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

Supplementary information for:

Time-resolved, broadband UV-absorption spectrometry measurements of Criegee intermediate kinetics using a new photolytic precursor: Unimolecular decomposition of CH_2OO and its reaction with formic acid

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Determination of the effective optical path length, the initial CH_2OO concentration, and the detection limit

Figure S1 (vertical right-hand side axis) shows the average number of passes (*NP*) of the 2 meters long confocal cavity as a function of wavelength. The number of passes were determined using a static 5 ppm NO_2 in N_2 -sample in reactor at 50 Torr and 296 K. The observed absorbance ($A_{NO2,\lambda}$) between wavelengths of 300 nm and 450 nm is

$$A_{NO2,\lambda} = \ln(I_{0,\lambda}/I_\lambda) = \sigma_{NO2,\lambda} \times [NO_2] \times NP_\lambda \times 2\ \text{m}, \quad \text{(S1)}$$

where $I_{0,\lambda}$ is the light intensity at wavelength λ in the absence of NO_2, I_λ is the light intensity at wavelength λ in the presence of the static NO_2 sample, $\sigma_{NO2,\lambda}$ is the NO_2 absorption cross-section at wavelength λ, $[NO_2]$ is the NO_2 concentration, and NP_λ is the number of beam passes at wavelength λ. The effective optical path length (OPL) (vertical left-hand side axis of Fig. S1) is calculated using an overlap length of 75 ± 0.5 cm between the probe and the photolysis beams, which was marked and determined with two irises while the flow tube reactor was uninstalled. Using Equation S1, the effective OPL is

$$OPL = 0.75\ \text{m} \times NP_\lambda = 0.75\ \text{m} \times A_{NO2,\lambda}/(\sigma_{NO2,\lambda} \times [NO_2] \times 2\ \text{m}). \quad \text{(S2)}$$

The average effective OPL at 338 nm (with the wavelength resolution of 4 nm) is about 80 m. The confocal cavity design [1] and its low finesse makes the cavity relatively insensitive to alignment and the effective OPL does not change greatly from day to day.

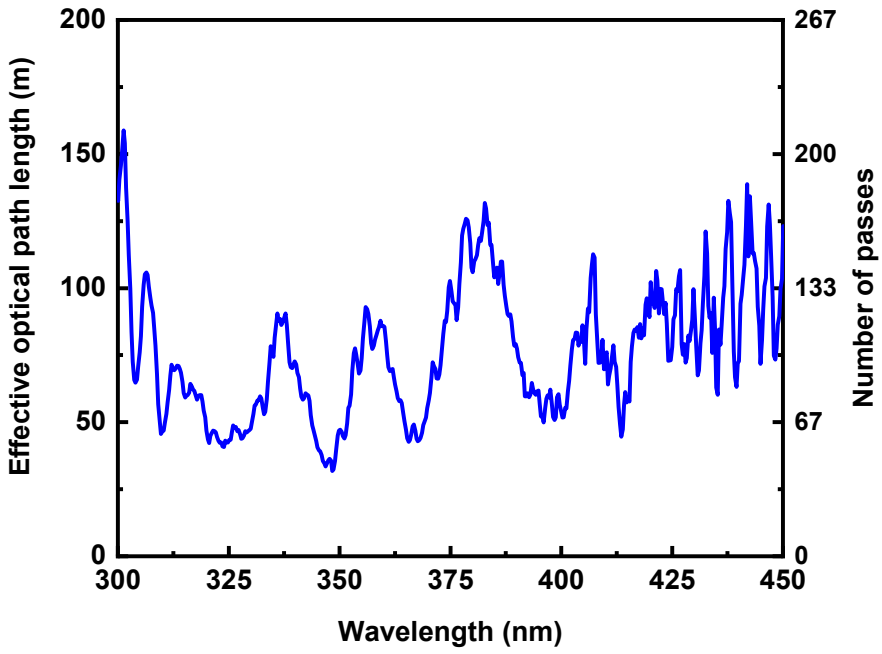

Figure S1. Determination of the effective optical path length of the TR-BB-CAES cavity.

Figure S4 presents a measured temporal absorbance profile ($A_{t,CH2OO} = \sigma_{CH2OO} \times [CH_2OO]_t \times OPL$) caused by CH_2OO at 338 nm with the presence of HCOOH (no absorption at 338 nm). The absorption cross-section of CH_2OO at 338 nm at is about 1.23×10^{-17} cm^2 $molecule^{-1}$ [2]. With the average effective OPL of about 80 m, the absorbance signal in Figure S4 (0.0085) gives the initial concentration of CH_2OO $\sim 8.5 \times 10^{10}$ molecules cm^{-3}. The initial concentration of CH_2I in the measurement was $\sim 2.2 \times 10^{11}$ molecules cm^{-3} (calculated assuming an unity quantum yield for the photodissociation of CH_2BrI at 213 nm). Assuming that the yield of reaction $CH_2I + O_2 \rightarrow CH_2OO$ is unity under experimental 5 Torr and 296 K conditions, the photodissociation quantum yield of the channel (R4a), $CH_2BrI + h\nu(213\ nm) \rightarrow CH_2I + Br$, can be estimated to be ~0.4. The observed signal-to-noise ratio (SNR) of the trace was ~35 for an averaging time of 1800 s (30 min). This gives a minimum detectable $[CH_2OO] \sim 2.4 \times 10^9$ molecule cm^{-3}.

Absorption cross-sections of the CH_2I_2 and CH_2IBr precursors and CH_2OO transient spectrum and absorbance signals utilizing these precursors

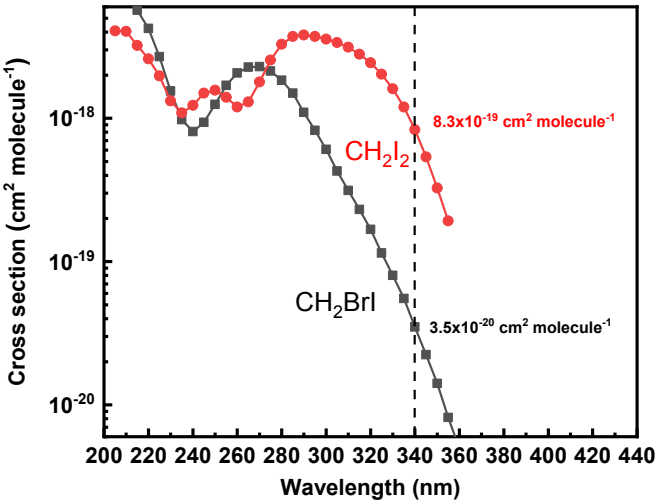

Figure S2. The absorption cross sections of CH_2I_2 and CH_2BrI precursors as function of wavelength [3].

Figure S2 shows the cross-sections of CH_2I_2 and CH_2BrI photolytic precursors as function of wavelength [3]. CH_2I_2 has more than 20 times stronger absorption cross-section than CH_2BrI at 340 nm region, where the absorption of CH_2OO has its maximum. Figure S3 shows a typical negative baseline shift for a measured absorbance signal that is caused by the depletion of CH_2I_2. The baseline is also non-constant, especially at longer delay times. However, the depletion of CH_2I_2 can be considered as a step function with a constant, negative baseline shift for shorter time scale (<10 ms). Depletion of CH_2IBr does not induce a negative baseline shift, because of its much smaller absorption cross-section at 340 region. In fact, the baseline is ~zero and constant even at longer measurement times as shown in figure S4.

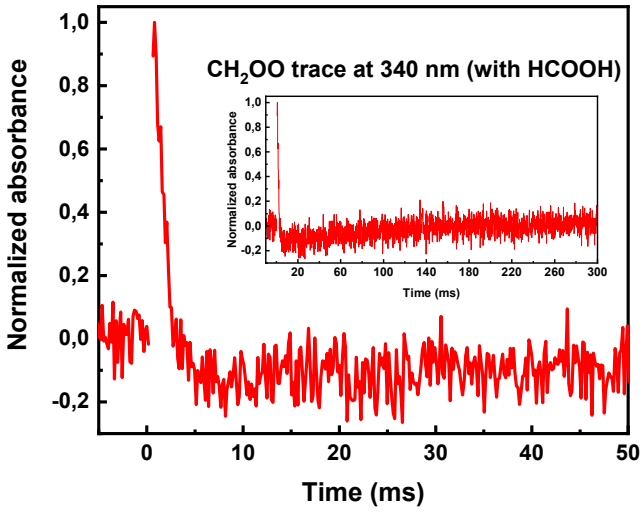

Figure S3. A transient absorbance signal of CH_2OO in reaction with HCOOH using CH_2I_2 photolytic precursor at 296 K and 5 Torr conditions.

