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Electronic Supplementary Material (ESI) for:

Solving the discrepancy between the direct and relative-rate determinations of unimolecular reaction kinetics of dimethyl-substituted Criegee intermediate $(CH_3)_2COO$ using a new photolytic precursor

Jari Peltola, Prasenjit Seal, Niko Vuorio, Petri Heinonen, and Arkke Eskola*
Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I. Virtasen aukio 1), FI-00014, Helsinki, Finland
*Corresponding author: arkke.eskola@helsinki.fi

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The determination of the effective optical path length, and the initial $(CH_3)_2COO$ concentration

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 (5.07 ± 0.10) ppm NO_2 in N_2 -sample in reactor at 20 Torr and 296 K. The observed absorbance ($A_{NO2,\lambda}$) between wavelengths of 300 nm and 450 nm is

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

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

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

The average effective OPL at 338 nm (with the wavelength resolution of 4 nm) is about 75 m. The initial concentration of $(CH_3)_2COO$ is calculated from the observed initial absorbance ($A_{0,(CH3)2COO}$) at 338 nm as

$$[(CH_3)_2COO]_0 = A_{0,(CH3)2COO}/(\sigma_{(CH3)2COO} \times OPL). \quad (S3)$$

The $(CH_3)_2COO$ absorption cross-section ($\sigma_{(CH3)2COO}$) at 338 nm at is about 1.70×10^{-17} cm^2 $molecule^{-1}$.[1]

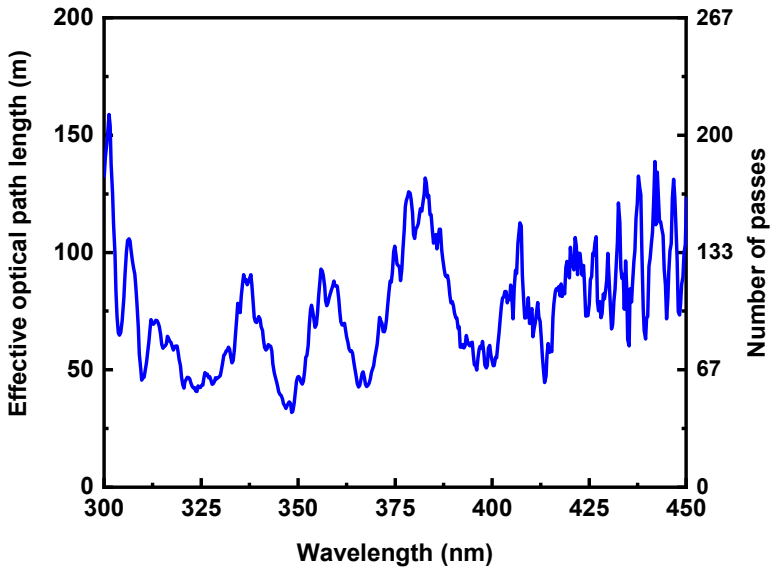

Figure S1. Determination of the effective optical path length of the TR-BB-CEAS cavity.

Synthesis of the 2-bromo-2-iodopropane precursor

2-Bromopropene (48.9 g, 0.40 mol) was dissolved in trifluoroacetic acid (150 mL) and potassium iodide (60.4 g, 0.364 mol) was added. The reaction was monitored by 1H NMR and stopped after 8 h reaction time at 43% conversion. The reaction mixture was diluted with pentane, washed 5 times with water and dried over $MgSO_4$. The evaporation of the solvent and distillation at reduced pressure (53–55 °C / 35 mmHg) gave the title compound (19.7 g, 20%). Traces of iodine were removed by shaking the neat compound with solid $Na_2S_2O_3$ followed by distillation in high vacuum. The distillate was collected into a receiver flask cooled in dry ice acetone bath. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.76 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.46, 27.06. IR (ATR, liquid film) ν_{max} / cm^{-1} 1152.2, 1086.2s, 566.0s, 459.3. According to NMR analysis, the residual trifluoroacetic acid concentration in the product is <0.01 wt%, resulting in $[CF_3COOH]_{max} < 2 \times 10^{10}$ molecule cm^{-3} in the reactor at the highest $[(CH_3)_2ClBr] = 6.3 \times 10^{13}$ molecule cm^{-3} used. Despite the very large bimolecular reaction rate coefficient, $k((CH_3)_2COO + CF_3COOH)(294K) = 6.1 \times 10^{-10}$ cm^3 s^{-1}, [2] the small residual $[CF_3COOH]$ had negligible (< 15 s^{-1}) effect on kinetics of $(CH_3)_2COO$.

The heating and cooling methods of the flow tube reactor

The method described in our previous publication[3] was used to heat the flow tube reactor. Two temperature-controlled custom-made aluminum blocks were placed around the quartz-glass reactor tube. Each aluminum block has four 300 W cartridge heaters that are regulated using a LabVIEW based PID-controller program. The gases were pre-heated close to the setpoint temperature before entering the reactor. Temperature of the gas flow was measured continuously using a K-type thermocouple, which tip was placed in the middle of reactor axial direction just outside the radial area filled by the photolysis beam. The linear gas flow speed was about 1 ms^{-1}, ensuring that the gas mixture was completely replaced between photolysis laser pulses with a repetition rate of 1 Hz. Complete axial temperature profile within the overlap volume of the probe and the photolysis beams were measured separately for all experimental conditions (temperature, pressure, and flow rate) used in this work. The observed temperature 2σ uncertainty in the measurement range 296–340 K was ≤ ±1.0 K.

For reactor cooling, the quartz-glass tube was replaced with a stainless steel reactor tube that was coated with halocarbon wax. Similar aluminum blocks to heating were constructed also for cooling. They were fitted with copper tubes connected to an external cooling bath circulation (Heto-Holten CBN 28-90/HMT 4000). Ethanol was employed as a heat transfer fluid below ambient temperature. The gases were pre-cooled close to the setpoint temperature before entering into the reactor. The observed temperature 2σ uncertainty in the measurement range 243–310 K was ≤ ±1.2 K.

Determination of k_{uni} from the absorption trace of $(CH_3)_2COO$ and the diffusion loss of $(CH_3)_2COO$

