0.4138235085	-0.1379958967
O	0.8844062411	-0.2531710694	-0.7998854491
C	-0.8986217495	-1.641672534	-0.2985261397
H	-0.4846609548	-2.3700467666	-0.983397016
O	1.5806872153	0.9248789814	-0.6602773858
H	-0.5045669659	0.3832759619	0.5277359647
C	-2.0342130008	-1.8725466217	0.3748582512
H	-2.5787483011	-2.7976857424	0.2575735925
H	-2.4427158467	-1.1398283059	1.0578336917
O	0.190572121	2.2938603698	1.3138344162
H	0.8308000711	1.9868878812	0.6390737596
H	0.6854765739	2.8229753542	1.9429882114

anti_Anti-$CH_2CHCHOO$ vinyl insertion 2a TS

C	-0.1534827795	0.0752187523	-0.0653278243
O	1.1441389696	0.0803384408	-0.0501809845
C	-0.9002639313	-0.9290983896	0.5139095523
H	-0.4081113061	-1.7828630345	0.9561212148
O	1.5991811703	1.4507111007	-0.0959478687
H	-0.6202240431	0.9727340228	-0.4500173042
C	-2.1772304093	-0.5502257911	0.891994027
H	-2.8059832107	-1.2126327977	1.4659656355
H	-2.6914597745	0.2411143936	0.3710375373
O	0.1005008263	2.0066775323	1.7749469081
H	1.0123796421	1.8117312541	0.7755692767
H	0.0482563946	2.9460301266	1.965596554
O	-1.9548278546	0.8033276537	2.4330071021
H	-1.0460224388	1.3593531598	2.1670838613
H	-1.743069275	0.3156102863	3.2360656526

anti_Anti-$CH_2CHCHOO$ vinyl insertion 2a vdW

C	0.1279212515	-0.7280517507	-0.4616369838
O	1.158054626	-0.3363157968	-1.0819569923
C	-0.7806736574	-1.6134686675	-1.1199355053
H	-0.5231933371	-1.9581598963	-2.1126395868
O	2.0128165297	0.5367448731	-0.4236964206
H	-0.0497952621	-0.3711745545	0.5489992351
C	-1.9170455656	-1.9752883092	-0.5068253982
H	-2.6251143474	-2.6374067914	-0.9833902454
H	-2.1602576265	-1.5964509708	0.4771537154
O	0.5153433063	2.3521034151	0.9129156958
H	1.1251581879	1.7465911159	0.4216402133
H	0.4056374705	3.1327485939	0.365651067
O	-1.3627082265	0.6419954895	1.9910168459
H	-0.7941036464	1.3797721672	1.6894473596
H	-1.3464517028	0.6797680823	2.9501740003

anti_Anti-$CH_2CHCHOO$ vinyl insertion 2b TS

C	-0.1515110641	0.0593654199	-0.0589638061
O	1.1457673541	0.0656226775	-0.0602215953
C	-0.9099948098	-0.9322093816	0.5224813477
H	-0.4340995553	-1.7771147051	0.9968234506
O	1.5875968537	1.4417273497	-0.0937849983
H	-0.6164072454	0.9584511252	-0.4466378903
C	-2.1968002734	-0.5412518972	0.8582683943
H	-2.8295833378	-1.1843515046	1.4481294186
H	-2.6978153891	0.2196004571	0.2808305181
O	0.1161761076	2.0484746871	1.7710745041
H	0.9848389457	1.80999048	0.7823322479
H	0.6364760713	2.2294225999	2.5580333774
O	-1.9021669837	0.7768751324	2.4001133882
H	-0.9988817124	1.3610825708	2.1342167743
H	-2.6294092015	1.4014837692	2.4998470386

anti_Anti-$CH_2CHCHOO$ vinyl insertion 2b vdW

C	-0.0246466842	-0.558070622	-0.6662911151
O	1.1517702241	-0.3491762045	-1.0808307301
C	-0.5818344187	-1.8676467411	-0.7983333524
H	0.0102298553	-2.6225098647	-1.2985460212
O	1.6726735863	0.9275588435	-0.9236733515
H	-0.5772058557	0.2567388102	-0.2067921125
C	-1.796864487	-2.1265097542	-0.293503198
H	-2.2394305973	-3.1087228586	-0.3726897525
H	-2.3573207515	-1.3581496211	0.2226236566

O	0.9583383406	1.8476692035	1.5192533477
H	1.2866855744	1.5635038213	0.6297108741
H	1.6635357133	1.662224141	2.1431492028
O	-1.6846910223	1.055331631	1.5145745098
H	-0.7828975972	1.3963911542	1.6849103573
H	-2.2673038801	1.8134880614	1.6008026851

anti_Syn-$CH_2CHCHOO$

C	-0.4660812677	0.4698466208	-0.1512969925
O	0.7915583659	0.3169924151	-0.1396846746
C	-1.3382935563	-0.5963533471	0.2614094319
O	1.5718443265	1.3588057509	-0.5404018503
H	-0.8318630836	1.4345782311	-0.4849968379
C	-0.9431393468	-1.8062524531	0.6822217295
H	-1.6678235895	-2.551379428	0.974605436
H	0.1019179174	-2.0747112823	0.7427513082
H	-2.3926267658	-0.3578255075	0.2119604497

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 1a TS

C	1.7158388553	-0.1479150043	0.0740802682
H	2.6858712104	-0.5721469961	0.2986488756
O	1.4833000254	1.0469806141	0.5085736645
O	2.6961187644	1.8149063495	0.3039363757
C	0.5772268598	-1.018543344	-0.1772807303
H	0.7913680616	-2.0778353814	-0.2201848946
C	-0.66032529	-0.5560370535	-0.3534387592
H	-0.8702175336	0.503949913	-0.3398295321
H	-1.4881664849	-1.2302552705	-0.5192586672
O	2.4553178668	0.5044558934	-1.6747008996
H	3.2420269165	0.0048647915	-1.9163312587
H	2.7702167484	1.2892234883	-0.9106414423

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 1a vdW

C	-0.2601041537	-0.4309759035	-0.080469974
H	0.5883803232	-0.6497295608	-0.7220550708
O	-0.2974191983	0.7017764089	0.4831831729
O	0.7356356088	1.5874714926	0.2765351251
C	-1.3311452746	-1.3710816074	0.1323950641
H	-1.2180339312	-2.3070267748	-0.3981458484
C	-2.4000191342	-1.1607379985	0.9120208638
H	-2.5358817915	-0.2355950676	1.4540460506
H	-3.16112293	-1.9191120645	1.0205608782
O	2.3219904259	0.3339537912	-1.6283958942
H	2.7330272809	0.8696703839	-2.3101465782

H	1.9072187747	0.9543379004	-0.9948467891

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 1b TS

C	1.6756238118	-0.0782795911	-0.0603509813
H	2.6245378691	-0.5148767946	0.2209877703
O	1.4232685943	1.1179194509	0.3587242704
O	2.6601353993	1.8690929677	0.2459337599
C	0.5521188814	-0.943736908	-0.4014052818
H	0.7997474777	-1.9831179991	-0.5676616295
C	-0.7050273094	-0.5099526406	-0.4944890482
H	-0.9561990299	0.5295679867	-0.3366027695
H	-1.5122299675	-1.1911004009	-0.7220997177
O	2.670979007	0.4703824852	-1.7034270995
H	2.0259286443	0.8102425307	-2.3339277528
H	2.8676096219	1.287759913	-0.9589145202

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 1b vdW

C	-0.2564826035	-0.4308992893	-0.0905798236
H	0.623682164	-0.6603155069	-0.6839503668
O	-0.3132499958	0.7041561507	0.4667814188
O	0.7384662022	1.5788397768	0.3145203022
C	-1.3470153424	-1.359592465	0.0659664098
H	-1.214403608	-2.2984842001	-0.4547615131
C	-2.4548854261	-1.1359148882	0.7850938616
H	-2.6109518518	-0.2075588179	1.3160719565
H	-3.2284065847	-1.8863250364	0.8539474028
O	2.414223192	0.3029519311	-1.4967033495
H	2.8674148904	0.8321596565	-2.1564639227
H	1.9715929636	0.9296476887	-0.888733376

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2a TS

C	1.7649747088	-0.1428065955	-0.3817022017
H	2.6472143043	-0.4695871794	0.154758239
O	1.4381026621	1.093732969	-0.236118939
O	2.5460813147	1.893036106	0.2682191882
C	0.6710881518	-1.1016058727	-0.6129052136
H	0.9909491136	-2.108234998	-0.8447554361
C	-0.6163319141	-0.7853810613	-0.5129467504
H	-0.933996735	0.2168658153	-0.2630631518
H	-1.3825775052	-1.5313252987	-0.6676223143
O	3.8061259078	1.8489536106	-1.8163354583
H	4.7546516794	1.8485432136	-1.666582653
H	3.2840675339	1.9854776462	-0.8340161521
O	2.7044520329	-0.3186556484	-2.0181646227