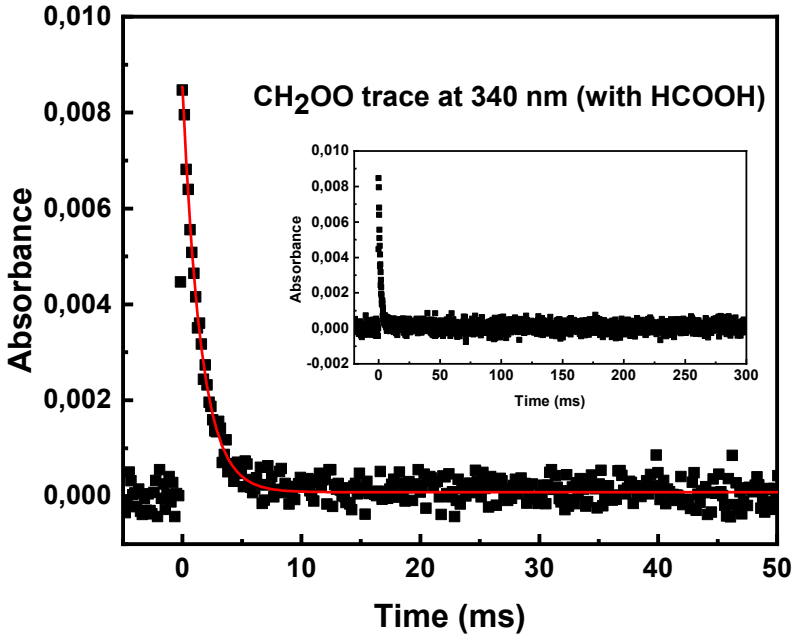

Figure S4. A transient absorbance signal of CH_2OO in reaction with HCOOH using CH_2IBr as photolytic precursor and measured at 296 K and 5 Torr conditions.

The transient absorption spectrum of CH_2OO corresponding to Fig. 3 in the manuscript is shown in Fig. S5 below. Photolysis of CH_2IBr at 213 nm, followed by reaction (R1), $CH_2I + O_2 \rightarrow CH_2OO + I$, was used for CH_2OO production. The spectrum was averaged over ~1000 s (with ~67 μs time resolution). The estimated initial CH_2OO concentration in the measurement was $\sim 2.0 \times 10^{11}$ molecule cm^{-3}.

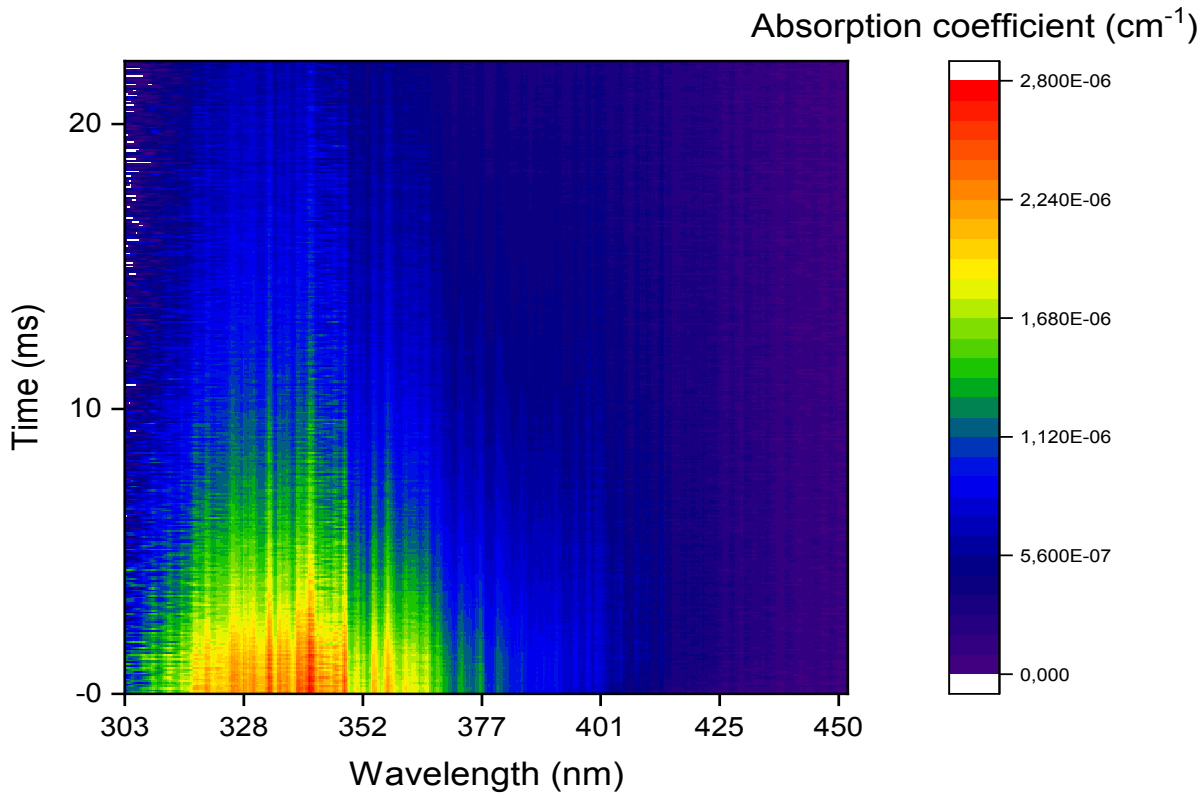

Figure S5. Transient absorption spectrum of CH_2OO using CH_2IBr as photolytic precursor and measured at 296 K and 10 Torr (N_2) pressure. The false-color scale indicates optical absorption per one centimeter. The initial CH_2OO concentration was $\sim 2.0 \times 10^{11}$ molecule cm^{-3}. The O_2 concentration was $\sim 3.8 \times 10^{16}$ molecule cm^{-3}.

Bimolecular CH_2OO + HCOOH reaction as a function of pressure at 296 K

HCOOH reactant concentration (partial pressure) in the reactor was calculated with accounting for the dimerization of the dilute HCOOH in helium mixture prepared in a bulb [4]. A small amount of (liquid) formic acid (Sigma-Aldrich, ≥96%) was first degassed by several freeze–pump–thaw cycles before evaporating it completely into the bulb. A typical sample consisted of about 3 Torr (4 mbar) of HCOOH mixed with He in total pressure of about 800 Torr. The measured HCOOH sample pressure (p_T) in the bulb is the sum of the partial pressures of monomer (p_M) and dimer (p_D), $p_T = p_M + p_D$. The equilibrium constant, K, for the reaction $(HCOOH)_2 \leftrightarrow 2$ HCOOH can be defined as

$K = p_M^2 / p_D = p_M^2 / (p_T - p_M)$.

From the equilibrium constant of the dimerization (3.91 mbar at 300 K [4]), the partial pressure of the monomer can be calculated as

$p_M = [(K^2 + 4Kp_T)^{1/2} - K]/2$.

Because, $p_D = p_T - p_M$ and noting that all the dimers dissociate to monomers in the reactor (high dilution), the total partial pressure, P_M, of monomers in the reactor is

$P_M = p_M + 2p_D = p_M + 2(p_T - p_M) = 2p_T - p_M$

$= 2p_T - [(K^2 + 4Kp_T)^{1/2} - K]/2$

In the main text, figure 7 shows the obtained pseudo-first-order decay coefficients (k_{obs}) of CH_2OO as function of [HCOOH] at different total pressures. A bimolecular rate coefficient $k(CH_2OO + HCOOH)$ is obtained from the slope of the equation $k_{obs} = k_{loss} + k(CH_2OO + HCOOH) \times [HCOOH]$ fitted to the data, while the intercept reflects the k_{loss}. The results are shown in Table S1 along with the experimental conditions. As mentioned in the main text, the reaction appears to be pressure independent over the range between 5 and 150 Torr considering the uncertainties of the measurements.

Table S1 Results and conditions of the experiments used to measure the bimolecular rate coefficient of CH_2OO + HCOOH reaction as a function of pressure at 296 K.