As is mentioned in the main text, the observed decay of $(CH_3)_2COO$ mainly contain contributions from the thermal unimolecular reaction and self-reaction, but also a small contribution from the gas diffusion loss and to some small extend from the possible reaction with other reactive species. The rate equation to describe the loss of $(CH_3)_2COO$ can be written as

$$-\frac{d[(\mathrm{CH_3})_2\mathrm{COO}]}{dt} = k_{\mathrm{uni}}[(\mathrm{CH_3})_2\mathrm{COO}] + 2k_{\mathrm{self}}[(\mathrm{CH_3})_2\mathrm{COO}]^2 + k_{\mathrm{bi}}[\mathrm{X}][(\mathrm{CH_3})_2\mathrm{COO}] + k_{\mathrm{loss}}[(\mathrm{CH_3})_2\mathrm{COO}] = (k_{\mathrm{uni}} + k_{\mathrm{loss}} + 2k_{\mathrm{self}}[(\mathrm{CH_3})_2\mathrm{COO}] + k_{\mathrm{bi}}[\mathrm{X}])[(\mathrm{CH_3})_2\mathrm{COO}], \quad \text{(S4)}$$

where k_{uni} is the unimolecular reaction rate coefficient, k_{self} is the rate coefficient for the self-reaction $(CH_3)_2COO$ + $(CH_3)_2COO$, [X] is the total concentration of other possible reactive species contributing to the bimolecular loss (originating, for example, from $(CH_3)_2COO$ + Br reaction) with a combined rate coefficient k_{bi}, and k_{loss} is the diffusion loss rate coefficient. Although the self-reaction rate coefficient for $(CH_3)_2COO$ is large, (6.0 ± 1.1) × 10^{-10} cm^3 $molecule^{-1}$ s^{-1},[4] the thermal unimolecular reaction is the main loss mechanism in the current system due to the low initial $(CH_3)_2COO$ concentration (typically $[(CH_3)_2COO]_0 < 10^{11}$ molecule cm^{-3}) used in the measurements. Thus, the decay traces of $(CH_3)_2COO$ were fitted to an integrated first order decay expression, which is derived from the simplified model (Equation S5), where the term $2k_{self}[(CH_3)_2COO] + k_{bi}[X]$ of Equation S4 is approximated as a constant $k_{eff}[X_{eff}]$[5]

$$-\frac{d[(\mathrm{CH_3})_2\mathrm{COO}]}{dt} = (k_{\mathrm{uni}} + k_{\mathrm{loss}} + k_{\mathrm{eff}}[\mathrm{X_{eff}}])[(\mathrm{CH_3})_2\mathrm{COO}] = k_{\mathrm{obs}}[(\mathrm{CH_3})_2\mathrm{COO}]. \quad \text{(S5)}$$

The integrated first-order decay expression is

$$[(CH_3)_2COO]_t = [(CH_3)_2COO]_0 \times exp(-k_{obs}), \quad \text{(S6)}$$

where k_{obs} is the obtained first-order decay rate coefficient, $[(CH_3)_2COO]_t$ is the $(CH_3)_2COO$ concentration at time t, $[(CH_3)_2COO]_0$ is the initial $(CH_3)_2COO$ concentration (at time t=0). This simplified method to describe the loss of $(CH_3)_2COO$ and the use of single-exponential fitting method has been tested previously by Smith et al.[5] in the similar unimolecular decompositioin study of $(CH_3)_2COO$. The single-exponential function fits reasonably well with the absorption traces, although the observed absorbance can be slightly higher than the fitted value just after the photolysis.

In the main text, Figure 2c shows the linear relationship of obtained first-order decay rate coefficients (k_{obs}) with respect to $[(CH_3)_2COO]_0$ under two different temperature and pressure conditions. The linear behavior suggests that $[X_{eff}]$ is proportional to $[(CH_3)_2COO]_0$. This is expected since most of the reactive species, as well as $(CH_3)_2COO$, are formed at small concentrations proportional to $[(CH_3)_2ClBr]_0$ and the laser pulse energy (assuming there are no other reactive species in the precursor mixture). Extrapolating the k_{obs} to zero $[(CH_3)_2COO]_0$ removes the effect of radical – radical processes. Hence, the unimolecular reaction rate coefficient of $(CH_3)_2COO$ can be determined from the intercept (k_{ic}) of the linear least squares fit to the obtained kinetic data.

As is mentioned in the main text, a constant positive baseline offset was observed when $(CH_3)_2ClBr$ was used as photolytic source, especially, in the kinetic measurements above room temperature (see Fig. 2a and Fig. S2). Depletion of $(CH_3)_2ClBr$ does not cause a negative baseline shift of the measured absorption signal, such as the use of $(CH_3)_2CI_2$ in the study of Smith et al.,[5] due to the significantly lower absorption of $(CH_3)_2ClBr$ at 340 nm region.

The offset value increases when $[(CH_3)_2COO]_0$ increases, but maintains its relative value with respect to absorbance (see Fig. S2). The offset is independent of pressure, but increases as temperature increases, indicating possible absorption by a formed (seemingly nonreactive within the experimental time-scale ~ 50 ms) product, which may have formed, for example, in the photodissociation of $(CH_3)_2ClBr$ (see Fig. 2 and Fig. S3). Overall, the positive baseline offset was between about 9% (at 243 K) and 20% (at 340 K) of the $(CH_3)_2COO$ absorption. The baseline offset has been taken into account in the fitting of the first-order single exponential decays. Assuming that formed product does not react with $(CH_3)_2COO$ (or other reactive species) and, therefore, does not decay within a (short) measurement timescale, we can use the following equation (Equation 3 in the main text) for the absorption traces,

$$A_t = A_0 \times exp(-k_{obst}) + A_{offset}, \quad \text{(S7)}$$

where k_{obs} is the obtained first-order decay rate coefficient, A_t is the absorbance at time t, A_0 is the initial absorbance (at time t=0), and A_{offset} is the constant absorbance caused by nonreactive species (formed at time t=0). Figure S3 shows two examples of measured transient absorption traces of $(CH_3)_2COO$ at 243 K and 340 K. The complete experimental conditions and results for the fittings of the data measured at different temperatures are shown in Table S2.

An exercise was performed to fit Figure S3b signal also with an expression $A_t = A_0 \times exp(-k_{obs}) + A_{offset} \times (1\text{-}exp(-k_{obs}))$, corresponding to situation where positive baseline offset is formed with the same rate as $(CH_3)_2COO$ is decayed. This would correspond to a situation, where $(CH_3)_2COO$ unimolecularly reacts and form a product that absorbs at the detection wavelength, see Figure S4. Interestingly, fits $A_t = A_0 \times exp(-k_{obst}) + A_{offset}$ and $A_t = A_0 \times exp(-k_{obs}) + A_{offset} \times (1\text{-}exp(-k_{obs}))$ returned very similar values,