H	2.0415114977	-0.2327234588	-2.7137925999
H	3.2826012474	0.6205407522	-2.0167839344

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2a vdW

C	-0.285180014	-0.6049652466	0.6700404005
H	0.7309456052	-0.9561996393	0.7908502345
O	-0.5007825403	0.6226646094	0.8530938141
O	0.5932966709	1.4086563297	1.2194079842
C	-1.3704980917	-1.4934854123	0.3333880579
H	-1.0635861883	-2.4946319685	0.0656356345
C	-2.6631263433	-1.1503125106	0.3516198863
H	-2.9832144237	-0.1552464428	0.6267707541
H	-3.4286332583	-1.8670102981	0.0929045397
O	1.9489023233	1.583480253	-1.1250629535
H	2.8662371157	1.8064550797	-0.9496863682
H	1.4850941871	1.6406550513	-0.2537510823
O	1.2217990887	-1.0186118281	-1.6711211408
H	0.9237802783	-1.1022087019	-2.579923737
H	1.5665625904	-0.1033652749	-1.590330024

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2b TS

C	1.7563909956	-0.181614582	-0.3337962076
H	2.5963513812	-0.5286149487	0.256315525
O	1.4651214607	1.0644383436	-0.2103126805
O	2.5816082691	1.8234941857	0.3382660846
C	0.6487529516	-1.0991975148	-0.6363101665
H	0.9440870034	-2.1039825604	-0.9049261558
C	-0.6315720962	-0.7538197865	-0.5534110854
H	-0.9298737883	0.2457140766	-0.2718181913
H	-1.4121777901	-1.4718288062	-0.7591670127
O	3.7749204448	1.8873747497	-1.7702688412
H	3.4517089775	2.5671929635	-2.3666471149
H	3.2575385363	1.9942037094	-0.7715318511
O	2.7332324574	-0.3034649242	-1.9770577923
H	3.4320015987	-0.9639068293	-1.9049949814
H	3.2354955983	0.6920969237	-1.9960195289

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2b vdW

C	-0.4777149566	-0.5130737141	0.3715064246
H	0.5151403676	-0.759946513	0.0041117198
O	-0.6477982432	0.5831762582	0.9764147319
O	0.451490396	1.4033706425	1.1714425738
C	-1.5966529662	-1.3975332982	0.1602581612
H	-1.3610358607	-2.2824213791	-0.4150605974

C	-2.8376051311	-1.1896648828	0.6186218865
H	-3.090910412	-0.3131818777	1.1983203049
H	-3.6255100976	-1.9013431197	0.4206215185
O	1.9755135372	1.5627018071	-1.0724904851
H	1.6796999894	2.3144940652	-1.5906071531
H	1.4424638434	1.5699658237	-0.2410574765
O	1.8193607103	-1.1188284352	-1.6861720355
H	2.6859570758	-1.5252245166	-1.7579552083
H	1.9811107476	-0.1555998601	-1.6232213651

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2c TS

C	1.7839348043	-0.2142056493	-0.3171367622
H	2.6165777622	-0.5870321573	0.267579843
O	1.5238374931	1.037954777	-0.1817871828
O	2.6710742972	1.7679206384	0.3375300838
C	0.6506446124	-1.1006075559	-0.6175902621
H	0.9173626882	-2.1159856384	-0.8761593528
C	-0.619145159	-0.715380484	-0.5494136894
H	-0.889095811	0.2958183666	-0.2812604044
H	-1.4194554327	-1.4110525725	-0.7561707002
O	3.635375174	1.9145197451	-1.880049659
H	4.5871162444	2.0396576979	-1.8876824892
H	3.2550700214	1.9796335076	-0.8100440511
O	2.751311269	-0.3530792739	-1.960018576
H	3.4533585186	-1.0067180457	-1.8666654493
H	3.2375295179	0.6541296446	-2.0165383484

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2c vdW

C	-0.30254014	-0.5761769298	0.6636049346
H	0.7149676656	-0.9159146771	0.8040623432
O	-0.530605282	0.6532293624	0.8172751284
O	0.5523703434	1.4564078992	1.1792792997
C	-1.376251843	-1.4811388826	0.3335956989
H	-1.0577673218	-2.4851740811	0.0913933047
C	-2.6718360161	-1.1488301697	0.3290442129
H	-3.003533615	-0.1508273684	0.5786199091
H	-3.4281467855	-1.8775619604	0.0769840033
O	1.9344787293	1.592054934	-1.1522698249
H	2.8477421219	1.8267088185	-0.9709816036
H	1.4597951203	1.6641069861	-0.2879456459
O	1.23585298	-1.0274772886	-1.6499978099
H	0.9494499416	-1.133338078	-2.5602135961
H	1.5719311012	-0.1077455644	-1.5851103543

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2d TS

C	1.7153299954	-0.1077267497	-0.4197623844
H	2.5848850629	-0.3895128219	0.1616323136
O	1.3411653607	1.1207851321	-0.3223404085
O	2.3910180937	1.9680957189	0.2284884969
C	0.6647468704	-1.109721648	-0.6687154223
H	1.0282123774	-2.1069365063	-0.8752576776
C	-0.6356676241	-0.8399194129	-0.6093601737
H	-0.9967806423	0.1530931297	-0.3826433715
H	-1.3694228376	-1.6159387812	-0.7733464081
O	3.939327048	1.783852176	-1.6376345497
H	3.8593185262	2.4983908311	-2.273816429
H	3.2579444737	1.9874247657	-0.77052269
O	2.7197678665	-0.2958015295	-2.0143974403
H	2.0774332707	-0.2001125746	-2.7272919129
H	3.3124551584	0.6324702708	-1.9775329424

anti_Syn-$CH_2CHCHOO$ carbonyl insertion 2d vdW

C	-0.471619174	-0.5021623879	0.3581269461
H	0.5138893203	-0.757651409	-0.0229044149
O	-0.6191495502	0.5856205172	0.983882141
O	0.4944608402	1.385252111	1.1830115934
C	-1.6060187172	-1.3654527751	0.1418305962
H	-1.3894191301	-2.2434599384	-0.4512309287
C	-2.8393548081	-1.1467759474	0.6154668053
H	-3.0737295773	-0.2769786289	1.212926002
H	-3.6399754927	-1.8426457969	0.4123510381
O	2.000151647	1.5611747009	-1.0720272809
H	1.7112821272	2.3265261133	-1.5739573997
H	1.4749132155	1.5617828614	-0.2356060823
O	1.796827771	-1.1062797723	-1.7315283148
H	2.6563253224	-1.5245715686	-1.8186821512
H	1.9740592061	-0.1469200793	-1.6530845498

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2a TS

C	-0.444691	0.367057	-0.442073
O	0.817284	0.309691	-0.143105
C	-1.359439	-0.434596	0.205614
O	1.425422	1.624332	-0.250464
H	-0.726141	1.1273	-1.163728
C	-0.987888	-1.125373	1.368236
H	-1.723063	-1.741117	1.863563
H	0.037945	-1.435115	1.487447
H	-2.398019	-0.356834	-0.075929

O	-0.867811	0.184697	2.754253	
H	-0.242116	0.993817	2.421652	
H	-0.420914	-0.202487	3.517652	
O	0.61461	2.041906	2.028097	
H	1.038456	1.959601	1.015073	
H	0.229062	2.915409	2.126977	

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2a vdW

C	-0.1231290862	-0.6189762873	-1.6437054898
O	0.2407154723	0.2000252662	-0.7566817915
C	-1.0498679088	-1.6707964376	-1.3267600248
O	1.1514841712	1.178660985	-1.1150404105
H	0.2986333832	-0.4818843728	-2.6344085263
C	-1.5283694453	-1.9073422713	-0.0948599724
H	-2.2229293913	-2.7202178231	0.0642000487
H	-1.2364899113	-1.3128006513	0.765106937
H	-1.3418832338	-2.2873403556	-2.1663658278
O	-0.4978415529	-0.0471089265	2.428355181
H	0.1033014198	0.6685669749	2.1359007817
H	-0.1946535389	-0.2877726927	3.3065836589
O	1.2387109326	1.9615152142	1.5045039836
H	1.3027872966	1.784914924	0.5363183396
H	0.9129603928	2.861165454	1.5834011127

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2b TS

C	-0.4706512412	0.3601023319	-0.4501138005
O	0.7783359544	0.3560019313	-0.1018917227
C	-1.3723013174	-0.4742432607	0.1774190848
O	1.3387756096	1.6943421377	-0.1901806745
H	-0.7561242543	1.1021628215	-1.1891081099
C	-1.0082477086	-1.1291632602	1.3658459164
H	-1.7199849083	-1.7847809714	1.8451827246
H	0.0242785266	-1.3860466099	1.5357464461
H	-2.4004580904	-0.4609983993	-0.1511482354
O	-0.9152953396	0.1354855731	2.7840963885
H	-0.2454037739	0.9228822728	2.50698276
H	-1.787679218	0.5446750088	2.8268217626
O	0.572909633	2.0286776896	2.1345992984
H	0.9719086123	1.9755574647	1.1260302227
H	1.3130423858	2.1780532403	2.727969539