T(K)	[He] (×10^{18} molecule cm^{-3})	[b]*p* (Torr)	[c][HCOOH] (×10^{13} molecule cm^{-3})	k_{loss} (s^{-1})	[d]*k* (×10^{-10} cm^3 $molecule^{-1}$ s^{-1})
Precursor: [a]CH_2BrI					
296	0.16	5	0.55–2.06	98	1.01±0.10
296	1.6	50	0.53–1.66	37	0.92±0.07
296	3.3	100	0.54–1.69	27	0.97±0.05
296	4.9	150	0.54–1.69	29	1.00±0.03

[a]Precursor concentrations used: (7.0-9.5) × 10^{12} molecule cm^{-3} for CH_2BrI. Estimated initial CH_2OO concentration was <1.0 × 10^{11} molecule cm^{-3}. [b]The fixed concentration of O_2 was ~3.8 × 10^{16} molecule cm^{-3} for all measurements. [c]HCOOH reactant concentration in the reactor is calculated with accounting for the dimerization of the dilute HCOOH in helium mixture prepared in a bulb [4]. [d] The statistical uncertainties shown are 2σ. Estimated overall uncertainties in the measured rate coefficients are about ±20%. The linear gas flow velocity was ~1.0 ms^{-1}.

As is mentioned in the main text, a positive baseline shift was observed at high pressures using CH_2IBr photolytic precursor, which may originate from an enhanced stabilization of ICH_2OO [5, 6], iodomethyl peroxy radical, at higher pressures. Figure 6 shows four measured transient absorbance traces of CH_2OO (with added HCOOH) over the pressure range between 5 and 150 Torr at 296 K utilizing 213 nm photolysis of CH_2IBr precursor for CH_2I radical production. The complete experimental conditions (and results) for the measurements are shown in Table S2. It is known that the reaction $CH_2I + O_2$ proceeds *via* two major channels [5, 6],

$CH_2I + O_2 \rightarrow CH_2OO + I$ (1)

$CH_2I + O_2 + M \rightarrow ICH_2OO + M$ (2)

where rate coefficients k_1 and k_2 depend on pressure, because stabilization of the adduct ICH_2OO depends on its collisions with third body molecules (M = helium, nitrogen). The reported UV cross-section of ICH_2OO [7, 8] is ~0.1 times that of the CH_2OO at 338 nm, which is in reasonable accordance with our observed positive base-line shifts (offsets) when taking into account the estimated pressure dependent yield of CH_2OO [5]. From 5 to 150 Torr, the background is increased by a factor of 3.5 while the CH_2OO absorption is decreased by 35%. In the

measurements (high [O_2]), the formation of CH_2OO and ICH_2OO is much faster ($k_1 + k_2 = 1.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} [5]) than the decay of CH_2OO. Thus, assuming that ICH_2OO does not react with other sample components and, therefore, does not decay within a short timescale (<30 ms), we can use the following fitting function for the high-pressure measurements:

$$A_t = A_{0,\,CH2OO} \times exp(-k't) + A_{0,\,ICH2OO},$$

where k' is the pseudo-first-order decay rate coefficient, A_t is the measured absorbance at time t, and $A_{0,\,CH2OO}$ and $A_{0,\,ICH2OO}$ are the initial absorbances caused by CH_2OO and ICH_2OO (at time t=0), respectively. Figure S7 shows that the baseline is constant at high pressures within a short timescale (< 30 ms) but decays to zero at longer timescale.

Table S2 Results and conditions of the experiments presented in Fig. S7 (with the added HCOOH).

T(K)	[He] (×10^{18} molecule cm^{-3})	[a]p (Torr)	[b]Initial [CH_2I] (×10^{11} molecule cm^{-3})	[c][HCOOH] (×10^{13} molecule cm^{-3})	[d]k (s^{-1})	ΔA (×10^{-3})	Baseline shift (×10^{-3})	ΔA Criegee (×10^{-3})
296	0.16	5	2.20	1.31	1593±138	7.66	0.13	7.53
296	1.6	50	2.95	1.17	878±58	6.97	0.31	6.66
296	3.3	100	2.22	1.31	1254±92	5.99	0.44	5.55
296	4.9	150	2.25	1.31	1306±104	5.55	0.49	5.06

[a]The fixed concentration of O_2 was ~3.8×10^{16} molecule cm^{-3} for all measurements. [b]Precursor CH_2BrI concentrations used: (7.2-9.5)×10^{12} molecule cm^{-3}. [c]The HCOOH reactant concentration in the reactor is calculated with accounting for the dimerization of the dilute HCOOH in helium mixture prepared in a bulb [4]. [d]The statistical uncertainties shown are 2σ. Estimated overall uncertainties in the measured rate coefficients are about ±20%. The linear gas flow velocity was ~1.0 ms^{-1}.

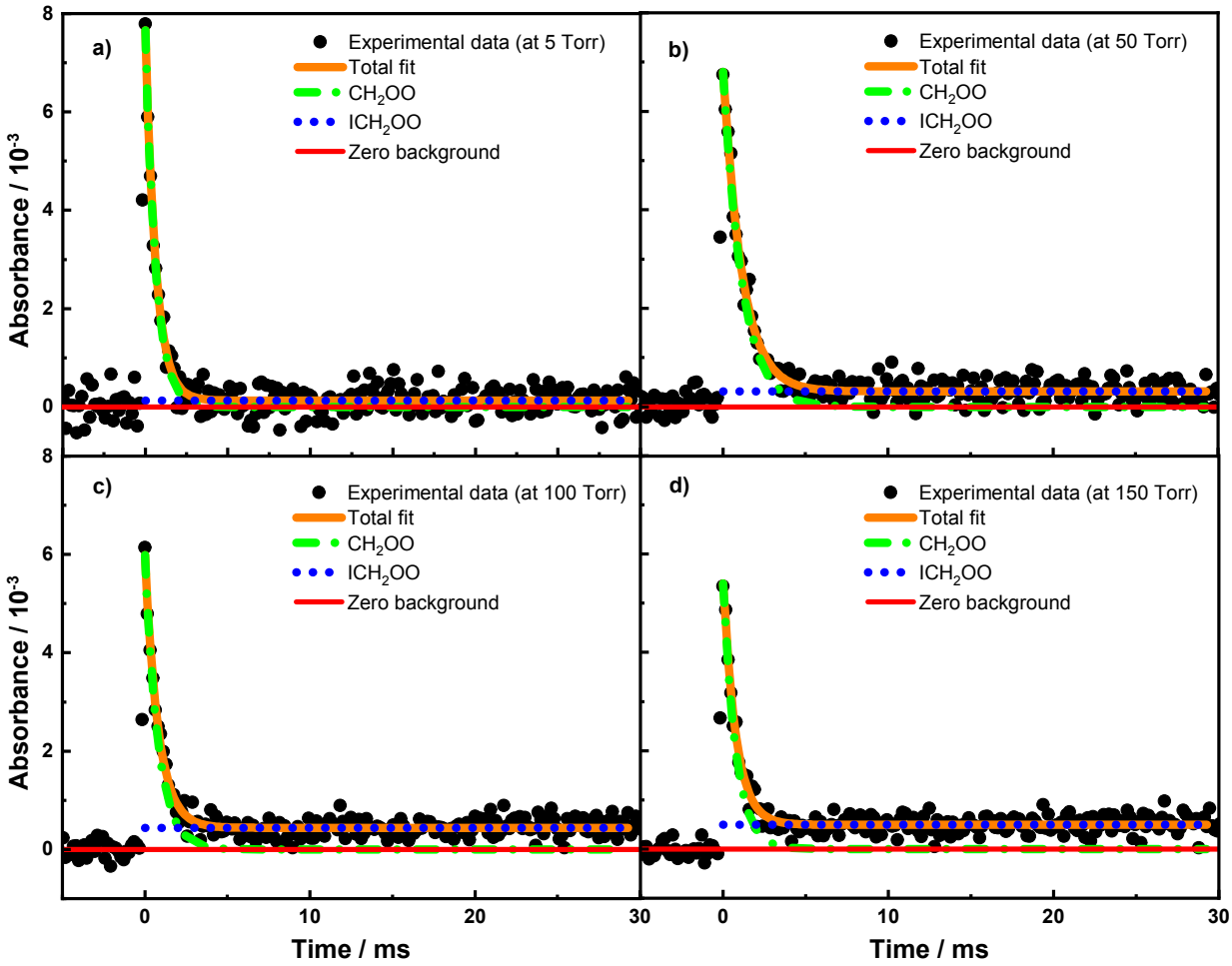

Figure S6. Measured transient absorbance signals of CH_2OO in reaction with HCOOH at a) 5 Torr, b) 50 Torr, c) 100 Torr, and d) 150 Torr. Photolysis of CH_2IBr at 213 nm used as source of CH_2I radical.

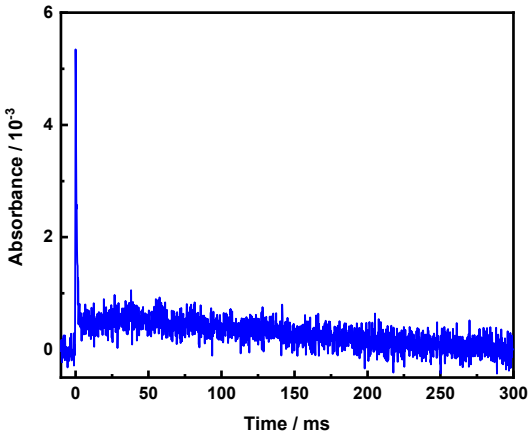

Figure S7. A transient absorbance signal of CH_2OO in reaction with HCOOH at 150 Torr and 296 K. CH_2IBr used as photolytic source.