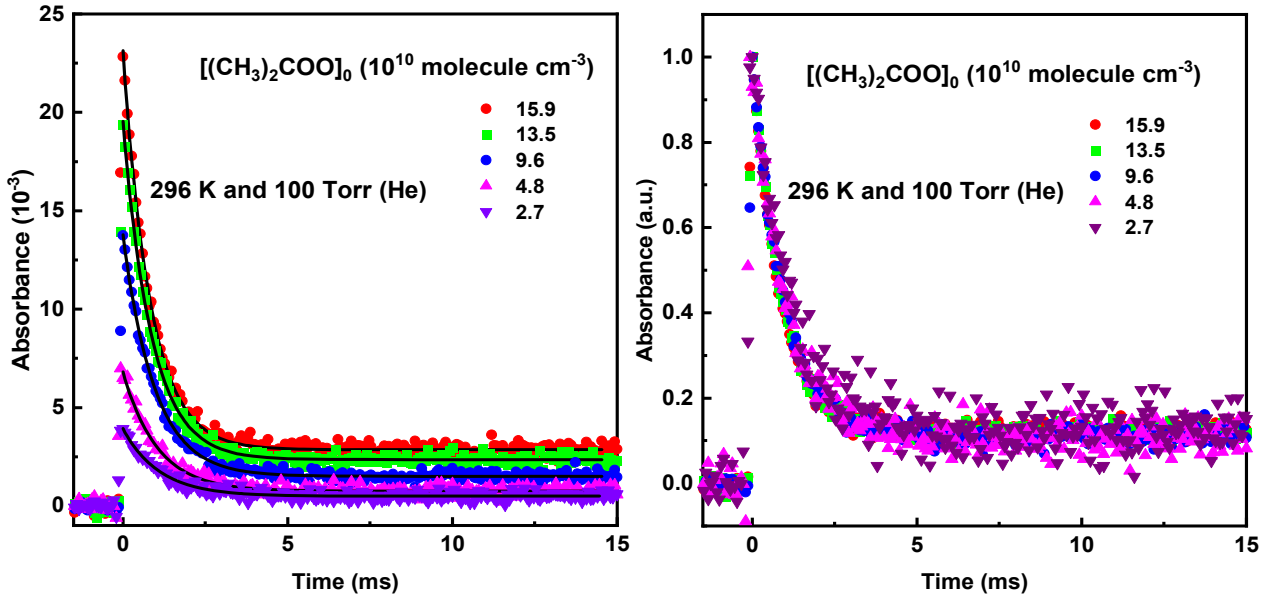

Figure S2. The decay trace of $(CH_3)_2COO$ for various initial $[(CH_3)_2COO]_0$ at 296 K and 100 Torr (in He). On the left is Figure 2a of the main text. On the right are the relative absorbances of Figure 2a. The $(CH_3)_2COO$ traces were probed at 338 nm with a time resolution of 67 μs.

k_{obs} = 5903 s^{-1} and k_{obs} = 6000 s^{-1}, giving difference < 2 %. This shows that regardless of the exact mechanism of positive baseline offset formation, the current fittings and results are reliable.

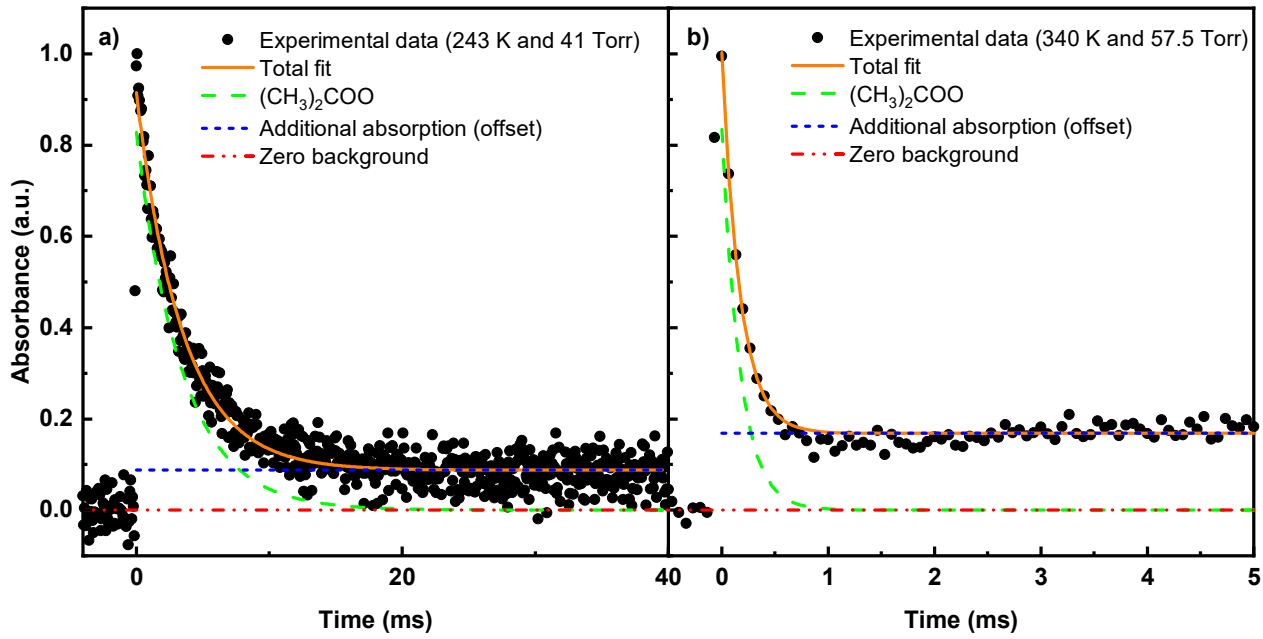

Figure S3. The transient absorption signals of $(CH_3)_2COO$ at a) 243 K and 41 Torr (in N_2) and at b) 340 K and 57.5 Torr (in He). $(CH_3)_2CIBr$ used as photolytic source. The $(CH_3)_2COO$ traces were probed at 338 nm with a time resolution of 67 µs.

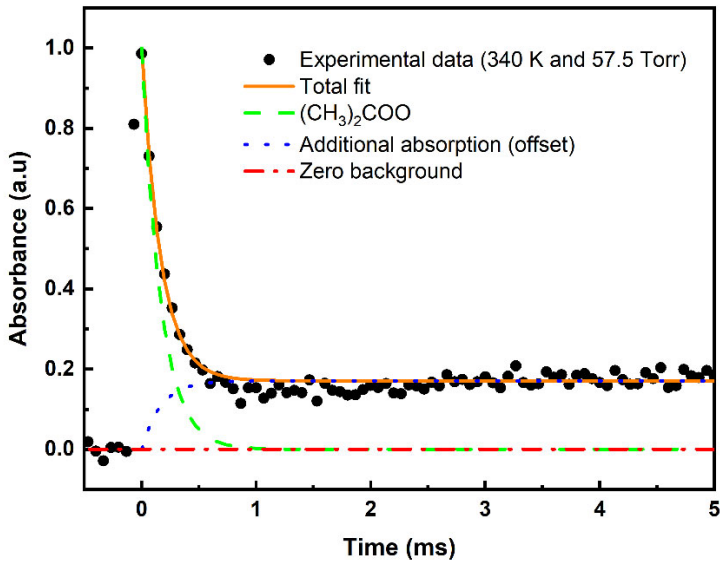

Figure S4. The transient absorption signal of $(CH_3)_2COO$ at 340 K and 57.5 Torr (in He) from Figure S3b fitted with function $A_t = A_0 \times exp(-k_{obs}) + A_{offset} \times (1\text{-}exp(-k_{obs}))$ and returning value k_{obs} = 6000 s^{-1}. This value can be compared with the original fitted value 5903 s^{-1} obtained using expression S7 above. $(CH_3)_2CIBr$ used as photolytic source. The $(CH_3)_2COO$ traces were probed at 338 nm with a time resolution of 67 µs.