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2b vdW

C	-0.1450158695	-0.5445293693	-1.6669990027
O	0.3203275086	0.1640431656	-0.7335417451

C	-1.0191070096	-1.6478311751	-1.3766260072
O	1.1395136611	1.2261096012	-1.0749983806
H	0.1488767216	-0.2733711767	-2.6760923989
C	-1.456818845	-1.9584523883	-0.1460101508
H	-2.1148612038	-2.8048910067	-0.00816125
H	-1.1808141192	-1.381335222	0.7308984557
H	-1.3211466887	-2.2273289639	-2.2387694501
O	-0.5786436238	-0.0669822267	2.4112615445
H	0.0427477282	0.6425372427	2.1475250443
H	-1.0980152867	0.3060262601	3.1269746925
O	1.1816442505	1.9536281282	1.5615595556
H	1.251756315	1.8056810367	0.5889989538
H	2.0784044612	1.8924740942	1.898887139

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2c TS

C	-0.4840687383	0.3368848936	-0.4938764958
O	0.7682597354	0.3686272918	-0.1593866004
C	-1.3623439376	-0.4898438393	0.1741750254
O	1.3080531734	1.7103699442	-0.3021324804
H	-0.789664174	1.0384712712	-1.2638843335
C	-0.9779214002	-1.0821181138	1.3917203289
H	-1.6643573089	-1.7500899769	1.8905070042
H	0.063539967	-1.2939469869	1.571328282
H	-2.3903642648	-0.5244163648	-0.1536687634
O	-0.9626961633	0.2305791839	2.7466962552
H	-0.2690433558	0.9916165528	2.4641144516
H	-1.8348043178	0.6388690691	2.6932562912
O	0.6816850969	1.9792500114	2.0688055381
H	1.0143507638	1.9834728089	1.0361590904
H	0.5723509341	2.8807770948	2.3763343364

anti_Syn-$CH_2CHCHOO$ vinyl insertion 2d TS

C	-0.436158	0.378848	-0.41224
O	0.824329	0.287341	-0.109258
C	-1.368884	-0.421963	0.20854
O	1.451214	1.596923	-0.174974
H	-0.698844	1.16734	-1.109936
C	-1.014756	-1.158238	1.349105
H	-1.764424	-1.774916	1.82106
H	0.003359	-1.4969	1.455848
H	-2.405016	-0.311018	-0.070515
O	-0.87023	0.09228	2.779621
H	-0.254103	0.921114	2.475081
H	-0.416434	-0.336659	3.515668

O	0.496445	2.033228	2.03567
H	1.004762	1.929342	1.055994
H	1.11583	2.413959	2.661654

syn_Anti-$CH_2CHCHOO$

C	0.4052042055	-0.2826414234	-0.4949473575
H	1.1803652634	-0.5775018896	-1.1915879921
O	-0.6640317954	-0.9575322569	-0.6396390836
O	-1.7297239675	-0.6997447797	0.1671916737
C	0.5864903833	0.7529967827	0.471242511
H	-0.2562113843	0.9609604659	1.1135459638
C	1.7464965267	1.4191531605	0.560651349
H	2.5820334315	1.1980996638	-0.0913975931
H	1.8888243368	2.2033692767	1.2897005289

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 1a TS

C	1.8860798124	-0.1312195438	-0.1293091949
O	1.4765534803	0.9923974453	0.3720571987
O	2.5973346467	1.9165203348	0.3056160537
O	2.5345609481	0.7252725553	-1.779538316
H	3.3729459418	0.3244247993	-2.0311719345
H	2.7490273307	1.4886161677	-0.9988674458
H	1.0703585872	-0.751359362	-0.4890311868
C	3.1088213741	-0.7923449986	0.3153651257
H	3.8101798925	-0.1740078547	0.856101595
C	3.2996956741	-2.0949936258	0.1078878367
H	2.5844377998	-2.6956908147	-0.4400819694
H	4.1770685124	-2.6014951029	0.4835732376

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 1a vdW

C	-0.7235341757	-0.5086460954	0.7467297706
O	-1.0279200003	0.7224007925	0.7545739474
O	-0.0706897072	1.6482245747	0.3958455701
O	0.514069051	0.8655995432	-2.1982728235
H	0.2684458293	1.5014489134	-2.8738848873
H	0.3160455732	1.3003743266	-1.3446267376
H	-1.5525140893	-1.1382087309	1.0499805614
C	0.5488269373	-1.0523141096	0.3950431987
H	1.3180250671	-0.3622971146	0.086495401
C	0.7444973047	-2.3773367545	0.4431845368
H	-0.041542343	-3.0587911709	0.7429085421
H	1.696558553	-2.8131421744	0.1780219205

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 1b TS

C	1.8809427597	-0.125053994	-0.1574443026
O	1.4454515348	0.9848585656	0.3598338114
O	2.5442783227	1.9367277536	0.2962157148
O	2.618662916	0.7353328861	-1.783148448
H	1.8712041848	1.029705846	-2.3172397308
H	2.7521990739	1.5085645811	-0.9834074554
H	1.0771403622	-0.7647321642	-0.5125702906
C	3.1201891372	-0.7655961424	0.2610040921
H	3.8413547704	-0.1353004802	0.7585674261
C	3.3035861666	-2.0714876623	0.0768966467
H	2.5729458702	-2.6829943681	-0.4374162727
H	4.1936259017	-2.5697668212	0.4329608088

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 1a vdW

C	-0.7121901217	-0.5306465462	0.7407159548
O	-1.0386636086	0.6945382214	0.7636573802
O	-0.0988873134	1.6416401865	0.4144535685
O	0.4952530812	0.9004667122	-2.1896882115
H	0.2370316447	1.5397499277	-2.8573149661
H	0.2909535348	1.3214582801	-1.330629554
H	-1.5291669812	-1.1785886273	1.0377643913
C	0.5691205685	-1.0471012219	0.3806065546
H	1.3252280652	-0.3397326501	0.0790736041
C	0.7886873321	-2.368861427	0.4126997233
H	0.0155712666	-3.0678684263	0.7055373029
H	1.7479635319	-2.784273429	0.140890252

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2a TS

C	2.0104792685	-0.2668680202	-0.342890368
O	1.532643445	0.9199121463	-0.1275329548
O	2.5334380632	1.8845243193	0.3001658466
O	3.6232167575	2.0147007046	-1.864417179
H	4.5759566328	2.1107862662	-1.795487027
H	3.1552423755	2.0683285273	-0.8226141835
O	2.7264691884	-0.2347674452	-2.1024635285
H	1.9660404005	-0.1351411353	-2.6882993437
H	3.2200539966	0.7648929323	-2.0874991726
H	1.2167558764	-0.9623826164	-0.5913511711
C	3.1591688791	-0.7910208478	0.4028104857
H	3.7789600181	-0.053570144	0.8880777405
C	3.365970279	-2.0989273286	0.5186460019
H	2.7334477853	-2.8256191694	0.0247318343
H	4.1824480342	-2.4859291891	1.1113420191

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2a vdW

C	-0.8345911451	-0.5851784287	0.6083569412
O	-1.1480183517	0.6390459485	0.5694229105
O	-0.2210289167	1.5678295377	1.0403147924
O	0.9395329886	1.8509845986	-1.4163488316
H	1.8615184788	2.1058078494	-1.336899469
H	0.5607543253	1.9044189383	-0.5072471478
O	0.1332644802	-0.7204793211	-2.1833243583
H	-0.2825204813	-0.664065942	-3.0468295015
H	0.480574746	0.1773384571	-2.0087660548
H	-1.5917712259	-1.2255545621	0.1738925505
C	0.3678549263	-1.1087138702	1.1766694259
H	1.0361013516	-0.4006715072	1.6413454142
C	0.6208879235	-2.4216595327	1.1138036888
H	-0.055503299	-3.1062370592	0.6191649145
H	1.5198851995	-2.8420851062	1.5407417251

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2b TS

C	2.069636026	-0.3197570684	-0.3619460514
O	1.6089776513	0.8716828395	-0.1554013287
O	2.6330846837	1.8165641552	0.2709231612
O	3.479355221	2.1045428721	-1.9845078618
H	2.96440108	2.7262834709	-2.504680843
H	3.102886379	2.1136885109	-0.9220444343
O	2.791275918	-0.2296649534	-2.1088383368
H	3.5847545972	-0.775676851	-2.144239972
H	3.1164735781	0.8340210588	-2.1709027884
H	1.2727581213	-0.9968400849	-0.6460567526
C	3.1951297787	-0.8695399448	0.404098661
H	3.8840041186	-0.1476811271	0.8146756516
C	3.3024447286	-2.1792953351	0.613097468
H	2.5885055946	-2.8848279932	0.2060644941
H	4.1060765239	-2.5877115497	1.209144933

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2b vdW

C	-0.7908499287	-0.668789559	0.604031374
O	-1.0917345582	0.5525560236	0.4868240468
O	-0.184469972	1.4994022111	0.9607497687
O	0.8492175913	2.0198169876	-1.5054595997
H	0.4049370368	2.7668436545	-1.9135415717
H	0.5061779632	1.9770507797	-0.5815470073
O	0.1055423028	-0.5962989887	-2.1709926441
H	0.7682392175	-0.9884331094	-2.7439250065
H	0.3798050062	0.3368931103	-2.0598027288