Unimolecular decomposition kinetics of CH_2OO as a function of pressure and temperature

As is mentioned in the main text, the positive baseline offset of the measured absorbance signal was also present at the high pressures in the unimolecular decomposition measurements when CH_2IBr was used as photolytic source. Figure S8 shows two examples of measured transient absorption traces of CH_2OO at 575 K. The complete experimental conditions and results for the fittings of the data are shown in Table S3. The offset value increased when the pressure increased as in the bimolecular CH_2OO + HCOOH reaction. At high temperatures (>550 K), the baseline offset decreased as the pressure increased. This might indicate a possible decomposition of ICH_2OO. Overall, positive baseline offset (when occurred) was between 0 and 20% of the CH_2OO absorption with an average of 5 %. The baseline offset has been taken into account in the fittings as explained above (see bimolecular CH_2OO + HCOOH reaction). Interestingly, at high temperatures, a small offset was present already at low pressures, which might indicate possible absorption by another formed product than ICH_2OO.

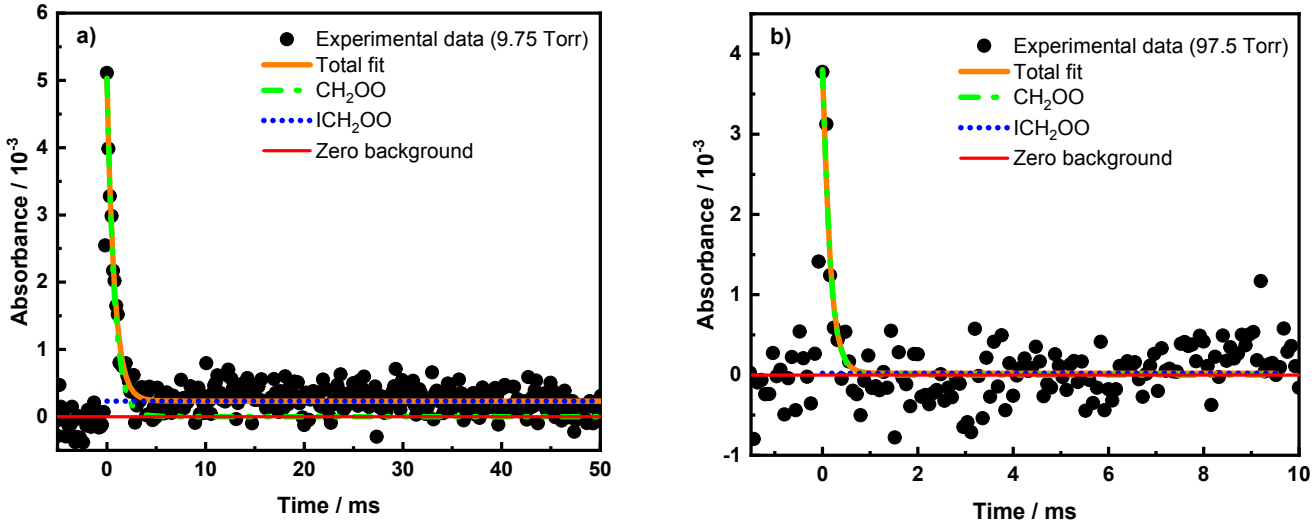

Figure S8. The transient absorption signals of CH_2OO at 575 K and at a) 9.75 Torr, b) 97.5 Torr. CH_2IBr used as photolytic source.

Table S3 Unimolecular decomposition kinetics of CH_2OO determined from the UV experiments. k_{obs} are the fitted single exponential decay rate coefficients of CH_2OO, with 2σ statistical uncertainties. k_{uni} are derived as $k_{uni} = k_{obs} - k_{loss}$. Troe fits to k_{obs} are derived using eqn (1).

T(K)	[He] ($\times 10^{18}$ molecule cm^{-3})	^{a}p (Torr)	Initial [CH_2I] ($\times 10^{11}$ molecule cm^{-3})	k_{obs} (s^{-1})	k_{loss} (s^{-1})	k_{uni} (s^{-1})	ΔA ($\times 10^{-3}$)	Baseline shift ($\times 10^{-3}$)	ΔA Criegee ($\times 10^{-3}$)
475	1.6	80.5	4.70	303 ± 13.	29	274	7.97	0.29	7.68
	3.3	160.5	4.74	444 ± 30.	24	420	7.00	0.52	6.48
	4.9	240.5	4.77	554 ± 48.	26	528	6.46	0.48	5.98
	6.5	320.5	4.78	629 ± 65.	19	610	5.86	0.47	5.39
	8.2	401.5	4.80	693 ± 56.	19	674	6.28	0.58	5.70
500	1.6	84.5	4.19	725 ± 52	29	696	7.55	0.30	7.25
	3.3	169	4.25	1029 ± 111	24	1005	6.99	0.39	6.60
	4.9	253.5	4.27	1407 ± 188	26	1381	6.38	0.39	5.99
	6.5	338	4.73	1732 ± 172	19	1713	5.95	0.28	5.67
525	0.33	17.75	3.06	608 ± 40	62	546	6.14	0.23	5.91
	1.6	89	4.13	1587 ± 149	29	1558	6.57	0.20	6.37
	3.3	177.5	4.19	2231 ± 269	24	2207	6.86	0.26	6.60
	4.9	266	4.22	3271 ± 407	26	3245	5.98	0.27	5.71
	6.5	355	4.28	3518 ± 536	19	3499	6.52	0.37	6.15
550	0.16	9.3	3.45	767 ± 58	100	667	5.59	0.38	5.21
	0.33	18.6	3.45	1133 ± 910	62	1071	5.50	0.25	5.25
	1.6	93	4.65	3083 ± 451	29	3054	5.30	0.19	5.11
	3.3	186	4.71	4296 ± 800	24	4272	5.47	0.18	5.29
	4.9	279	4.75	06199 ± 1683	26	6173	4.42	0.26	4.16
575	0.16	9.75	3.14	1319 ± 119	100	1219	5.06	0.28	4.78
	0.33	19.45	3.14	1878 ± 233	62	1816	4.07	0.21	3.86
	1.6	97.5	4.27	06635 ± 1791	29	6606	3.80	0.02	3.78
600	0.16	10.15	3.20	2170 ± 351	100	2070	4.23	0.23	4.00
	0.33	20.3	3.20	3093 ± 610	62	3031	3.84	0.11	3.73

^{a}The fixed concentration of O_2 was ~3.9×10^{16} molecule cm^{-3} for all measurements.

Figure S9 shows the observed experimental decays of CH_2OO as function of temperature at the fixed total density of 1.6×10^{17} molecule cm^{-3} using CH_2IBr as photolytic source. The data shows that the measured decay is almost constant between the temperatures 296 and 375 K, while the exponential increasing unimolecular decomposition starts at 425 K.