The diffusion loss (k_{loss}), which originates from the diffusion out of the measurement volume (mainly in radial direction), was determined by measuring the diffusion loss of CH_2OO under the same experimental conditions with the TR-BB-CEAS-apparatus. The thermal decomposition rate coefficient of CH_2OO is negligible below 375 K.[3,6] Approximating the diffusivities of CH_2OO and $(CH_3)_2COO$ with those of HCOOH and $CH_3(CH_3)CHCOOH$,[7] we obtain for the k_{uni} = $k_{ic}((CH_3)_2COO)$ – $k_{loss}((CH_3)_2COO)$ = $k_{ic}((CH_3)_2COO)$ – $D(CH_3(CH_3)CHCOOH)/D(HCOOH) \times k_{loss}(CH_2OO)$ = $k_{ic}((CH_3)_2COO) – 0.52 \times k_{loss}(CH_2OO)$ at a given temperature and total density. All the transient absorption traces of CH_2OO were measured at 338 nm and fitted to first-order, single exponential decay function. The initial CH_2OO concentration used in the measurements was below 2.0×10^{11} molecule cm^{-3}**,** which efficiently suppressed radical-radical, especially CH_2OO - CH_2OO, reactions. The values of $k_{loss}(CH_2OO)$ at each total density stay almost constant in all temperatures. The diffusion depends on the buffer-gas and Table S1 presents the obtained $k_{loss}(CH_2OO)$ values in the experimental conditions used in this work. The $k_{loss}(CH_2OO)$ values measured in helium buffer-gas (296–340 K) are taken from our previous unimolecular decomposition study of CH_2OO.[3]

Table S1 The obtained $k_{loss}(CH_2OO)$ values in the experimental conditions used in this work. The $k_{loss}(CH_3)_2COO)$ values are calculated as $0.52 \times k_{loss}(CH_2OO)$.

T(K)	[a][N_2] ($\times 10^{18}$ molecule cm^{-3})	k_{loss} (CH_2OO) (s^{-1})	k_{loss} ($(CH_3)_2COO$) (s^{-1})	*T*(K)	[a][He] ($\times 10^{18}$ molecule cm^{-3})	[b]k_{loss} (CH_2OO) (s^{-1})	k_{loss} ($(CH_3)_2COO$) (s^{-1})
243–	0.16	30	16	296–	0.16	100	52
310	0.33	20	10	340	0.33	62	32
	1.6	10	5		1.6	29	15
	3.3	7	4		3.3	24	12
	6.5	5	3		6.5	19	10

[a]The fixed O_2 concentration was ~4×10^{16} molecule $cm^{-3}$and the initial CH_2OO concentration was below 2.0×10^{11} molecule cm^{-3}. [b]Taken from our previous study.[3]

Table S2 Results and conditions of the unimolecular reaction kinetic experiments of $(CH_3)_2COO$ presented in this study. Some of the pressures have been measured twice and the average of the measurements is reported in the article.

T(K)	Total number density ($\times10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times10^{-3}$)	Baseline shift ($\times10^{-3}$)	ΔA Criegee ($\times10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times10^{10}$ molecule cm^{-3})
243	0.16	N_2	4.1	222 ± 7	3.99	5.66	2772	8.42	0.87	7.55	5.92
	0.16	N_2	4.1	166 ± 8	2.06	5.66	2228	4.65	0.42	4.23	3.32
	0.16	N_2	4.1	141 ± 9	1.12	5.66	3664	2.73	0.28	2.45	1.92
	0.16	N_2	4.1	311 ± 10	5.15	4.53	1775	12.17	1.28	10.89	8.54
	0.16	N_2	4.1	258 ± 7	4.23	4.53	3352	9.75	0.96	8.79	6.90
	0.16	N_2	4.1	171 ± 8	2.20	4.53	2196	4.95	0.32	4.63	3.63
	0.16	N_2	4.1	139 ± 10	1.22	4.53	3238	2.83	0.20	2.63	2.06
	0.33	N_2	8.2	352 ± 11	5.26	4.53	1792	13.95	1.38	12.57	9.86
	0.33	N_2	8.2	299 ± 9	4.26	4.53	2097	11.37	1.05	10.32	8.09
	0.33	N_2	8.2	197 ± 9	2.20	4.53	2209	5.88	0.48	5.40	4.24
	0.33	N_2	8.2	151 ± 9	1.21	4.53	3722	3.26	0.30	2.96	2.32
	1.6	N_2	41	288 ± 10	4.63	3.96	1504	10.07	0.96	9.11	7.15
	1.6	N_2	41	236 ± 8	3.75	3.96	2431	8.06	0.75	7.31	5.73
	1.6	N_2	41	160 ± 9	1.91	3.96	2962	4.00	0.35	3.65	2.86
	1.6	N_2	41	114 ± 10	1.47	3.96	5007	2.20	0.16	2.04	1.60
	3.3	N_2	82	223 ± 6	5.50	3.96	3307	8.34	0.89	7.45	5.84
	3.3	N_2	82	202 ± 8	4.44	3.96	2103	6.89	0.60	6.29	4.94
	3.3	N_2	82	122 ± 8	2.30	3.96	3134	3.38	0.23	3.15	2.47
	3.3	N_2	82	97 ± 8	1.28	3.96	6139	1.88	0.18	1.70	1.34
	3.3	N_2	82	240 ± 9	4.79	3.96	2148	7.68	0.69	6.99	5.48
	3.3	N_2	82	201 ± 8	3.89	3.96	3234	5.93	0.48	5.45	4.28
	3.3	N_2	82	133 ± 7	2.04	3.96	6152	2.91	0.18	2.73	2.14
	3.3	N_2	82	77 ± 8	1.12	3.96	9108	1.44	0.00	1.44	1.13

T(K)	Total number density ($\times10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times10^{-3}$)	Baseline shift ($\times10^{-3}$)	ΔA Criegee ($\times10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times10^{10}$ molecule cm^{-3})
253	0.16	N_2	4.3	288 ± 10	4.67	5.66	1301	10.96	1.18	9.78	7.67
	0.16	N_2	4.3	264 ± 10	3.74	5.66	1432	9.33	0.93	8.40	6.59
	0.16	N_2	4.3	191 ± 7	1.97	5.66	3823	4.60	0.39	4.21	3.30
	0.16	N_2	4.3	155 ± 9	1.08	5.66	5048	2.58	0.22	2.36	1.85
	0.16	N_2	4.3	301 ± 10	4.75	3.96	1932	10.41	1.12	9.29	7.29
	0.16	N_2	4.3	284 ± 9	3.87	3.96	3650	8.73	0.90	7.83	6.14
	0.16	N_2	4.3	198 ± 10	2.02	3.96	3335	4.31	0.43	3.88	3.04
	0.16	N_2	4.3	165 ± 15	1.12	3.96	3011	2.44	0.25	2.19	1.72
	0.33	N_2	8.5	345 ± 9	4.78	4.53	2470	12.55	1.20	11.35	8.90
	0.33	N_2	8.5	311 ± 8	3.85	4.53	2449	10.65	0.98	9.67	7.59
	0.33	N_2	8.5	217 ± 8	1.99	4.53	2776	5.33	0.46	4.87	3.82
	0.33	N_2	8.5	157 ± 8	1.13	4.53	5331	2.93	0.26	2.67	2.10
	0.33	N_2	8.5	397 ± 11	4.83	4.53	2042	13.24	1.34	11.90	9.34
	0.33	N_2	8.5	334 ± 9	3.93	4.53	3262	10.15	0.97	9.18	7.20
	0.33	N_2	8.5	228 ± 9	2.04	4.53	3737	5.04	0.39	4.65	3.65
	0.33	N_2	8.5	193 ± 11	1.12	4.53	6186	3.28	0.30	2.98	2.33
	1.6	N_2	42.6	334 ± 11	4.63	4.53	2295	6.82	0.61	6.21	4.87
	1.6	N_2	42.6	283 ± 9	3.78	4.53	2984	5.39	0.47	4.92	3.86
	1.6	N_2	42.6	202 ± 10	1.96	4.53	4163	2.56	0.20	2.36	1.85
	1.6	N_2	42.6	165 ± 14	1.09	4.53	4611	1.40	0.14	1.26	0.99
	1.6	N_2	42.6	361 ± 9	4.75	4.53	2786	12.32	1.29	11.03	8.65
	1.6	N_2	42.6	319 ± 10	3.83	4.53	2429	10.19	1.07	9.12	7.15
	1.6	N_2	42.6	218 ± 10	1.97	4.53	3255	5.11	0.50	4.61	3.61
	1.6	N_2	42.6	172 ± 12	1.09	4.53	3553	2.89	0.32	2.57	2.02
	3.3	N_2	85.3	325 ± 12	4.79	4.53	1540	10.27	0.74	9.53	7.47
	3.3	N_2	85.3	290 ± 11	3.86	4.53	2105	8.56	0.70	7.86	6.16
	3.3	N_2	85.3	211 ± 11	2.01	4.53	3313	4.29	0.41	3.88	3.04
	3.3	N_2	85.3	149 ± 12	1.11	4.53	3895	2.31	0.19	2.12	1.66