H	-1.5372377476	-1.3262897989	0.1757237158
C	0.3855704028	-1.1680636649	1.2458143802
H	1.0734544885	-0.4362116749	1.6396976066
C	0.5856585131	-2.4880878292	1.3416354795
H	-0.1174968197	-3.200034333	0.9289509584
H	1.461662504	-2.8901918087	1.829711228

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2c TS

C	2.2021599855	-0.233371397	-0.2658387057
O	1.8002950438	0.9837609764	-0.0835480758
O	2.8957321101	1.9188004445	0.133680819
O	3.2314672177	2.0942907424	-2.264421048
H	4.1159061658	2.3665463573	-2.519609789
H	3.1293793524	2.161818734	-1.1425974582
O	2.7285942254	-0.2831138288	-2.0703488977
H	3.5207214278	-0.8279939349	-2.1327699805
H	3.0185673578	0.7758067767	-2.2719257826
H	1.3583443388	-0.8978505921	-0.4104588843
C	3.3879716068	-0.7728998525	0.4143845468
H	4.1239532146	-0.0456417841	0.7208632515
C	3.4948521028	-2.0725927898	0.6786540409
H	2.734179882	-2.7826638737	0.3780747772
H	4.3456169688	-2.4675879784	1.2154791864

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2c vdW

C	-0.7680345128	-0.5521973944	0.7543205486
O	-1.1296784485	0.6551090875	0.6538094156
O	-0.1906776277	1.6459254176	0.9370914949
O	0.6710656549	1.7534651976	-1.6529100068
H	1.5858653241	2.0398368893	-1.7022780241
H	0.3965481582	1.8726808027	-0.7131108126
O	-0.1200538452	-0.8950950467	-2.1111744026
H	-0.6333085385	-0.9233558871	-2.9220206997
H	0.2108693239	0.0236310512	-2.051140963
H	-1.5451501136	-1.2479101069	0.4640836721
C	0.5101539283	-0.9920168514	1.2187962784
H	1.1998748696	-0.2288541523	1.5438636401
C	0.8035788822	-2.2979691433	1.2327238287
H	0.1014761979	-3.0405134911	0.8770576974
H	1.7605277471	-2.6555183726	1.5843443331

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2d TS

C	1.9632930486	-0.3114865429	-0.3295219207
O	1.4810528525	0.8802004609	-0.1522512619

O	2.4788489631	1.8711080382	0.2171132906
O	3.7789840719	1.7604998943	-1.8201309335
H	3.6134983626	2.4769938348	-2.437142538
H	3.1744571201	1.9303341763	-0.8498770309
O	2.6015152689	-0.3468783889	-2.1280519137
H	1.8145549372	-0.1891239833	-2.6631820436
H	3.1707786183	0.6123097594	-2.123913484
H	1.1690237806	-1.0254154052	-0.5151004204
C	3.1537347356	-0.7943543706	0.3746668482
H	3.8395227107	-0.0409353168	0.7281055251
C	3.3276951513	-2.0923986325	0.6024759547
H	2.6296451048	-2.8367296161	0.2407487212
H	4.1804472738	-2.4529139077	1.1596072069

syn_Anti-$CH_2CHCHOO$ carbonyl insertion 2d vdW

C	-0.8728651884	-0.5156312724	0.6449847304
O	-1.2310442808	0.6960218169	0.5856584356
O	-0.3027558195	1.670387926	0.9544272443
O	1.1995196439	1.5427135957	-1.2986076795
H	1.1947083855	2.3672231537	-1.7901992563
H	0.688460901	1.7184049427	-0.4709372115
O	-0.0389931952	-0.8349047857	-2.161930048
H	-0.4669943386	-0.7206740103	-3.0135057057
H	0.4359146732	0.0035578641	-1.9955734461
H	-1.6358853217	-1.1960126744	0.288464459
C	0.3840758371	-0.9794081679	1.142305567
H	1.0582100118	-0.2372739395	1.5405583685
C	0.6819086564	-2.2835012926	1.0897946409
H	0.0010058802	-3.0035750544	0.6556014294
H	1.623862155	-2.6595861018	1.4618694721

syn_Anti-$CH_2CHCHOO$ vinyl insertion 1a TS

C	0.3729533754	0.1452428281	-0.3951727235
H	1.0315904068	0.011915925	-1.2487147578
O	-0.8354718872	-0.263613404	-0.6524023163
O	-1.8142653913	0.4023939171	0.1704633479
C	0.7216242085	0.7829459486	0.7891071283
H	0.0975212589	0.558600114	1.6434993866
C	1.1501988525	2.0857246478	0.6588242051
H	1.6303041977	2.4323378867	-0.2441020236
H	1.2214903814	2.7294924132	1.5210734556
O	-0.7577254039	2.6438212335	0.0188759301
H	-1.4536105545	1.4609498461	0.1186955002
H	-1.2170522044	3.4702945239	0.2091055174

syn_Anti-$CH_2CHCHOO$ vinyl insertion 1a vdW

C	0.7060397744	-0.8010849788	-0.4333574221
H	1.4430775432	-1.2063966211	-1.1174724881
O	-0.469870746	-1.1855567526	-0.7119321152
O	-1.5165134389	-0.7546341531	0.0760791305
C	1.0700763004	0.05802314	0.6471925216
H	0.2772813915	0.4351864622	1.2734681959
C	2.3572881753	0.3769062059	0.8413317246
H	3.1410212678	0.0004494934	0.1962600029
H	2.6575706011	1.0281248296	1.6490452817
O	-1.3522072154	1.994454335	-0.2386764216
H	-1.5786057702	1.0479460601	-0.1395227846
H	-2.0995628834	2.3916929794	-0.6911666255

syn_Anti-$CH_2CHCHOO$ vinyl insertion 2a TS

C	0.4369376405	-0.2556434263	-0.396262246
H	1.1731210469	-0.4851175896	-1.1616163478
O	-0.6544567383	-0.9350006431	-0.5783055612
O	-1.7594452749	-0.4350419483	0.1932332596
C	0.6592401657	0.6703711087	0.5962351473
H	-0.0612852901	0.7289447947	1.3965345881
C	1.5158743265	1.7417013914	0.3648332603
H	2.236042419	1.6870194223	-0.441048951
H	1.7726684558	2.4126480989	1.1678679733
O	0.3625475437	3.0983689264	-0.428421959
H	0.6705145571	3.2888288979	-1.3216125173
H	-0.6202394616	2.5672296009	-0.5257783651
O	-1.7252996717	1.8452577544	-0.6509174257
H	-1.8079385703	0.7104592268	-0.2141580392
H	-2.5533141883	2.318469815	-0.5489314062

syn_Anti-$CH_2CHCHOO$ vinyl insertion 2a vdW

C	0.7475260987	-1.4621879929	0.1606787628
H	1.437561806	-2.251947776	-0.1167670604
O	-0.4566855733	-1.8598425501	0.1532522299
O	-1.4557197596	-0.9640292819	0.4976381443
C	1.1970291459	-0.1469034522	0.4777532678
H	0.471274104	0.6050985528	0.7473493753
C	2.504871899	0.1417366874	0.4020474933
H	3.240672538	-0.6006410335	0.1186888145
H	2.8605332157	1.1393102035	0.6146457812
O	0.0045251899	2.8487658168	0.1477327953
H	-0.5341285284	3.4722606898	0.6399337018

H	-0.6175246638	2.3643304691	-0.4271664157
O	-1.5570510617	1.0415719267	-1.3244928127
H	-1.6064057032	0.2835215161	-0.6952260471
H	-2.4165037074	1.0992892244	-1.7473970303

syn_Anti-$CH_2CHCHOO$ vinyl insertion 2b TS

C	0.4973677897	-0.2589652322	-0.4077180661
H	1.2805420084	-0.4484466955	-1.1362601616
O	-0.5636012383	-0.9598878527	-0.6665661114
O	-1.7228200761	-0.5156231846	0.059694637
C	0.6410006832	0.6511375685	0.6145649701
H	-0.1250444766	0.6813388724	1.3732504994
C	1.4775338022	1.746221438	0.4307637473
H	2.2434111584	1.7200380042	-0.3304908404
H	1.6644770231	2.4231451393	1.2503515282
O	0.3724343263	2.9989822289	-0.5701881632
H	0.2428078478	3.8068717394	-0.0605097461
H	-0.6235926227	2.4764504109	-0.6261588417
O	-1.766888229	1.8122472685	-0.6377152028
H	-1.7904714407	0.6481618362	-0.305700324
H	-2.2732911358	1.9329490886	-1.444362305

syn_Syn-$CH_2CHCHOO$

C	0.7649524651	-0.4023726008	-0.5514802227
H	1.5245304826	-0.8772098767	-1.1599139207
O	-0.3582342471	-0.9939212872	-0.6831049297
O	-1.43930077	-0.5410407993	0.0051385692
C	1.0859508727	0.7281929335	0.2525999871
H	2.1237605436	1.0294667745	0.1784701939
C	0.2519170882	1.4190032789	1.0559419421
H	-0.7835452194	1.14282359	1.1494166527
H	0.6337467844	2.2638949871	1.6138357282