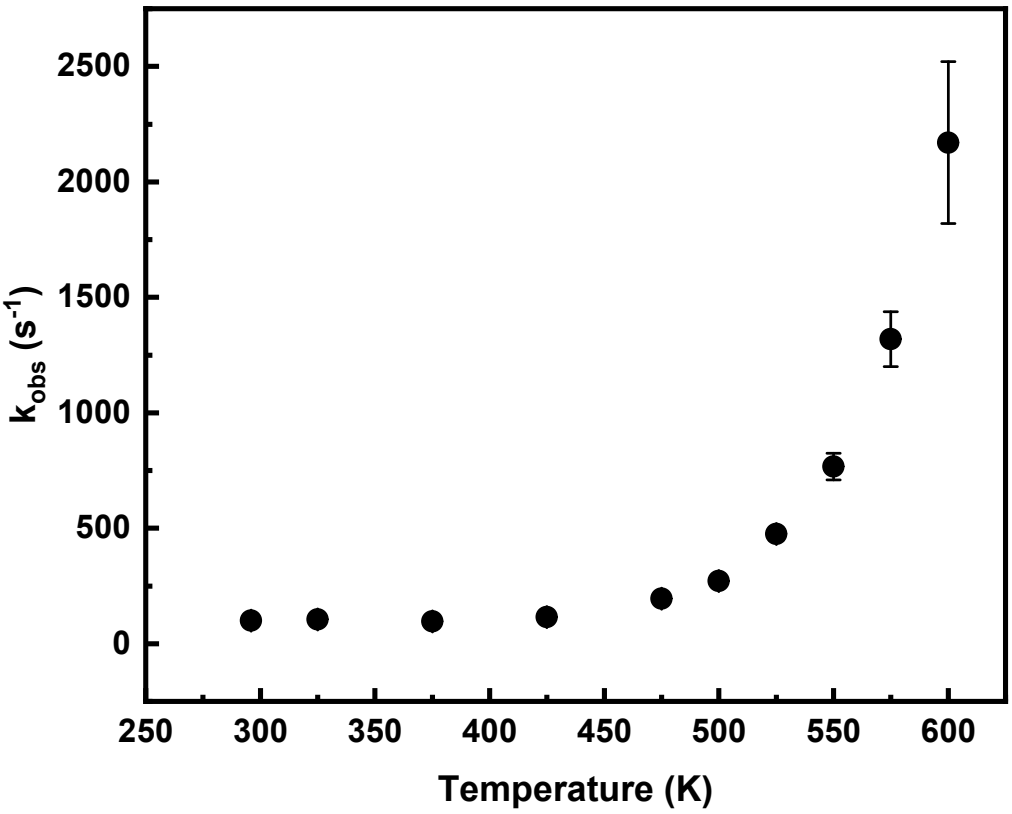

Figure S9. The observed experimental decays of CH_2OO as a function of temperature at fixed total density of 1.6×10^{17} molecule cm^{-3} using CH_2IBr as photolytic source.

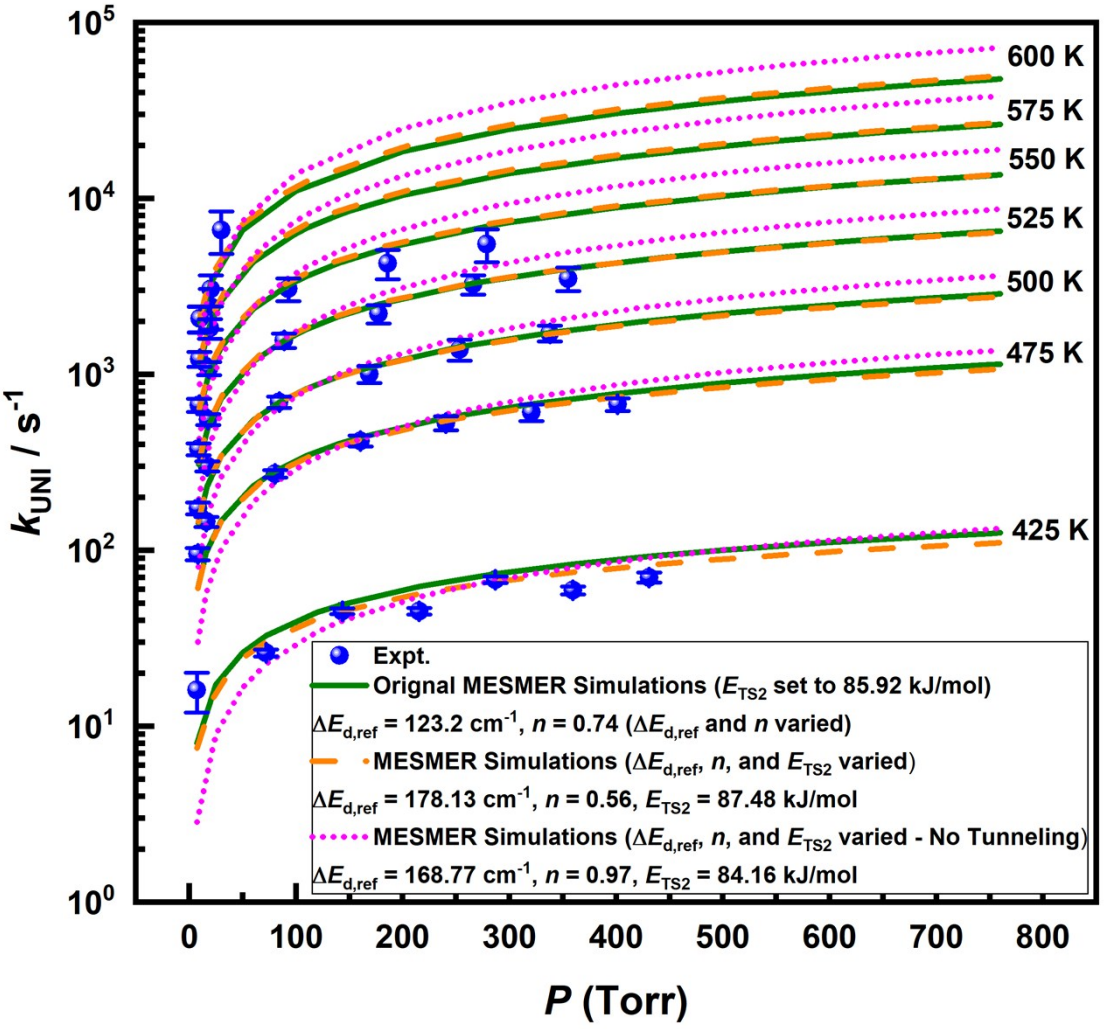

Figure S10. Results of MESMER simulations with different options: Original simulation from Figure 8, a simulation by varying $\langle \Delta E \rangle_{down,\ ref}$, n, and E_{TS2} parameters, and a simulation by varying $\langle \Delta E \rangle_{down,\ ref}$, n, and E_{TS2} parameters without tunneling (tunneling turned off). Results of experiments (solid blue points) are also shown with 2σ statistical uncertainties.

References

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! First column: pressure (atm), second column: pre-exponential factor (cm^3 s^{-1} or s^{-1}), third column: exponent of T, fourth column: activation energy (cal/mol)

CH2OO => H2 + CO2 7.2766e+23 -5.24416 19453.4
PLOG/ 0.001 7.2766e+23 -5.24416 19453.4/
PLOG/ 0.005 3.90896e+24 -5.22622 20112.3/
PLOG/ 0.01 7.83197e+24 -5.21458 20395.1/
PLOG/ 0.025 1.90299e+25 -5.19511 20767.6/
PLOG/ 0.05 3.60445e+25 -5.17606 21047.1/
PLOG/ 0.1 6.52253e+25 -5.15102 21323/
PLOG/ 0.25 1.26483e+26 -5.1019 21676.3/
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PLOG/ 1 2.01579e+26 -4.95687 22158.2/
PLOG/ 2.5 1.40535e+26 -4.7725 22409/
PLOG/ 5 6.05632e+25 -4.55768 22538.1/
PLOG/ 7.5 2.75541e+25 -4.39302 22580.5/
PLOG/ 10 1.35185e+25 -4.25597 22592.6/
PLOG/ 50 1.64503e+22 -3.13351 22303.3/
PLOG/ 100 2.29837e+20 -2.47473 21972.4/

CH2OO => H2O + CO 3.91274e+51 -14.012 29310.7
PLOG/ 0.001 3.91274e+51 -14.012 29310.7/
PLOG/ 0.005 2.88152e+81 -23.1545 40179.9/
PLOG/ 0.01 1.10875e+112 -32.683 50915.1/
PLOG/ 0.025 1.12012e-63 22.9236 -6407.84/
PLOG/ 0.05 3.71563e-98 34.0674 -16687.6/
PLOG/ 0.1 9.37228e-154 52.2098 -31702.4/

CH2OO => HCO + OH 6.07947e+21 -5.23032 19490

PLOG/ 0.001 6.07947e+21 -5.23032 19490/

PLOG/ 0.005 3.42826e+22 -5.21469 20150.1/

PLOG/ 0.01 7.00748e+22 -5.20396 20433.3/

PLOG/ 0.025 1.74573e+23 -5.18554 20806.2/

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PLOG/ 0.1 6.17796e+23 -5.14225 21362/

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PLOG/ 0.75 1.90912e+24 -4.98554 22104.8/