T(K)	Total number density ($\times10^{18}$ molecule cm^{-3})	Buffer gas	[a] p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times10^{-3}$)	Baseline shift ($\times10^{-3}$)	ΔA Criegee ($\times10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times10^{10}$ molecule cm^{-3})
263	0.16	N_2	4.4	327 ± 10	4.67	4.53	1914	10.08	0.96	9.12	7.16
	0.16	N_2	4.4	302 ± 10	3.81	4.53	2010	8.23	0.75	7.48	5.87
	0.16	N_2	4.4	229 ± 11	1.94	4.53	3517	4.03	0.34	3.69	2.89
	0.16	N_2	4.4	200 ± 11	1.04	4.53	7885	2.29	0.21	2.08	1.63
	0.16	N_2	4.4	356 ± 15	4.75	3.96	1306	9.83	0.95	8.88	6.96
	0.16	N_2	4.4	318 ± 11	3.89	3.96	2716	8.07	0.79	7.28	5.71
	0.16	N_2	4.4	253 ± 12	2.04	3.96	3362	4.24	0.31	3.93	3.08
	0.16	N_2	4.4	208 ± 17	1.13	3.96	3652	2.32	0.15	2.17	1.71
	0.33	N_2	8.9	377 ± 13	4.74	4.53	1481	12.23	1.14	11.09	8.70
	0.33	N_2	8.9	350 ± 10	3.85	4.53	2302	10.33	0.87	9.46	7.42
	0.33	N_2	8.9	247 ± 11	1.99	4.53	2988	5.02	0.43	4.59	3.60
	0.33	N_2	8.9	230 ± 13	1.13	4.53	4789	3.09	0.26	2.83	2.22
	0.33	N_2	8.9	380 ± 13	4.83	3.96	1849	10.78	1.13	9.65	7.57
	0.33	N_2	8.9	330 ± 13	3.92	3.96	1746	8.72	0.84	7.88	6.18
	0.33	N_2	8.9	253 ± 13	2.05	3.96	3108	4.36	0.40	3.96	3.11
	0.33	N_2	8.9	222 ± 18	1.13	3.96	2914	2.62	0.22	2.40	1.88
	1.6	N_2	44.3	345 ± 12	4.60	4.53	1669	9.81	1.05	8.76	6.87
	1.6	N_2	44.3	316 ± 11	3.78	4.53	2438	8.28	0.83	7.45	5.84
	1.6	N_2	44.3	233 ± 11	2.30	4.53	3167	4.26	0.39	3.87	3.03
	1.6	N_2	44.3	206 ± 16	1.08	4.53	3540	2.44	0.23	2.21	1.74
	1.6	N_2	44.3	300 ± 13	4.71	3.96	1754	7.30	0.64	6.66	5.22
	1.6	N_2	44.3	280 ± 13	3.83	3.96	2300	5.78	0.44	5.34	4.19
	1.6	N_2	44.3	226 ± 15	1.99	3.96	3905	3.01	0.26	2.75	2.15
	1.6	N_2	44.3	175 ± 15	1.09	3.96	6874	1.62	0.11	1.51	1.18
	3.3	N_2	88.7	411 ± 13	4.78	4.53	1612	11.95	1.15	10.80	8.47
	3.3	N_2	88.7	357 ± 11	3.81	4.53	2372	9.94	0.89	9.05	7.09
	3.3	N_2	88.7	259 ± 10	1.99	4.53	3792	5.10	0.50	4.60	3.60

T(K)	3.3 Total number density ($\times10^{18}$ molecule cm^{-3})	N_2 Buffer gas	88.7 ^{a}p (Torr)	198 ± 14 k_{obs} (s^{-1})	1.09 $[(CH_3)_2ClBr]_0$ ($\times10^{13}$ molecule cm^{-3})	4.53 Laser intensity (mJ cm^{-2})	3776 Number of average	2.38 ΔA ($\times10^{-3}$)	0.03 Baseline shift ($\times10^{-3}$)	2.35 ΔA Criegee ($\times10^{-3}$)	1.84 $[(CH_3)_2COO]_0$ ($\times10^{10}$ molecule cm^{-3})
263	3.3	N_2	88.7	408 ± 12	4.75	3.96	2037	11.74	1.06	10.68	8.38
	3.3	N_2	88.7	250 ± 12	2.03	3.96	2989	4.83	0.39	4.44	3.48
	3.3	N_2	88.7	210 ± 17	1.11	3.96	3730	2.58	0.32	2.26	1.77
273	0.16	N_2	4.6	419 ± 14	4.67	4.53	2014	10.21	1.04	9.17	7.19
	0.16	N_2	4.6	384 ± 12	3.81	4.53	2716	8.46	0.81	7.65	6.00
	0.16	N_2	4.6	307 ± 14	1.95	4.53	3636	4.23	0.32	3.91	3.07
	0.16	N_2	4.6	286 ± 18	1.13	4.53	5282	2.55	0.22	2.33	1.83
	0.16	N_2	4.6	423 ± 21	5.03	3.96	1158	8.83	0.81	8.02	6.29
	0.16	N_2	4.6	307 ± 17	2.14	3.96	5115	3.39	0.28	3.11	2.44
	0.16	N_2	4.6	285 ± 24	1.18	3.96	6285	1.92	0.14	1.78	1.40
	0.33	N_2	9.2	421 ± 15	4.91	3.96	2017	9.31	0.90	8.41	6.60
	0.33	N_2	9.2	406 ± 18	3.97	3.96	1976	7.67	0.66	7.01	5.50
	0.33	N_2	9.2	308 ± 14	2.07	3.96	4961	3.81	0.30	3.51	2.75
	0.33	N_2	9.2	316 ± 29	1.13	3.96	4116	2.14	0.17	1.97	1.55
	1.6	N_2	46	574 ± 16	5.09	4.53	1624	15.82	1.53	14.29	11.21
	1.6	N_2	46	532 ± 14	4.09	4.53	2229	13.08	1.24	11.84	9.29
	1.6	N_2	46	402 ± 14	2.12	4.53	3714	6.41	0.57	5.84	4.58
	1.6	N_2	46	324 ± 19	1.16	4.53	4400	3.43	0.29	3.14	2.46
	3.3	N_2	92.1	493 ± 20	4.83	3.96	1842	10.18	0.80	9.38	7.35
	3.3	N_2	92.1	469 ± 18	3.92	3.96	2105	9.19	0.65	8.54	6.70
	3.3	N_2	92.1	366 ± 21	2.05	3.96	3492	4.16	0.33	3.83	3.01
	3.3	N_2	92.1	330 ± 29	1.13	3.96	4324	2.42	0.17	2.25	1.76
283	0.16	N_2	4.8	523 ± 22	4.78	4.53	2182	8.79	0.90	7.89	6.19
	0.16	N_2	4.8	422 ± 22	3.00	4.53	2142	5.78	0.52	5.26	4.12
	0.16	N_2	4.8	405 ± 26	2.07	4.53	3146	3.94	0.34	3.60	2.82
	0.16	N_2	4.8	403 ± 28	1.13	4.53	5974	2.48	0.25	2.23	1.75