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 1a TS

C	1.8927194096	-0.0521068357	-0.03122508
O	1.4610263316	1.128746787	0.2737851309
O	2.5099375922	2.087419324	-0.0538709367
O	2.4049529269	0.4853911888	-1.8596158024
H	3.2606535918	0.09927416	-2.073967372
H	2.6107546044	1.3947855614	-1.2616960166
H	1.0706685231	-0.7377308508	-0.2200516378
C	3.1476224005	-0.667697168	0.4166663836
H	3.2337556982	-1.7157927876	0.1554425012
C	4.0755030827	-0.080199092	1.1716112134

H	4.0044935276	0.9668415363	1.4254957308
H	4.9147503114	-0.6512238234	1.5441008856

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 1a vdW

C	-0.7167941752	-0.8593847335	0.8672908568
O	-0.7773037657	-0.1993532734	-0.219515842
O	0.3766604555	0.2977963975	-0.760131888
O	-0.3932353738	1.0934652393	-3.3975980903
H	-0.4179053432	2.0526767401	-3.3841074181
H	-0.1235789067	0.8354027987	-2.4978036629
H	-1.703653845	-1.1859567856	1.1722249564
C	0.4242176388	-1.1866844477	1.6548571682
H	0.1861443781	-1.7658625606	2.538321924
C	1.7067812729	-0.8563837918	1.4035628045
H	1.9743653443	-0.28245436	0.5339858126
H	2.4795563199	-1.1771472229	2.0895413788

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 1b TS

C	1.8904510042	-0.0090478623	-0.0480131955
O	1.4743421438	1.1715783167	0.2844967856
O	2.5248853084	2.1268639808	-0.0561254538
O	2.4838789591	0.5173695641	-1.8661365007
H	1.6937199111	0.6997708708	-2.38884422
H	2.6607807934	1.4236561967	-1.257307719
H	1.0605967894	-0.6905101879	-0.2247871543
C	3.155243114	-0.6346848799	0.3428400357
H	3.2761619615	-1.6448252477	-0.0259514633
C	4.0558835185	-0.0905299651	1.1582343023
H	3.9524054742	0.9259265552	1.5070172699
H	4.9130070224	-0.6637213413	1.4829013132

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 1b vdW

C	-0.7131478991	-0.8637302803	0.8567350137
O	-0.7789446392	-0.1829964943	-0.2169149761
O	0.3750656272	0.3036220979	-0.76693246
O	-0.4218695062	1.1607317706	-3.3769735378
H	-0.429213972	2.1198218563	-3.3458352572
H	-0.1427508274	0.8815810231	-2.486407158
H	-1.7007618501	-1.1784531916	1.1715277241
C	0.4340783154	-1.2253299215	1.6198939954
H	0.1996238913	-1.816282808	2.4965022458
C	1.7182218019	-0.9130472307	1.3540520937
H	1.9823035257	-0.3281129878	0.490760137
H	2.4958355327	-1.2597958336	2.0216741793

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2a TS

C	1.9854212336	-0.1286535049	-0.2669644299
O	1.490858831	1.066567139	-0.2016965752
O	2.4474442825	2.1229231538	0.0869123619
O	3.6114342386	1.9316500584	-2.0413232551
H	4.5621220914	2.0206428373	-1.9383757816
H	3.1149602591	2.1344990406	-1.0454829935
O	2.7335862776	-0.3367704747	-1.99565163
H	1.9876746534	-0.3377176894	-2.6074402308
H	3.215607225	0.6656451743	-2.1019546062
H	1.1839296008	-0.8376218091	-0.4524523983
C	3.1174830166	-0.6609287132	0.5079153447
H	3.3599718946	-1.6842827879	0.2539879811
C	3.7482625841	-0.0378624913	1.4995095194
H	3.5235376723	0.9863521759	1.7508286375
H	4.5011561395	-0.5642941088	2.0704520558

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2a vdW

C	-0.9711241339	-0.7375277391	0.5911906873
O	-1.1865474529	0.4851953572	0.3320142347
O	-0.2618607424	1.433361898	0.7394958817
O	0.815755723	1.5465177968	-1.8080579206
H	1.7206456664	1.8668595184	-1.7951647122
H	0.467683493	1.6831567683	-0.8996525179
O	0.2589406869	-1.2078751371	-2.0578214878
H	-0.0584837152	-1.3887712915	-2.9455270759
H	0.5124302627	-0.2639313116	-2.0629742141
H	-1.7530464167	-1.3619126644	0.1782770322
C	0.1019704064	-1.3352318379	1.3186540428
H	0.0543937674	-2.4161604981	1.3400824241
C	1.1049268558	-0.6994968483	1.9503942795
H	1.1753439137	0.374097963	1.9403236911
H	1.8489686857	-1.2788379737	2.4809796552

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2b TS

C	2.1545774283	-0.155410118	-0.1893383061
O	1.7630124625	1.0743580115	-0.0848468432
O	2.8370332665	2.0438013989	0.0673134397
O	3.3380509949	1.982412618	-2.3034267735
H	2.7382490309	2.5222632435	-2.8243475185
H	3.1302531657	2.1555885013	-1.2070327873
O	2.6809560317	-0.3411695288	-1.9982382167
H	3.4946012134	-0.8567022817	-2.0368293368

H	2.9712851252	0.7163926793	-2.2479672491
H	1.2862772842	-0.7912879433	-0.3225459897
C	3.2903484932	-0.7825146108	0.505517152
H	3.3274202627	-1.8570029838	0.3654916069
C	4.1661801325	-0.1837428733	1.3101190822
H	4.1453119254	0.8835723446	1.4600658251
H	4.9082851829	-0.7756154574	1.828978915

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2b vdW

C	-0.8519839221	-0.7730021145	0.7341395166
O	-1.1132413343	0.4398245969	0.4727262045
O	-0.1566909867	1.4070815897	0.7422799328
O	0.6332398051	1.5380768207	-1.8907643751
H	0.1534294026	2.2187521985	-2.3689015173
H	0.3862715132	1.6517650944	-0.9459466115
O	-0.2149881039	-1.1434576287	-2.0999668574
H	0.3907017958	-1.6355301676	-2.6587759423
H	0.0904818551	-0.2155449592	-2.1420614199
H	-1.6691057918	-1.4159782003	0.4326083435
C	0.3076016639	-1.3386274242	1.3457835668
H	0.265863675	-2.4173734274	1.4248541257
C	1.3824510024	-0.6777744523	1.8124727665
H	1.4505711221	0.393601945	1.7407061191
H	2.1901783037	-1.2346888709	2.268894148

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2c TS

C	2.1810112322	-0.1512947688	-0.1939239076
O	1.8173325942	1.086500694	-0.0842426443
O	2.9152327449	2.0273031003	0.0781061045
O	3.211239722	2.0313321591	-2.3289167876
H	4.0889653239	2.2846035993	-2.624087259
H	3.1342348617	2.1823919338	-1.2124141522
O	2.76185923	-0.3377600015	-1.9763133669
H	3.5918761591	-0.8272283462	-1.968056303
H	3.0170948509	0.7254269884	-2.2428421258
H	1.3004453949	-0.7642174086	-0.3537876346
C	3.2800876507	-0.8110854933	0.5321571089
H	3.311358588	-1.8827017069	0.3701488458
C	4.1217128326	-0.2391037646	1.3904003587
H	4.1012909978	0.8249695319	1.5635378208
H	4.8339518172	-0.8480625168	1.9309179422

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2c vdW

C	-0.8985039044	-0.7377207953	0.7228942602

O	-1.1459057997	0.4858532163	0.498637841
O	-0.1728989998	1.4321409049	0.7777497462
O	0.545355025	1.550807075	-1.8932262811
H	1.4438657413	1.8702898775	-2.0037708879
H	0.3253050771	1.6854507428	-0.9453475701
O	-0.0438716883	-1.2024378383	-2.0708858821
H	-0.4802433784	-1.3807852636	-2.9071124156
H	0.2076891368	-0.25871273	-2.1084826943
H	-1.73043651	-1.3603433671	0.4196022324
C	0.2634572283	-1.3382472005	1.2949075353
H	0.2179206981	-2.4191833813	1.3200654952
C	1.3443552668	-0.705031629	1.7846768163
H	1.4140646768	0.3685210418	1.7676196173
H	2.1533994304	-1.2863956531	2.2068361874

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2d TS

C	2.1075364452	-0.1958165101	-0.2418368686
O	1.60490347	0.9916233802	-0.1060702792
O	2.5730138599	2.0636526347	0.0554714333
O	3.6289566973	1.8144734802	-2.1134186323
H	3.3112815375	2.4448230238	-2.7644162016
H	3.1505305952	2.0442435905	-1.1022724553
O	2.5992072424	-0.3885672962	-2.0675949603
H	1.7660847721	-0.3639073382	-2.5524640167
H	3.0894466544	0.6083723309	-2.2185850843
H	1.2997810083	-0.9175878104	-0.3160282244
C	3.3468797655	-0.7102352419	0.3577193809
H	3.5515281396	-1.7368099395	0.0843037294
C	4.1295365003	-0.0684378695	1.2210223699
H	3.9483849755	0.9604608222	1.4865507226
H	4.9675613369	-0.5848732568	1.6690250867

syn_Syn-$CH_2CHCHOO$ carbonyl insertion 2d vdW

C	-0.8698318468	-0.7621005994	0.6954721453
O	-1.1009408298	0.4580764773	0.4399373549
O	-0.1339926911	1.4040725276	0.7454468365
O	0.7296420436	1.546388948	-1.8637590657
H	0.275968134	2.240906714	-2.3474709224
H	0.4592260889	1.6552807035	-0.9248146251
O	-0.1630584588	-1.1161551925	-2.124154131
H	0.4481986482	-1.6140995202	-2.6715839279
H	0.1609212435	-0.1938932358	-2.1481605229
H	-1.6904372859	-1.3862406526	0.3651946569
C	0.2617985899	-1.3559577682	1.3322019881