PLOG/ 1 1.9394e+24 -4.94385 22196.9/

PLOG/ 2.5 1.32798e+24 -4.75395 22447.5/

PLOG/ 5 5.56771e+23 -4.53273 22576.9/

PLOG/ 7.5 2.47472e+23 -4.36316 22619.4/

PLOG/ 10 1.18934e+23 -4.22201 22631.4/

PLOG/ 50 1.1639e+20 -3.06161 22336.1/

PLOG/ 100 1.33826e+18 -2.37237 21992.5/

CH2OO => cyc-H2COO 5.54832e+29 -8.76493 31340

PLOG/ 0.001 5.54832e+29 -8.76493 31340/

PLOG/ 0.005 1.24837e+32 -9.01464 33264.4/

PLOG/ 0.01 9.53569e+32 -9.08128 34065.7/

PLOG/ 0.025 1.06926e+34 -9.13297 35098/

PLOG/ 0.05 5.40525e+34 -9.14444 35857/

PLOG/ 0.1 2.24429e+35 -9.13002 36594.1/

PLOG/ 0.25 1.01072e+36 -9.06149 37524.7/

PLOG/ 0.5 2.12156e+36 -8.95734 38181.9/

PLOG/ 0.75 2.62636e+36 -8.86721 38540.4/

PLOG/ 1 2.69826e+36 -8.78669 38780/

PLOG/ 2.5 1.19895e+36 -8.41049 39436.2/

PLOG/ 5 1.95715e+35 -7.9659 39786.2/

PLOG/ 7.5 3.66585e+34 -7.62404 39912.9/

PLOG/ 10 8.12701e+33 -7.33936 39960.9/

PLOG/ 50 6.32675e+27 -5.00902 39425.7/

PLOG/ 100 4.31404e+23 -3.54825 38637.4/

CH2OO => open-H2COO 6.88542e+19 -6.64394 19515.3

PLOG/ 0.001 6.88542e+19 -6.64394 19515.3/

PLOG/ 0.005 1.65008e+21 -6.61198 20161.7/

PLOG/ 0.01 6.3492e+21 -6.59549 20440.1/

PLOG/ 0.025 4.39473e+22 -6.59495 20833.2/

PLOG/ 0.05 3.23082e+23 -6.66777 21210/

PLOG/ 0.1 2.16198e+24 -6.72797 21575.9/

PLOG/ 0.25 2.22179e+25 -6.78317 22039/

PLOG/ 0.5 1.06533e+26 -6.79881 22370.1/

PLOG/ 0.75 2.39494e+26 -6.7937 22553.3/

PLOG/ 1 4.01014e+26 -6.78224 22677.1/

PLOG/ 2.5 1.35182e+27 -6.68933 23026.3/

PLOG/ 5 1.39385e+27 -6.49947 23185.9/

PLOG/ 7.5 9.18228e+26 -6.33001 23226.8/

PLOG/ 10 5.8592e+26 -6.18964 23237.5/

PLOG/ 50 7.28885e+23 -4.84875 22736.3/

PLOG/ 100 4.56791e+24 -4.93337 23198.7/

cyc-H2COO => CH2OO 1.46959e+28 -8.16471 58385.8

PLOG/ 0.001 1.46959e+28 -8.16471 58385.8/

PLOG/ 0.005 3.30657e+30 -8.41442 60310.1/

PLOG/ 0.01 2.52573e+31 -8.48106 61111.5/

PLOG/ 0.025 2.83215e+32 -8.53276 62143.8/

PLOG/ 0.05 1.43169e+33 -8.54422 62902.8/

PLOG/ 0.1 5.94447e+33 -8.5298 63639.8/

PLOG/ 0.25 2.67712e+34 -8.46128 64570.5/

PLOG/ 0.5 5.61941e+34 -8.35713 65227.7/

PLOG/ 0.75 6.95645e+34 -8.26699 65586.2/

PLOG/ 1 7.14691e+34 -8.18647 65825.8/

PLOG/ 2.5 3.17566e+34 -7.81028 66482/

PLOG/ 5 5.18393e+33 -7.36568 66832/

PLOG/ 7.5 9.70976e+32 -7.02382 66958.7/

PLOG/ 10 2.15261e+32 -6.73914 67006.7/

PLOG/ 50 1.67577e+26 -4.4088 66471.5/

PLOG/ 100 1.14266e+22 -2.94803 65683.2/

cyc-H2COO => H2 + CO2 6.62704e+14 -2.60186 11243.5

PLOG/ 0.001 6.62704e+14 -2.60186 11243.5/

PLOG/ 0.005 6.47902e+15 -2.65203 12344.5/

PLOG/ 0.01 1.4922e+16 -2.65365 12808.8/

PLOG/ 0.025 4.35762e+16 -2.65362 13420/

PLOG/ 0.05 9.50236e+16 -2.65245 13873.2/

PLOG/ 0.1 1.78869e+17 -2.63468 14298.9/

PLOG/ 0.25 2.5109e+17 -2.54746 14787.3/

PLOG/ 0.5 2.01027e+17 -2.41686 15095.4/

PLOG/ 0.75 1.4791e+17 -2.31578 15256.2/

PLOG/ 1 1.11367e+17 -2.23462 15364/

PLOG/ 2.5 3.38521e+16 -1.93446 15683.2/

PLOG/ 5 1.06042e+16 -1.67017 15901.3/

PLOG/ 7.5 4.71609e+15 -1.49761 16013.3/

PLOG/ 10 2.44798e+15 -1.36441 16081.7/

PLOG/ 50 8.01729e+12 -0.350608 16154.8/

PLOG/ 100 3.3684e+11 0.170782 16060.3/

cyc-H2COO => HCO + OH 4.37681 0.34889 29841.6

PLOG/ 0.001 4.37681 0.34889 29841.6/

PLOG/ 0.005 9656.15 -0.408793 28806.6/

PLOG/ 0.01 217120 -0.704712 28346.7/

PLOG/ 0.025 5.29077e+31 -8.87945 35953.2/

PLOG/ 0.05 5.18226e+17 -4.31501 30388.4/

PLOG/ 0.1 4.14514e+12 -2.5726 27773.9/

PLOG/ 0.25 2.25092e+11 -2.00315 26076.1/

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PLOG/ 0.75 4.76839e+12 -2.21312 24898.6/

PLOG/ 1 1.78775e+13 -2.3363 24667.4/

PLOG/ 2.5 2.65203e+15 -2.82047 24162.1/

PLOG/ 5 1.39453e+17 -3.19407 24020.5/

PLOG/ 7.5 1.12663e+18 -3.37632 24017.2/

PLOG/ 10 4.10007e+18 -3.47837 24039.7/

PLOG/ 50 1.03654e+20 -3.50985 24307.7/

PLOG/ 100 2.11215e+20 -3.44541 24626.7/

cyc-H2COO => open-H2COO 9.4046e+19 -6.01748 17281.2

PLOG/ 0.001 9.4046e+19 -6.01748 17281.2/

PLOG/ 0.005 1.6416e+23 -6.53639 17211.5/

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PLOG/ 0.025 3.0001e+25 -6.80792 17465.7/

PLOG/ 0.05 2.91881e+26 -6.95155 17695/

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PLOG/ 0.75 1.2028e+29 -7.22308 18390.4/

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PLOG/ 5 1.78354e+29 -6.95846 18367.4/

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PLOG/ 10 2.63394e+28 -6.58724 18085.8/

PLOG/ 50 1.43574e+23 -4.66237 16509.4/

PLOG/ 100 3.13179e+22 -4.32819 16480.9/

open-H2COO => CH2OO 2.58719e+19 -6.51112 32337.6

PLOG/ 0.001 2.58719e+19 -6.51112 32337.6/

PLOG/ 0.005 6.20018e+20 -6.47916 32984/

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PLOG/ 0.025 1.65132e+22 -6.46213 33655.5/

PLOG/ 0.05 1.21398e+23 -6.53495 34032.3/

PLOG/ 0.1 8.12363e+23 -6.59515 34398.2/

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PLOG/ 2.5 5.07945e+26 -6.55651 35848.6/

PLOG/ 5 5.23738e+26 -6.36665 36008.2/

PLOG/ 7.5 3.45024e+26 -6.1972 36049.1/

PLOG/ 10 2.20159e+26 -6.05682 36059.8/

PLOG/ 50 2.73878e+23 -4.71593 35558.6/

PLOG/ 100 1.71639e+24 -4.80055 36021/

open-H2COO => H2 + CO2 1.81904e+25 -7.14568 13739.8

PLOG/ 0.001 1.81904e+25 -7.14568 13739.8/

PLOG/ 0.005 3.31149e+29 -7.95106 14977.7/

PLOG/ 0.01 7.38061e+30 -8.16118 15584.9/

PLOG/ 0.025 9.0363e+31 -8.24221 16301.3/

PLOG/ 0.05 7.52554e+32 -8.35248 16942.7/

PLOG/ 0.1 3.54832e+33 -8.39991 17532.1/

PLOG/ 0.25 9.70152e+33 -8.34013 18186.6/

PLOG/ 0.5 8.68686e+33 -8.18799 18567.5/

PLOG/ 0.75 5.7289e+33 -8.05369 18748.9/

PLOG/ 1 3.66136e+33 -7.93865 18858.8/

PLOG/ 2.5 3.60232e+32 -7.4548 19097/

PLOG/ 5 1.08077e+32 -7.17192 19357.8/

PLOG/ 7.5 1.30675e+31 -6.81378 19324.4/

PLOG/ 10 2.05032e+30 -6.51201 19255.2/

PLOG/ 50 2.774e+25 -4.7205 18836.2/

open-H2COO => H2O + CO 1.14689 2.83014 -9536.37

PLOG/ 0.001 1.14689 2.83014 -9536.37/

PLOG/ 0.005 0.748355 3.11599 -8864.94/

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open-H2COO => HCO + OH 1.00801e+11 -4.17029 32315.6