T(K)	Total number density ($\times10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times10^{-3}$)	Baseline shift ($\times10^{-3}$)	ΔA Criegee ($\times10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times10^{10}$ molecule cm^{-3})
283	0.16	N_2	4.8	628 ± 21	5.02	4.53	2161	12.79	1.56	11.239	8.81
	0.16	N_2	4.8	542 ± 19	4.09	4.53	2842	10.14	1.11	9.03	7.08
	0.16	N_2	4.8	433 ± 27	2.16	4.53	2586	4.85	0.46	4.39	3.44
	0.16	N_2	4.8	416 ± 37	1.19	4.53	3739	2.79	0.22	2.57	2.01
	0.33	N_2	9.6	547 ± 23	4.90	3.40	2135	8.42	0.82	7.60	5.96
	0.33	N_2	9.6	505 ± 29	3.98	3.40	1772	6.64	0.61	6.03	4.73
	0.33	N_2	9.6	432 ± 29	2.08	3.40	4443	3.24	0.26	2.98	2.34
	0.33	N_2	9.6	354 ± 35	1.15	3.40	6517	1.78	0.17	1.61	1.26
	1.6	N_2	47.8	740 ± 19	4.89	5.10	1995	16.20	1.55	14.65	11.50
	1.6	N_2	47.8	680 ± 20	3.97	5.10	2078	13.53	1.28	12.25	9.61
	1.6	N_2	47.8	564 ± 25	2.05	5.10	2988	6.81	0.61	6.20	4.86
	1.6	N_2	47.8	523 ± 33	1.13	5.10	4377	3.82	0.34	3.48	2.73
	3.3	N_2	95.5	643 ± 25	4.83	3.96	2286	9.87	0.80	9.07	7.12
	3.3	N_2	95.5	625 ± 34	3.90	3.96	1744	7.86	0.64	7.22	5.67
	3.3	N_2	95.5	527 ± 43	2.01	3.96	2587	3.91	0.33	3.58	2.81
	3.3	N_2	95.5	454 ± 50	1.11	3.96	4175	2.17	0.18	1.99	1.56
296	0.16	N_2	5	851 ± 54	4.99	3.96	2548	7.04	0.72	6.32	4.96
	0.16	N_2	5	758 ± 54	4.08	3.96	3042	5.19	0.49	4.70	3.69
	0.16	N_2	5	690 ± 75	2.14	3.96	5022	2.46	0.21	2.25	1.77
	0.16	N_2	5	657 ± 105	1.19	3.96	7000	1.39	0.14	1.25	0.99
	0.33	N_2	10	962 ± 41	4.79	3.96	1929	12.79	1.47	11.32	8.88
	0.33	N_2	10	921 ± 38	3.90	3.96	2999	10.35	1.13	9.22	7.23
	0.33	N_2	10	791 ± 52	2.03	3.96	2891	5.31	0.50	4.81	3.77
	0.33	N_2	10	697 ± 61	1.10	3.96	5173	2.94	0.25	2.69	2.11
	0.33	N_2	10	1191 ± 29	6.23	3.40	1904	18.71	3.05	15.66	12.28
	0.33	N_2	10	1066 ± 29	5.04	3.40	2035	15.35	2.39	12.96	10.17
	0.33	N_2	10	917 ± 29	3.40	3.40	2574	10.68	1.51	9.16	7.19

	0.33	N_2	10	807 ± 39	1.79	3.40	4333	5.34	0.63	4.71	3.70
T(K)	Total number density ($\times 10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times 10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times 10^{-3}$)	Baseline shift ($\times 10^{-3}$)	ΔA Criegee ($\times 10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times 10^{10}$ molecule cm^{-3})
296	1.6	N_2	50	1289 ± 31	6.09	3.40	2303	19.61	2.57	17.04	13.37
	1.6	N_2	50	1195 ± 26	4.90	3.40	3407	15.84	2.05	13.79	10.82
	1.6	N_2	50	1083 ± 29	3.31	3.40	3587	11.13	1.33	9.80	7.69
	1.6	N_2	50	1010 ± 41	1.75	3.40	4254	6.19	0.70	5.49	4.31
	6.5	N_2	200	1335 ± 31	6.28	3.40	1718	21.55	2.65	18.90	14.82
	6.5	N_2	200	1304 ± 34	5.04	3.40	1535	18.52	2.18	16.34	12.82
	6.5	N_2	200	1180 ± 29	3.40	3.40	3393	13.12	1.44	11.68	9.16
	6.5	N_2	200	1056 ± 40	1.78	3.40	3937	7.18	0.81	6.37	5.00
310	0.33	N_2	10.5	1602 ± 68	4.20	3.40	2260	12.78	1.94	10.84	8.50
	0.33	N_2	10.5	1569 ± 62	3.42	3.40	2374	10.53	1.51	9.02	7.07
	0.33	N_2	10.5	1428 ± 52	2.60	3.40	3525	8.29	1.13	7.16	5.62
	0.33	N_2	10.5	1331 ± 82	1.79	3.40	3091	5.66	0.71	4.95	3.89
	1.6	N_2	52.3	1972 ± 61	6.14	3.40	1942	18.64	2.44	16.20	12.71
	1.6	N_2	52.3	1934 ± 71	4.95	3.40	2031	15.41	1.96	13.45	10.55
	1.6	N_2	52.3	1827 ± 69	3.34	3.40	2829	10.73	1.28	9.45	7.41
	1.6	N_2	52.3	1501 ± 126	1.74	3.40	2027	5.59	0.68	4.91	3.85
296	0.16	He	5	848 ± 26	5.82	3.40	1067	16.00	2.20	13.80	10.8
	0.16	He	5	800 ± 24	4.72	3.40	1365	13.56	1.66	11.90	9.33
	0.16	He	5	750 ± 26	3.25	3.40	1602	9.71	1.04	8.67	6.80
	0.16	He	5	654 ± 38	1.71	3.40	1936	4.95	0.48	4.47	3.51
	0.16	He	5	668 ± 42	0.92	3.40	4442	2.88	0.28	2.60	2.04
	0.33	He	10	845 ± 23	5.91	3.40	1626	19.49	2.31	17.18	13.5
	0.33	He	10	798 ± 22	4.77	3.40	1708	16.40	1.79	14.61	11.5
	0.33	He	10	728 ± 22	3.28	3.40	1697	11.82	1.16	10.66	8.36
	0.33	He	10	682 ± 33	1.72	3.40	1674	6.23	0.49	5.74	4.50
	0.33	He	10	661 ± 41	0.92	3.40	3122	3.52	0.28	3.24	2.54