H	0.1975695254	-2.4344469406	1.3987064084
C	1.3358351326	-0.7205433756	1.8347160615
H	1.4260956939	0.3499988477	1.7761469579
H	2.1201880125	-1.2973909332	2.3068757855

syn_Syn-$CH_2CHCHOO$ vinyl insertion 1a TS

C	0.893647	-0.44015	-0.563702
H	1.682934	-1.038169	-1.007893
O	-0.252428	-0.844493	-1.002048
O	-1.413677	-0.116902	-0.606981
C	1.219997	0.630103	0.2527
H	2.259185	0.925689	0.2201
C	0.322096	1.412519	0.978303
H	-0.570146	0.972604	1.38572
H	0.710809	2.277892	1.496228
O	-0.795478	2.263572	-0.414051
H	-1.543258	2.756892	-0.051907
H	-1.135114	1.263798	-0.628229

syn_Syn-$CH_2CHCHOO$ vinyl insertion 1a vdW

C	1.1823939681	-0.6797111893	-0.3153734341
H	1.6868443463	-1.263839531	-1.0755368935
O	0.1622238723	-0.0938279598	-0.8016247608
O	-0.6045708528	0.6919794395	0.0141911225
C	1.6864055472	-0.6442544986	1.0165531036
H	2.5800401157	-1.2399750015	1.155009656
C	1.173357382	0.0353257294	2.0616135438
H	0.2873476797	0.6359575644	1.9549948483
H	1.6645740156	-0.0245526227	3.023776001
O	-2.2907858115	2.1161984782	-1.8053671075
H	-3.1627709293	1.7265187263	-1.7122646504
H	-1.7283833331	1.629087865	-1.1765794287

syn_Syn-$CH_2CHCHOO$ vinyl insertion 1b TS

C	0.914422	-0.537038	-0.514713
H	1.714204	-1.14106	-0.93143
O	-0.224421	-0.983341	-0.925482
O	-1.406051	-0.279808	-0.551803
C	1.222643	0.583392	0.243435
H	2.258505	0.891148	0.202053
C	0.309921	1.378787	0.936264
H	-0.576441	0.94763	1.364563
H	0.673985	2.276464	1.415842
O	-0.94906	2.158085	-0.389119

H	-0.424396	2.493716	-1.125463
H	-1.198087	1.151493	-0.611236

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2a TS

C	-0.8096010309	0.7213023564	0.9565127595
O	-0.0080525867	-0.0293838122	1.6434566619
O	0.2199918998	-1.3409591139	1.1226363281
O	1.782201944	-1.0380210164	-0.7640627044
H	2.3568442587	-1.798206535	-0.8815577014
H	1.1996972445	-1.1831746541	0.1239200784
O	-0.1162280477	-0.6048989854	-2.2835474666
H	-0.0365189214	0.3207966464	-2.5440764116
H	0.7503966553	-0.8244381019	-1.705821192
H	-0.9260655507	1.6742025604	1.4640312957
C	-1.4824663819	0.5212381431	-0.2296383971
H	-2.0555887297	1.3764670859	-0.5623700564
C	-1.4857535615	-0.6352398277	-1.042421726
H	-1.170730221	-1.5634947588	-0.5998827751
H	-2.2602590409	-0.7063979468	-1.792196803

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2a vdW

C	-0.7655893034	1.1466139918	1.3725689218
O	0.1026322613	0.3575565778	1.8662836589
O	0.3034599781	-0.8690351623	1.2615248843
O	2.2176510799	-0.6674124168	-0.69038147
H	2.8324412045	-1.4019363595	-0.6244421926
H	1.616753395	-0.7483651088	0.0837147179
O	0.3665541389	-0.4189835432	-2.7944420999
H	0.7305401714	0.1593465915	-3.4685165207
H	1.0774042299	-0.5250082962	-2.1330735295
H	-0.8250718995	2.0570971388	1.9585366876
C	-1.5855131957	0.9944032276	0.2216369389
H	-2.2021884701	1.8605703567	0.0171320693
C	-1.6372510384	-0.0678704153	-0.6099089941
H	-1.0493245762	-0.9489292534	-0.4333898981
H	-2.2844449757	-0.0402703286	-1.4744341739

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2b TS

C	-0.7988710937	0.7168506852	0.9186541239
O	0.0090879955	-0.0160341507	1.6213999626
O	0.2603699158	-1.3347740216	1.123941473
O	1.7945948387	-1.0529256921	-0.7752701204
H	2.5062991437	-0.4262879734	-0.6260138989
H	1.2168828579	-1.1599840615	0.1315139262

O	-0.083908121	-0.5478805367	-2.2834407737
H	-0.1468795205	-1.303069591	-2.8823958272
H	0.7901674038	-0.7091102181	-1.6872693859
H	-0.9221786258	1.6769780728	1.4108370316
C	-1.4664423235	0.4959051495	-0.2637299861
H	-2.0242845722	1.3482988746	-0.6254133919
C	-1.4620282037	-0.6742961055	-1.0518510972
H	-1.144218909	-1.5899499773	-0.5837074952
H	-2.236508786	-0.753720454	-1.8016895407

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2b vdW

C	-0.7542799954	1.1843861433	1.2354717963
O	0.1302777834	0.476016111	1.8160098785
O	0.3400641767	-0.8199956767	1.3794459667
O	2.1491673616	-0.8415588863	-0.6771656552
H	3.0017940229	-0.4757138485	-0.4322159991
H	1.5972292027	-0.8334793537	0.1364594322
O	0.3764517021	-0.1252211252	-2.7344171773
H	0.5605457884	-0.6905295339	-3.4883874142
H	1.0694623599	-0.3379314767	-2.0807776645
H	-0.8163461588	2.1633883958	1.6977710543
C	-1.5880155821	0.8761546315	0.1278312358
H	-2.2165905027	1.7020220794	-0.1798305617
C	-1.6331789331	-0.2830665358	-0.5617220928
H	-1.0295884947	-1.1261093147	-0.2798967007
H	-2.290713731	-0.3696366097	-1.4141900983

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2c TS

C	-0.7651777169	0.7073711503	0.9253910869
O	-0.0147092158	-0.0671119326	1.6469986734
O	0.1986185957	-1.3849976177	1.1284689079
O	1.739516885	-0.985332881	-0.7332392677
H	2.4159137706	-1.6587908938	-0.8320308289
H	1.147226901	-1.1917783829	0.1574400831
O	-0.1469981238	-0.6782059155	-2.276615831
H	-0.2700400444	-1.4574190706	-2.8332707578
H	0.7373043123	-0.8443702305	-1.6874946774
H	-0.842479949	1.6753811531	1.411119029
C	-1.4252875102	0.5173983947	-0.2664243346
H	-1.9207609316	1.4000223522	-0.6457135569
C	-1.5065510362	-0.6665240183	-1.0319338167
H	-1.2560651971	-1.5914793585	-0.5418356295
H	-2.2949119996	-0.706014839	-1.7706623798

syn_Syn-$CH_2CHCHOO$ vinyl insertion 2d TS

C	-0.8441998126	0.744621478	0.9478886025
O	0.009173303	0.0474197435	1.6298420241
O	0.274918567	-1.2734267499	1.1511810198
O	1.7826455487	-1.1168207103	-0.7936169746
H	2.5915021852	-0.6171307329	-0.6650203515
H	1.2341767514	-1.1539533121	0.122138677
O	-0.0898992061	-0.4946939833	-2.2829045443
H	-0.0670099068	0.4478287035	-2.4874326495
H	0.7823138359	-0.7055026947	-1.7171376987
H	-1.0039989027	1.6961994653	1.4463267693
C	-1.5235831491	0.4949089142	-0.2243212298
H	-2.1586051608	1.3081788572	-0.5500874948
C	-1.4466659449	-0.655191957	-1.0437268506
H	-1.0623277343	-1.5612524575	-0.6091014829
H	-2.216086954	-0.778971904	-1.7917799359

anti-CHCCHOO

C	0.4333782279	-0.1654038816	-0.0686382025
H	0.2984471888	0.9086274428	-0.1224781485
O	-0.5654099176	-0.8636440526	0.298988616
O	-1.7114899042	-0.217412026	0.5925922704
C	1.6374952816	-0.8066959963	-0.3804643716
C	2.7039261319	-1.2872504251	-0.6643779965
H	3.6384949915	-1.7276900612	-0.9114781673

anti-CHCCHOO 1a TS

C	1.0677812171	0.2163912086	-0.056088682
H	1.1512720592	0.6285466021	0.9418090416
O	0.0070226965	-0.4666725672	-0.3379197453
O	-1.0982253847	0.2428932391	0.2688849976
O	0.3094467042	1.9239245207	-0.694231201
H	-0.5652299722	1.3888947176	-0.246750681
H	0.5554880769	2.6352539866	-0.0931477877
C	2.247062497	-0.0769747166	-0.7888100447
C	3.2732280257	-0.3049589029	-1.3660432431
H	4.1726178605	-0.5154196481	-1.8910355846

anti-CHCCHOO 1a vdW

C	0.4359333108	-0.1523594893	-0.0680742428
H	0.3120154023	0.9262265991	-0.1298698881
O	-0.5553819148	-0.8625470069	0.2922234752
O	-1.7277604614	-0.2415118892	0.6020536721
O	-1.1674239563	2.4480711541	0.0956736035