PLOG/ 0.001 1.00801e+11 -4.17029 32315.6/

PLOG/ 0.005 4.91316e+17 -5.7072 31439.2/

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PLOG/ 5 6.59677e-284 89.1003 -94463.1/

PLOG/ 7.5 1.63871e-247 77.9465 -80792.9/

PLOG/ 10 6.79706e-225 71.0287 -72239.1/

PLOG/ 50 5.43412e+146 -45.9574 50866.4/

open-H2COO => cyc-H2COO 1.32423e+21 -6.48388 3056.46

PLOG/ 0.001 1.32423e+21 -6.48388 3056.46/

PLOG/ 0.005 2.31148e+24 -7.00278 2986.7/

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PLOG/ 0.05 4.10988e+27 -7.41794 3470.26/

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PLOG/ 0.25 2.50592e+29 -7.63488 3942.11/

PLOG/ 0.5 9.15912e+29 -7.67943 4095.32/

PLOG/ 0.75 1.69361e+30 -7.68948 4165.63/

PLOG/ 1 2.43637e+30 -7.68818 4204.93/

PLOG/ 2.5 4.61132e+30 -7.62012 4254.66/

PLOG/ 5 2.51134e+30 -7.42486 4142.65/

PLOG/ 7.5 9.60689e+29 -7.22913 3997.62/

PLOG/ 10 3.70875e+29 -7.05364 3861.02/

PLOG/ 50 2.02162e+24 -5.12877 2284.65/

PLOG/ 100 4.40977e+23 -4.79459 2256.07/

t-HCOOH => H2O + CO 0.331107 3.51493 59011.6

PLOG/ 0.001 0.331107 3.51493 59011.6/

PLOG/ 0.005 0.0186741 4.13581 59573.5/

PLOG/ 0.01 0.00356049 4.45738 59746.5/

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PLOG/ 1 5.8271e-14 8.3644 58464.4/

PLOG/ 2.5 5.5576e-17 9.37677 57749.1/

PLOG/ 5 4.58921e-19 10.068 57224/

PLOG/ 7.5 3.85222e-20 10.4232 56944.3/

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Mesmer input file:

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   <atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.867884" />
  </atomArray>
  <bondArray>
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  </bondArray>
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   </property>
   <property title="basis">
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   </property>
   <property title="File Format">
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   </property>
   <property title="Energy" dictRef="me:ZPE">
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   </property>
   <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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   </property>
   <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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   </property>
   <property title="Rotational Constants" dictRef="me:rotConsts">
    <array units="cm-1">18.639</array>
   </property>
   <property title="Symmetry Number" dictRef="me:symmetryNumber">
    <scalar>1</scalar>
   </property>
  </propertyList>
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  </molecule>

  <molecule id="TS2">
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/>
    <atom id="a2" elementType="H" x3="-0.751427" y3="-1.179626" z3="-0.599619" />
    <atom id="a3" elementType="O" spinMultiplicity="2" x3="1.079044" y3="-0.266315" z3="0.071832" />
    <atom id="a4" elementType="O" x3="-0.102117" y3="0.666740" z3="-0.079469" />
    <atom id="a5" elementType="H" x3="-1.760091" y3="-0.192024" z3="0.629509" />
   </atomArray>
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    <bond atomRefs2="a4 a1" order="1" />
    <bond atomRefs2="a4 a3" order="1" />
    <bond atomRefs2="a1 a5" order="1" />
   </bondArray>
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    </property>
    <property title="basis">
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    </property>
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    </property>
    <property title="ImaginaryFrequency" dictRef="me:imFreqs">
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    </property>
    <property title="Rotational Constants" dictRef="me:rotConsts">
     <array units="cm-1">1.450 0.515 0.396</array>
    </property>
    <property title="Symmetry Number" dictRef="me:symmetryNumber">
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    </property>
    <property dictRef="me:frequenciesScaleFactor" >
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    </property>
                                <property title="Transition State Optical Symmetry Number"
dictRef="me:TSOpticalSymmetryNumber">
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    </property>
   </propertyList>
   <me:DOSCMethod  name="QMRotors" />
  </molecule>
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     <atom id="a2" elementType="O" spinMultiplicity="2" x3="-1.286740" y3="-0.274126" z3="-0.015250"
/>
     <atom id="a3" elementType="H" x3="0.597517" y3="1.026027" z3="0.221192" />
     <atom id="a4" elementType="O" x3="1.322320" y3="-0.101944" z3="-0.102124" />
     <atom id="a5" elementType="H" x3="1.580000" y3="-0.775200" z3="0.545500" />
    </atomArray>
    <bondArray>
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     <bond atomRefs2="a2 a1" order="1" />
     <bond atomRefs2="a1 a3" order="1" />
    </bondArray>
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     </property>
     <property title="basis">
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     </property>
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     </property>
     <property title="ImaginaryFrequency" dictRef="me:imFreqs">
      <scalar units="cm-1">1732.01</scalar>
     </property>
     <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">2.779 0.282 0.260</array>
     </property>
     <property title="Symmetry Number" dictRef="me:symmetryNumber">
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     </property>
     <property dictRef="me:frequenciesScaleFactor" >
      <scalar>1</scalar>
     </property>
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     </property>
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    <me:DOSCMethod  name="QMRotors" />
   </molecule>

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     <atom id="a2" elementType="H" x3="0.077251" y3="1.156579" z3="-0.893125" />
     <atom id="a3" elementType="O" spinMultiplicity="2" x3="-1.080675" y3="-0.349410" z3="-0.008378"
/>
     <atom id="a4" elementType="O" spinMultiplicity="2" x3="1.082576" y3="-0.347479" z3="0.008142" />
     <atom id="a5" elementType="H" x3="-0.082728" y3="1.153978" z3="0.893960" />
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     <bond atomRefs2="a3 a1" order="1" />
     <bond atomRefs2="a1 a4" order="1" />
     <bond atomRefs2="a1 a5" order="1" />
    </bondArray>
    <propertyList>
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     </property>
     <property title="basis">
      <scalar>def2TZVP (5D, 7F)</scalar>
     </property>
     <property title="File Format">
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     </property>
                                    <property title="Energy" dictRef="me:ZPE">
      <scalar units="kJ/mol">-33.67</scalar>
     </property>
     <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
      <array units="cm-1">956.40 1019.93 1137.56 1238.96 1451.80 1627.75 3155.88 3214.58</array>
     </property>
     <property title="ImaginaryFrequency" dictRef="me:imFreqs">
      <scalar units="cm-1">1562.28</scalar>
     </property>
     <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">1.449 0.431 0.355</array>
     </property>
     <property title="Symmetry Number" dictRef="me:symmetryNumber">
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     </property>
     <property dictRef="me:frequenciesScaleFactor" >
      <scalar>1</scalar>
     </property>
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     </property>
    </propertyList>
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   </molecule>

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/>
      <atom id="a2" elementType="O" spinMultiplicity="2" x3="1.081266" y3="-0.349366" z3="-0.008389"
/>
      <atom id="a3" elementType="C" x3="0.001678" y3="0.543652" z3="0.000184" />
      <atom id="a4" elementType="H" x3="0.083738" y3="1.153956" z3="0.893694" />
      <atom id="a5" elementType="H" x3="-0.076810" y3="1.156232" z3="-0.893095" />
     </atomArray>
     <bondArray>
      <bond atomRefs2="a5 a3" order="1" />
      <bond atomRefs2="a2 a3" order="1" />
      <bond atomRefs2="a3 a1" order="1" />
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     </bondArray>
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      </property>
      <property title="basis">
       <scalar>def2TZVP (5D, 7F)</scalar>
      </property>
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      </property>
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      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
       <array units="cm-1">957.65 1015.74 1131.98 1239.04 1449.94 1625.08 3156.65 3214.81</array>
      </property>
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       <scalar units="cm-1">1538.52</scalar>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
       <array units="cm-1">1.451 0.431 0.355</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
       <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor" >
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      </property>
     </propertyList>
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    </molecule>