T(K)	Total number density ($\times 10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times 10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times 10^{-3}$)	Baseline shift ($\times 10^{-3}$)	ΔA Criegee ($\times 10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times 10^{10}$ molecule cm^{-3})
296	1.6	He	50	1082 ± 25	5.82	3.40	1271	20.30	2.50	17.80	14.0
	1.6	He	50	1044 ± 26	4.67	3.40	1409	17.20	2.05	15.15	11.9
	1.6	He	50	953 ± 31	3.19	3.40	1575	12.07	1.34	10.73	8.41
	1.6	He	50	838 ± 41	1.67	3.40	2517	6.14	0.63	5.51	4.32
	1.6	He	50	799 ± 55	0.89	3.40	3422	3.63	0.37	3.26	2.56
	3.3	He	100	1203 ± 26	5.91	3.40	1101	23.14	2.85	20.29	15.9
	3.3	He	100	1160 ± 23	4.77	3.40	1919	19.56	2.35	17.21	13.5
	3.3	He	100	1046 ± 26	3.24	3.40	2636	13.79	1.50	12.29	9.64
	3.3	He	100	957 ± 45	1.69	3.40	2284	7.16	0.75	6.41	5.03
	3.3	He	100	888 ± 63	0.90	3.40	2809	4.07	0.49	3.58	2.81
	6.5	He	200	1283 ± 28	5.96	3.40	1340	23.92	2.77	21.15	16.6
	6.5	He	200	1141 ± 39	3.26	3.40	1199	14.58	1.56	13.02	10.2
	6.5	He	200	1002 ± 54	1.71	3.40	1637	7.64	0.77	6.87	5.38
	6.5	He	200	946 ± 66	0.91	3.40	2547	4.46	0.50	3.96	3.11
310	0.16	He	5.2	1122 ± 43	5.82	3.40	1260	14.50	2.14	12.36	9.70
	0.16	He	5.2	1068 ± 42	4.72	3.40	1503	11.85	1.64	10.21	8.01
	0.16	He	5.2	1044 ± 52	3.24	3.40	1725	8.30	0.96	7.34	5.76
	0.16	He	5.2	970 ± 70	1.71	3.40	2940	4.31	0.47	3.84	3.01
	0.16	He	5.2	908 ± 85	0.92	3.40	5272	2.44	0.29	2.15	1.69
	0.33	He	10.5	1303 ± 48	5.91	3.40	1449	17.06	2.54	14.52	11.39
	0.33	He	10.5	1220 ± 41	4.77	3.40	1538	14.37	1.90	12.47	9.78
	0.33	He	10.5	1179 ± 45	3.27	3.40	2449	10.44	1.22	9.22	7.23
	0.33	He	10.5	1060 ± 64	1.72	3.40	3106	5.30	0.58	4.72	3.71
	0.33	He	10.5	1140 ± 100	0.92	3.40	4148	3.37	0.37	3.00	2.36
	1.6	He	52.3	1660 ± 51	5.82	3.40	1835	16.90	2.23	14.67	11.51
	1.6	He	52.3	1641 ± 44	4.67	3.40	2399	14.72	1.86	12.86	10.08

	1.6	He	52.3	1548 ± 47	3.19	3.40	3666	10.45	1.19	9.26	7.26
	1.6	He	52.3	1454 ± 85	1.66	3.40	4082	5.23	0.58	4.65	3.65

T(K)	Total number density ($\times 10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times 10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times 10^{-3}$)	Baseline shift ($\times 10^{-3}$)	ΔA Criegee ($\times 10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times 10^{10}$ molecule cm^{-3})
310	3.3	He	104.8	2049 ± 56	5.86	3.40	2745	19.34	2.61	16.73	13.12
	3.3	He	104.8	1929 ± 50	4.72	3.40	3666	16.58	2.15	14.43	11.31
	3.3	He	104.8	1804 ± 66	3.24	3.40	3087	11.60	1.38	10.22	8.01
	3.3	He	104.8	1608 ± 86	1.69	3.40	4239	5.95	0.73	5.22	4.09
	6.5	He	209.5	1941 ± 73	5.91	3.40	1659	17.05	1.96	15.09	11.83
	6.5	He	209.5	1942 ± 69	4.77	3.40	1670	15.91	1.76	14.15	11.10
	6.5	He	209.5	1894 ± 75	3.24	3.40	2259	11.44	1.26	10.18	7.99
	6.5	He	209.5	1704 ± 106	1.70	3.40	3646	5.97	0.63	5.34	4.19
323	0.16	He	5.5	1686 ± 82	5.86	3.40	1438	12.57	1.98	10.59	8.31
	0.16	He	5.5	1634 ± 94	4.72	3.40	1785	10.16	1.47	8.69	6.81
	0.16	He	5.5	1461 ± 88	3.23	3.40	2623	6.99	0.95	6.04	4.73
	0.16	He	5.5	1536 ± 143	1.72	3.40	4146	3.73	0.46	3.27	2.56
	0.33	He	10.9	2022 ± 73	5.91	3.40	2011	15.37	2.49	12.88	10.1
	0.33	He	10.9	1977 ± 84	4.77	3.40	2045	12.52	1.95	10.57	8.29
	0.33	He	10.9	1790 ± 82	3.27	3.40	3284	8.94	1.23	7.71	6.05
	0.33	He	10.9	1757 ± 131	1.72	3.40	4029	4.76	0.59	4.17	3.27
	1.6	He	54.5	2690 ± 120	5.86	3.40	2442	13.90	1.97	11.93	9.36
	1.6	He	54.5	2672 ± 121	4.77	3.40	3118	11.87	1.59	10.28	8.06
	1.6	He	54.5	2558 ± 110	3.23	3.40	4692	8.53	1.06	7.47	5.86
	1.6	He	54.5	2461 ± 180	1.68	3.40	5515	4.30	0.51	3.79	2.98
	3.3	He	109	3132 ± 103	5.86	3.40	3190	17.73	2.34	15.39	12.1
	3.3	He	109	3046 ± 112	4.77	3.40	3402	15.62	2.05	13.57	10.6
	3.3	He	109	2877 ± 143	3.24	3.40	2615	10.69	1.37	9.32	7.31
	3.3	He	109	2852 ± 202	1.69	3.40	5575	5.58	0.67	4.91	3.85