H	-1.6223564282	1.6113701138	0.3104360364
H	-1.8190430598	3.0226597717	-0.3121300833
C	1.6366710072	-0.8039185639	-0.3803922434
C	2.7000128704	-1.2906892872	-0.6628333873
H	3.6333522298	-1.7346704023	-0.9089639424

anti-CHCCHOO 1b TS

C	0.0401651525	1.0243142173	0.1312591549
H	0.0341837791	0.9072707408	1.2071739684
O	-0.8148641053	0.3461126998	-0.5648865983
O	-0.8692674348	-0.9671119506	0.0386551831
O	1.4514617468	-0.3518300553	0.1667250335
H	0.5060533327	-0.9332764914	0.1407241835
H	1.8354271925	-0.3958206647	-0.7171392906
C	0.5220642807	2.234110302	-0.4361861156
C	0.9424646415	3.2695703128	-0.8719404356
H	1.3081259842	4.1856763393	-1.2669711033

anti-CHCCHOO 1b vdW

C	0.0599710783	0.4611761934	-0.0398148512
H	0.941009442	-0.0905936069	0.2793092596
O	-1.0437757476	-0.1601483199	-0.1519905863
O	-1.0809947847	-1.4885506806	0.1482092275
O	1.5789072455	-2.0655436476	0.7776788141
H	0.6252880768	-2.143112441	0.5833806343
H	1.9876629346	-2.8879965878	0.4991930941
C	0.0830880869	1.8279441331	-0.3484502363
C	0.1813298995	3.0016293085	-0.5938601411
H	0.2528597688	4.0386076488	-0.8138182146

anti-CHCCHOO 2a TS

C	1.2362085021	-0.301335993	-0.2272840059
H	1.9312876855	-1.0260656951	-0.6323871257
O	1.6935594456	0.8894939489	-0.0231134575
O	2.8559987577	1.1462053237	-0.8548305668
O	0.2553153178	-0.3011197225	-1.8100464434
H	-0.6120437571	0.0604534852	-1.5903108929
H	0.7831185309	0.4489384704	-2.4148793075
O	1.5692431415	1.4338411424	-2.9230581553
H	2.2366847131	1.4076658586	-2.0572654813
H	2.0696131664	1.1731407285	-3.7004910251
C	0.2470742338	-0.7435013633	0.7133399607
C	-0.5578456871	-1.1481564425	1.5029575628
H	-1.2666841902	-1.4999047113	2.2116496979

anti-CHCCHOO 2a vdW

C	0.2231437661	-0.6082065984	0.7735203391
H	0.6329007907	-1.3237715771	0.073754312
O	0.7150744232	0.5560585089	0.8051708839
O	1.7543819925	0.807804761	-0.0683012181
O	-1.0387504423	-0.746179682	-1.6746309064
H	-1.9788172088	-0.5924229217	-1.7949491838
H	-0.5895452887	0.0293804913	-2.070902706
O	0.4422471188	1.4804214357	-2.38606409
H	0.9970407433	1.3747069098	-1.5811410215
H	1.0496993853	1.456663331	-3.129495131
C	-0.8075406064	-0.927821945	1.6711671106
C	-1.6764487568	-1.2756563165	2.4253401739
H	-2.446691917	-1.5681713969	3.0961574373

anti-CHCCHOO 2b TS

C	1.8466787698	-1.3303440859	-0.6760902664
H	2.3945854329	-2.2547686365	-0.8166462646
O	2.5605791577	-0.2782998075	-0.4569438376
O	3.9133543169	-0.4641544381	-0.9565305236
O	3.3254429666	-0.1340881982	-3.3026667814
H	3.2438580996	0.7917142067	-3.5458497038
H	3.7096172563	-0.1959096801	-2.2745495881
O	1.2965440436	-1.1979640358	-2.4663311703
H	2.1585359676	-0.7000357223	-2.9484285724
H	1.2046392549	-2.0779627639	-2.8502618161
C	0.5790433196	-1.3711297756	-0.0122060705
C	-0.4641837003	-1.4643268117	0.568872262
H	-1.3889151653	-1.5308532011	1.0871104126

anti-CHCCHOO 2b vdW

C	-0.1222925933	-0.5309437136	0.8639543944
H	0.2695670404	-1.4020311143	0.356232234
O	0.6110657018	0.4958597547	0.9440228378
O	1.8716092837	0.3990356984	0.3879255605
O	1.4653441663	0.8602112498	-2.2810335576
H	1.4646330089	1.8025145678	-2.4658447645
H	1.7239170099	0.7711981227	-1.3364861342
O	-0.8629448017	-0.5648784977	-1.8354681755
H	-0.0963905005	-0.0419922113	-2.1485183
H	-1.0396130124	-1.2084195648	-2.5255010514
C	-1.3948493385	-0.5002579279	1.4517521715
C	-2.4889062127	-0.5504442309	1.9468851485

H	-3.457168752	-0.5777241329	2.3833906365

anti-CHCCHOO 2c TS

C	1.2335196761	-0.3295293164	-0.2238455992
H	1.9413520864	-1.0754811541	-0.5663304163
O	1.7013279971	0.8638156461	-0.0709652497
O	2.8827122115	1.0566122029	-0.8946130312
O	0.258149345	-0.2890263794	-1.8167017265
H	0.3135717827	-1.1477419598	-2.2514097745
H	0.7998196113	0.4613248982	-2.4304751647
O	1.5596051678	1.4608732627	-2.90556296
H	2.2611495863	1.3834335299	-2.0560254212
H	2.0356325406	1.2661806973	-3.7164736137
C	0.2169054873	-0.7198657328	0.7060048102
C	-0.5961185146	-1.0993306052	1.4994339923
H	-1.3211740274	-1.4183796494	2.2069513344

anti-CHCCHOO 2c vdW

C	0.2124455059	-0.5914982774	0.7870938855
H	0.640415279	-1.312518818	0.1040302913
O	0.6935018231	0.5774751298	0.81154396
O	1.7453696558	0.8270153285	-0.0474036779
O	-1.0060645736	-0.773370989	-1.6800456792
H	-1.9452646555	-0.629543296	-1.8181060083
H	-0.5569740802	0.0008824064	-2.0789927277
O	0.4671971104	1.4569292458	-2.3960000673
H	1.009045139	1.3669833527	-1.5804166611
H	1.0874747629	1.428821778	-3.1286105441
C	-0.8306255147	-0.908499727	1.671260444
C	-1.7092556044	-1.2541403418	2.4151079081
H	-2.4882948477	-1.5446827921	3.0765598765

anti-CHCCHOO 2d TS

C	1.852923785	-1.2931767279	-0.6811881218
H	2.3927310568	-2.2084553923	-0.8901876534
O	2.5647289747	-0.2497608978	-0.4085355657
O	3.9131065434	-0.3918320248	-0.9316309919
O	3.3289939085	-0.1571199132	-3.2976435599
H	3.3189821928	0.7552989409	-3.597017439
H	3.700949101	-0.1819158046	-2.2700373596
O	1.2771298276	-1.1808230983	-2.4487130147
H	2.1208388356	-0.6789623041	-2.9384947396
H	0.5249154493	-0.5770762794	-2.4437696741
C	0.5981249731	-1.3721904965	0.0103104141

C	-0.440778776	-1.476862444	0.5975761575
H	-1.3568794719	-1.565501408	1.1280024581

anti-CHCCHOO 2d vdW

C	-0.3192558571	-0.3271212701	0.7666546321
H	-0.4386941179	-0.5229699499	-0.3011639253
O	0.8055534456	0.037955078	1.2285977632
O	1.8609177593	0.1562762045	0.366785676
O	1.4098443174	0.9638863756	-2.230427992
H	1.5560043229	1.9107506096	-2.2904306978
H	1.6152162287	0.709648574	-1.303985625
O	-0.9759300922	-0.3925654738	-2.274259483
H	-0.1738572402	0.1354138198	-2.4626002536
H	-1.0061665526	-1.0779945942	-2.9456741572
C	-1.3855357564	-0.4524865395	1.6694750291
C	-2.349425794	-0.5860769291	2.3765408576
H	-3.1928526635	-0.6989739048	3.0127141758

syn-CHCCHOO

C	-0.846588585	1.1355265099	-0.0192614881
H	-1.198133844	2.148307903	-0.157559975
O	-1.2079127504	0.3420058608	-0.9514202516
O	-0.8324282641	-0.947919107	-0.893394652
C	-0.0731565514	0.7476877179	1.0775423816
C	0.5893695125	0.4868718689	2.047812449
H	1.1757404825	0.2316352465	2.8960575361

syn-CHCCHOO 1a TS

C	0.9540190435	0.2920903979	0.1690087161
H	1.8682092676	-0.0149155532	-0.3286583401
O	-0.0721991261	-0.417930923	-0.16107998
O	-1.2458039474	0.3727825316	0.1459571241
O	0.37434098	1.846542701	-0.8838936873
H	-0.5705556758	1.4387108453	-0.5122793488
H	0.5530523991	2.6458476223	-0.3762743922
C	1.0839116622	0.9349023079	1.4376252257
C	1.3316484519	1.415620066	2.5087591771
H	1.513528545	1.8334974041	3.4683057355

syn-CHCCHOO 1a vdW

C	0.6167982372	-1.2498699664	0.2797753667
H	1.3258905718	-2.0667664279	0.2633990162
O	-0.3866963214	-1.4416913009	-0.479927758
O	-1.3499198242	-0.4851147882	-0.5469781643