    <molecule id="TS6b" >
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/>
      <atom id="a2" elementType="C" x3="0.027402" y3="0.374178" z3="-0.018033" />
      <atom id="a3" elementType="H" x3="0.025218" y3="1.377809" z3="-0.429595" />
      <atom id="a4" elementType="O" spinMultiplicity="2" x3="-1.178195" y3="-0.251886" z3="-0.048014"
/>
      <atom id="a5" elementType="H" x3="-0.174688" y3="0.428668" z3="1.127464" />
     </atomArray>
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      <bond atomRefs2="a4 a2" order="1" />
      <bond atomRefs2="a1 a2" order="1" />
      <bond atomRefs2="a2 a5" order="1" />
     </bondArray>
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      </property>
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       <scalar units="kJ/mol">-41.29</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
       <array units="cm-1">654.05 1068.23 1174.01 1254.46 1418.50 1547.10 2604.37 3230.72</array>
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      <property title="Rotational Constants" dictRef="me:rotConsts">
       <array units="cm-1">2.318 0.367 0.336</array>
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    <atom id="a2" elementType="H" x3="-1.294872" y3="-0.069855" z3="-0.916990" />
    <atom id="a3" elementType="O" x3="0.395537" y3="0.786423" z3="-0.000009" />
    <atom id="a4" elementType="O" x3="0.475400" y3="-0.742493" z3="-0.000029" />
    <atom id="a5" elementType="H" x3="-1.294950" y3="-0.069824" z3="0.917024" />
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    <bond atomRefs2="a1 a5" order="1" />
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    </property>
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3328.88</array>
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    </property>
    <property dictRef="me:sigma" >
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    </property>
    <property dictRef="me:epsilon" >
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    </property>
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    </property>
   </propertyList>
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   <me:DistributionCalcMethod  name="Boltzmann" />
   <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1" referenceTemperature="298.0">123.214</me:deltaEDown>
    <me:deltaEDownTExponent referenceTemperature="298.0">0.741299</me:deltaEDownTExponent>
   </me:energyTransferModel>
  </molecule>
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```
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     <atom id="a3" elementType="O" spinMultiplicity="2" x3="-1.184776" y3="-0.288599" z3="-0.000109"
/>
     <atom id="a4" elementType="O" spinMultiplicity="2" x3="1.186034" y3="-0.287931" z3="-0.000048"
/>
     <atom id="a5" elementType="H" x3="0.000956" y3="1.047999" z3="-0.888505" />
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     <bond atomRefs2="a3 a1" order="1" />
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    </bondArray>
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     </property>
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     </property>
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3249.40</array>
     </property>
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     </property>
     <property title="Symmetry Number" dictRef="me:symmetryNumber">
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     </property>
     <property dictRef="me:sigma" >
      <scalar>3.79</scalar>
     </property>
     <property dictRef="me:epsilon" >
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     </property>
     <property dictRef="me:frequenciesScaleFactor" >
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     </property>
    </propertyList>
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    <me:DistributionCalcMethod  name="Boltzmann" />
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     <me:deltaEDown units="cm-1" referenceTemperature="298.0">123.214</me:deltaEDown>
     <me:deltaEDownTExponent referenceTemperature="298.0">0.741299</me:deltaEDownTExponent>
    </me:energyTransferModel>
   </molecule>

   <molecule id="t-HCOOH" >
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     <atom id="a1" elementType="O" x3="1.128563" y3="-0.264126" z3="0.000004" />
     <atom id="a2" elementType="C" x3="0.126590" y3="0.402678" z3="-0.000028" />
     <atom id="a3" elementType="H" x3="0.112189" y3="1.484238" z3="0.000104" />
     <atom id="a4" elementType="O" x3="-1.106977" y3="-0.091127" z3="-0.000006" />
     <atom id="a5" elementType="H" x3="-1.044420" y3="-1.058283" z3="0.000076" />
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     <bond atomRefs2="a2 a3" order="1" />
     <bond atomRefs2="a4 a5" order="1" />
    </bondArray>
    <propertyList>
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     </property>
     <property title="basis">
      <scalar>def2TZVP (5D, 7F)</scalar>
     </property>
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3732.96</array>
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     </property>
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      <scalar>3.79</scalar>
     </property>
     <property dictRef="me:epsilon" >
      <scalar>520.0</scalar>
     </property>
     <property dictRef="me:frequenciesScaleFactor" >
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     </property>
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   <me:DistributionCalcMethod  name="Boltzmann" />
   <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1" referenceTemperature="298.0">123.214</me:deltaEDown>
    <me:deltaEDownTExponent referenceTemperature="298.0">0.741299</me:deltaEDownTExponent>
   </me:energyTransferModel>
  </molecule>

</moleculeList>

<reactionList>

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    </reactant>
   </reactantList>
   <productList>
    <product>
     <molecule ref="cyc-H2COO" role="modelled" />
    </product>
   </productList>
   <me:transitionState>
    <molecule ref="TS2" role="transitionState" />
   </me:transitionState>
                <me:tunneling name="Eckart" />
   <me:MCRCMethod name="RRKM" />
  </reaction>

  <reaction id="R2">
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    <reactant>
     <molecule ref="cyc-H2COO" role="modelled" />
    </reactant>
   </reactantList>
   <productList>
    <product>
     <molecule ref="H2" role="sink" />
    </product>
    <product>
     <molecule ref="CO2" role="sink" />
    </product>
   </productList>
   <me:transitionState>
    <molecule ref="TS6" role="transitionState" />
   </me:transitionState>
                <me:tunneling name="Eckart" />
   <me:MCRCMethod name="RRKM" />
  </reaction>
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  <reactant>
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  </reactant>
 </reactantList>
 <productList>
  <product>
   <molecule ref="open-H2COO" role="modelled" />
  </product>
 </productList>
 <me:transitionState>
  <molecule ref="TS6a" role="transitionState" />
 </me:transitionState>
                <me:tunneling name="Eckart" />
 <me:MCRCMethod name="RRKM" />
</reaction>

<reaction id="R4" reversible="true">
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   <molecule ref="open-H2COO" role="modelled" />
  </reactant>
 </reactantList>
 <productList>
  <product>
   <molecule ref="t-HCOOH" role="modelled" />
  </product>
 </productList>
 <me:transitionState>
  <molecule ref="TS6b" role="transitionState" />
 </me:transitionState>
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 <me:MCRCMethod name="RRKM" />
</reaction>

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   <molecule ref="t-HCOOH" role="modelled" />
  </reactant>
 </reactantList>
 <productList>
  <product>
   <molecule ref="H2O" role="sink" />
  </product>
  <product>
   <molecule ref="CO" role="sink" />
  </product>
 </productList>
 <me:transitionState>
  <molecule ref="TS4" role="transitionState" />
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    </me:transitionState>
                    <me:tunneling name="Eckart" />
    <me:MCRCMethod name="RRKM" />
   </reaction>

   <reaction id="R5">
    <reactantList>
     <reactant>
      <molecule ref="t-HCOOH" role="modelled" />
     </reactant>
    </reactantList>
    <productList>
     <product>
      <molecule ref="HCO" role="sink" />
     </product>
     <product>
      <molecule ref="OH" role="sink" />
     </product>
    </productList>
     <me:MCRCMethod xsi:type="MesmerILT">
     <me:preExponential units="cm3molecule-1s-1" >1.83e-10</me:preExponential>
     <me:activationEnergy  units="kJ/mol" reverse="true">0.00</me:activationEnergy>
     <me:TInfinity>298.0</me:TInfinity>
     <me:nInfinity >0.0</me:nInfinity>
    </me:MCRCMethod>
   </reaction>

  </reactionList>

  <me:conditions>

   <me:bathGas>He</me:bathGas>

   <me:PTs>

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error="9.5">145</me:experimentalRate>
       </me:PTpair>
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error="13">272</me:experimentalRate>
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<me:PTpair units="Torr" P="401.5" T="475" precision="qd" bathGas="He" >
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error="29">376</me:experimentalRate>
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error="40">553</me:experimentalRate>
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error="351">2071</me:experimentalRate>
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   <me:InitialPopulation>
    <me:molecule ref="CH2OO" me:population="1.0" />
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 </me:conditions>

 <me:modelParameters>
  <me:grainSize units="cm-1">100</me:grainSize>
  <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
 </me:modelParameters>

 <me:control>
  <me:printSpeciesProfile />
  <me:eigenvalues>3</me:eigenvalues>
  <me:calcMethod  name="simpleCalc" />
 </me:control>
 <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
  <dc:title>Project name</dc:title>
  <dc:source>CH2OO_decomp-full.xml</dc:source>
  <dc:creator>Mesmer v5.2</dc:creator>
  <dc:date>20190826_122934</dc:date>
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    <dc:contributor>praseal</dc:contributor>
  </metadataList>
</me:mesmer>
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