O	-0.1159491342	1.9740401453	-1.3327934374
H	-0.6201286081	1.1882062702	-1.0575613552
H	-0.4982914784	2.236357873	-2.1735637602
C	0.8005966032	-0.1097168908	1.0612332235
C	1.0118678189	0.8682440904	1.7288640643
H	1.1754041352	1.7501539952	2.2987688043

syn-CHCCHOO 1b TS

C	0.067095935	0.8924914284	0.3811268336
H	0.3764036188	1.8476108337	-0.0332560239
O	-0.8716475455	0.3174480699	-0.299298914
O	-0.8275039152	-1.0906953423	0.0414907534
O	1.4813111337	-0.3803776954	-0.1401673554
H	0.5787430923	-1.0030459919	-0.0957329653
H	1.6614744383	-0.2384210264	-1.0778071175
C	0.2408923738	0.7087500144	1.7827712118
C	0.3771514375	0.7055437921	2.9741014511
H	0.4807153912	0.6694470575	4.0304941863

syn-CHCCHOO 1b vdW

C	-0.8494013774	1.1406027047	-0.0188340016
H	-1.1991122189	2.1532508969	-0.1693219285
O	-1.1990162959	0.3458302075	-0.9499857098
O	-0.8197501604	-0.9572411849	-0.8758502438
O	2.0331852016	-1.048112506	-0.6747362979
H	1.0639544153	-1.115776777	-0.7338203234
H	2.3652340592	-1.5132111026	-1.4463049198
C	-0.0931780112	0.7628904644	1.090164283
C	0.5804940685	0.4861283573	2.0474222668
H	1.1868533192	0.2126549397	2.876181875

syn-CHCCHOO 2a TS

C	1.370126704	-0.3292959118	-0.3580062965
H	0.6337298284	-0.6943225515	0.3492321818
O	1.7644681826	0.8662554694	-0.0653510587
O	2.8463211699	1.3363753957	-0.9072517567
O	0.1639439635	-0.1968386985	-1.7883686204
H	-0.5922231093	0.2950414123	-1.4441132871
H	0.7200326428	0.5083838616	-2.432341161
O	1.5307824399	1.4410501314	-2.9732377021
H	2.2004552841	1.4798252985	-2.0993001444
H	2.0339974545	1.1169940868	-3.7246054962
C	2.2597866049	-1.3029992385	-0.9167542537
C	2.9628297408	-2.1990679376	-1.2873434317

H	3.609341054	-2.9712263078	-1.6243369734

syn-CHCCHOO 2a vdW

C	-0.1254029014	-0.4704503599	1.2159239231
H	-0.9907003471	-0.7258949663	1.8111791792
O	0.1388665021	0.7673013692	1.2018827242
O	1.1999052894	1.189898403	0.4339595981
O	-2.0903187827	-0.3497985498	-0.8810263378
H	-2.9871121711	-0.0096419543	-0.9242142116
H	-1.5373552644	0.3204387002	-1.3299919193
O	-0.2963227381	1.5698071684	-1.8619864571
H	0.3308638112	1.5605546934	-1.1066235869
H	0.229503157	1.3734211568	-2.6410555685
C	0.6285099657	-1.4442691753	0.5520166522
C	1.2239092736	-2.3550753708	0.0410551913
H	1.7633992058	-3.1427901145	-0.425109187

syn-CHCCHOO 2b TS

C	2.0499943164	-1.454921263	-0.7356707804
H	1.0880025384	-1.4269460343	-0.2382412603
O	2.7399503891	-0.3909537213	-0.5014538899
O	4.0632549925	-0.4443717891	-1.0975607026
O	3.2063086586	0.0643523652	-3.3308623425
H	3.0651137699	1.0049309114	-3.4656796119
H	3.7099951282	-0.0775068171	-2.3665068406
O	1.3166307481	-1.2086086884	-2.4466597863
H	2.1000864374	-0.5997426068	-2.9337166356
H	1.3056729219	-2.0624646554	-2.8959568644
C	2.6701994704	-2.7391070385	-0.889656412
C	3.0834349242	-3.8625310672	-0.9490279296
H	3.491820025	-4.8415291155	-1.003513094

syn-CHCCHOO 2b vdW

C	-0.5536997869	-0.2764139035	1.1453254692
H	-1.5785776676	-0.218460015	1.4838709274
O	0.0336647736	0.8431714297	1.0993681075
O	1.3295783445	0.8683258691	0.6304764247
O	0.6056473098	1.3697600932	-1.984003982
H	0.6577262656	2.3097981313	-2.1737279193
H	1.0105627289	1.255892245	-1.0962438836
O	-1.8562311637	0.2193605329	-1.303391121
H	-1.0561994715	0.659091711	-1.6561458886
H	-2.1554430917	-0.3659391193	-2.0030815236
C	0.054179046	-1.4947723688	0.8196049632

C	0.502547806	-2.5869290425	0.5932147598
H	0.924916907	-3.538509563	0.3810766665

syn-CHCCHOO 2c TS

C	1.390563335	-0.3365660461	-0.3997668358
H	0.6000989828	-0.5825366638	0.2992542957
O	1.8395820056	0.8572599968	-0.2093978309
O	2.9458700998	1.1803245203	-1.0916884971
O	0.2430831588	-0.2191268962	-1.8694812327
H	0.345338847	-1.0274018607	-2.3857402276
H	0.6974239341	0.6094992405	-2.4486771497
O	1.3892705398	1.6708063837	-2.9139619949
H	2.18653749	1.5598242591	-2.1644566429
H	1.772860555	1.5559637175	-3.7867779256
C	2.2508511179	-1.4089874489	-0.8148908327
C	2.8963088969	-2.3854486367	-1.0728509776
H	3.5035295973	-3.2248224555	-1.3071212581

syn-CHCCHOO 2c vdW

C	-0.1711332021	-0.4572078745	1.2231178242
H	-1.0510095436	-0.7200370281	1.7932552141
O	0.087700085	0.7817717002	1.2234207825
O	1.1671448009	1.2136264885	0.4869476591
O	-2.0792900125	-0.3330003871	-0.925423017
H	-2.9762283156	0.0032029539	-0.9908352112
H	-1.5176530399	0.3425114672	-1.3553065639
O	-0.2686331024	1.600800212	-1.8461336197
H	0.3380993674	1.5897884157	-1.0742707244
H	0.2788386509	1.4116918611	-2.6119808381
C	0.6049507934	-1.4236838256	0.5742010738
C	1.218205144	-2.3287588024	0.0742930042
H	1.7737813744	-3.1112661806	-0.3816345835

syn-CHCCHOO 2d TS

C	1.9945059768	-1.4452418879	-0.7159160504
H	1.0447407919	-1.5401482808	-0.2015671462
O	2.6143538002	-0.3603146682	-0.3797131044
O	3.9492152476	-0.2675693915	-0.9380678721
O	3.28574894	-0.1894241533	-3.2870128462
H	3.2644193841	0.7034887039	-3.6400031328
H	3.6824475125	-0.1541530389	-2.2512857283
O	1.2249394292	-1.1524508123	-2.4053932564
H	2.0883606673	-0.6849889793	-2.9198283502
H	0.5760625699	-0.4529839455	-2.2606703314

C	2.695333466	-2.6589879826	-1.0016545438
C	3.2063302859	-3.7295791464	-1.1650261387
H	3.6910673689	-4.6619294472	-1.3182573192

syn-CHCCHOO 2d vdW

C	-0.5408501785	-0.2638617344	1.1828784964
H	-1.549562808	-0.2867251434	1.5706439476
O	0.0108696019	0.873771546	1.2573918376
O	1.2825152375	1.0068134372	0.7458813461
O	0.675779432	1.0508312109	-1.9422763757
H	0.8619842839	1.918307145	-2.3094811573
H	1.0148482954	1.075488743	-1.019939848
O	-1.9094228207	0.1317137015	-1.3060745287
H	-1.074826983	0.4867023864	-1.6703117806
H	-2.5957198111	0.736969851	-1.5961790115
C	0.0818582989	-1.406585191	0.6714336908
C	0.5452688571	-2.437883512	0.2633218286
H	0.9752095945	-3.3342914403	-0.1116084452