T(K)	Total number density ($\times 10^{18}$ molecule cm^{-3})	Buffer gas	^{a}p (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ ($\times 10^{13}$ molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA ($\times 10^{-3}$)	Baseline shift ($\times 10^{-3}$)	ΔA Criegee ($\times 10^{-3}$)	$[(CH_3)_2COO]_0$ ($\times 10^{10}$ molecule cm^{-3})
323	6.5	He	218	3380 ± 116	5.96	3.40	2556	17.96	2.11	15.85	12.4
	6.5	He	218	3290 ± 117	4.77	3.40	3531	15.16	1.73	13.43	10.5
	6.5	He	218	3157 ± 148	3.27	3.40	4912	10.83	1.25	9.58	7.51
	6.5	He	218	3086 ± 251	1.70	3.40	4344	5.76	0.65	5.11	4.01
330	0.16	He	5.6	1969 ± 86	5.82	3.40	3017	10.74	1.77	8.97	7.04
	0.16	He	5.6	1894 ± 87	4.72	3.40	3249	9.00	1.36	7.64	5.99
	0.16	He	5.6	1805 ± 109	3.24	3.40	3330	6.28	0.83	5.45	4.28
	0.16	He	5.6	1692 ± 168	1.72	3.40	4564	3.20	0.40	2.80	2.19
	0.33	He	11.2	2613 ± 91	5.91	3.40	2945	13.20	2.27	10.93	8.57
	0.33	He	11.2	2461 ± 110	4.77	3.40	3059	11.15	1.82	9.33	7.32
	0.33	He	11.2	2365 ± 119	3.26	3.40	4387	7.99	1.14	6.85	5.37
	0.33	He	11.2	2240 ± 198	1.71	3.40	5029	3.93	0.58	3.35	2.63
	1.6	He	55.7	3698 ± 198	5.86	3.40	2176	12.99	1.94	11.05	8.67
	1.6	He	55.7	3595 ± 187	4.72	3.40	3371	10.828	1.61	9.21	7.22
	1.6	He	55.7	3567 ± 195	3.22	3.40	4807	7.52	0.99	6.53	5.12
	1.6	He	55.7	3444 ± 363	1.67	3.40	5380	3.93	0.50	3.43	2.69
	3.3	He	111.5	4066 ± 143	5.91	3.40	3667	16.10	2.16	13.94	10.94
	3.3	He	111.5	3918 ± 178	4.77	3.40	4257	13.48	1.73	11.75	9.21
	3.3	He	111.5	3770 ± 254	3.23	3.40	3650	9.47	1.16	8.31	6.52
	3.3	He	111.5	3825 ± 320	1.69	3.40	5031	4.83	0.53	4.30	3.37
340	0.16	He	5.8	2708 ± 147	5.86	3.40	4419	8.63	1.47	7.16	5.62
	0.16	He	5.8	2501 ± 148	4.72	3.40	3807	7.07	1.13	5.94	4.66
	0.16	He	5.8	2333 ± 163	3.23	3.40	5303	5.05	0.72	4.33	3.40
	0.16	He	5.8	1963 ± 230	1.73	3.40	5739	2.54	0.35	2.19	1.71
	0.33	He	11.7	3174 ± 193	5.96	3.40	3170	9.86	1.73	8.13	6.38
	0.33	He	11.7	3161 ± 187	4.77	3.40	3617	8.33	1.29	7.04	5.52

	0.33	He	11.7	2902 ± 206	3.26	3.40	5401	5.78	0.80	4.98	3.91
	0.33	He	11.7	3063 ± 345	1.70	3.40	7015	3.26	0.42	2.84	2.23
T(K)	Total number density (×10^{18} molecule cm^{-3})	Buffer gas	[a]*p* (Torr)	k_{obs} (s^{-1})	$[(CH_3)_2ClBr]_0$ (×10^{13} molecule cm^{-3})	Laser intensity (mJ cm^{-2})	Number of average	ΔA (×10^{-3})	Baseline shift (×10^{-3})	ΔA Criegee (×10^{-3})	$[(CH_3)_2COO]_0$ (×10^{10} molecule cm^{-3})
340	1.6	He	57.5	5963 ± 313	5.86	3.40	4432	12.41	2.12	10.29	8.07
	1.6	He	57.5	5573 ± 361	4.72	3.40	4988	10.47	1.64	8.83	6.92
	1.6	He	57.5	5129 ± 369	3.21	3.40	4176	7.14	1.07	6.07	4.76
	1.6	He	57.5	4958 ± 606	1.67	3.40	5920	3.71	0.54	3.17	2.49

[a]*The fixed concentration of O_2 was ~4.0 × 10^{16} molecule cm^{-3} for all measurements.*

UV spectra and absorption cross sections

Figure S6 shows measured "raw" cross section of acetone oxide $(CH_3)_2COO$ with contribution from iodine oxide IO at longer wavelengths, obtained from the measured absorbance shown in Figure S5 using $[(CH_3)_2COO] = 5.5 \times 10^{10}$ molecule cm^{-3} (determined at 340 nm), and known iodine oxide IO cross section. The concentration of acetone oxide, $[(CH_3)_2COO]$, was calculated using equation (S3) with the measured absorbance and using absorption cross section data from Huang et al..[8] In the recording of the UV spectrum about 3500 measurements were averaged. Figure S6 shows the distinct peaks of IO and consequently absorption cross section of IO from literature was used to determine the $[IO] = 2 \times 10^{10}$ molecule cm^{-3}.[9]

Figure S7 shows the cross section of $(CH_3)_2COO$ determined in this work after subtraction of the contribution of IO to the spectrum. Note that the $(CH_3)_2COO$ concentration used for recording the spectra is about an order of magnitude bigger than the concentrations typically used for the kinetic measurements.

In figure S8, the transmission of the optical cavity mirrors is shown below the "raw" cross section of $(CH_3)_2COO$ from figure S6.

Figure S9 shows comparison between the CH_2OO cross sections measured in this work (CH_2IBr / 213 nm / O_2 / N_2 environment) to those reported earlier by us and Ting et al.[3,10] The differences between the cross sections recorded by us are caused by different set of mirrors used for the optical cavity for the two measurements.

Figure S10 shows a comparison of the cross sections of acetone oxide determined in this work using 2,2-bromoiodomethane $(CH_3)_2CIBr$ ($(CH_3)_2CIBr$ / 213 nm / O_2 / N_2 environment) and 2,2-diiodopropane $(CH_3)_2CI_2$ ($(CH_3)_2CI_2$ / 266 nm / O_2 / N_2 environment). The differences between the two are due to changes made to the experimental setup to accommodate using the different precursor molecules (i.e, changing the wavelength of the laser and adjusting the mirror system for the absorption spectroscopy).

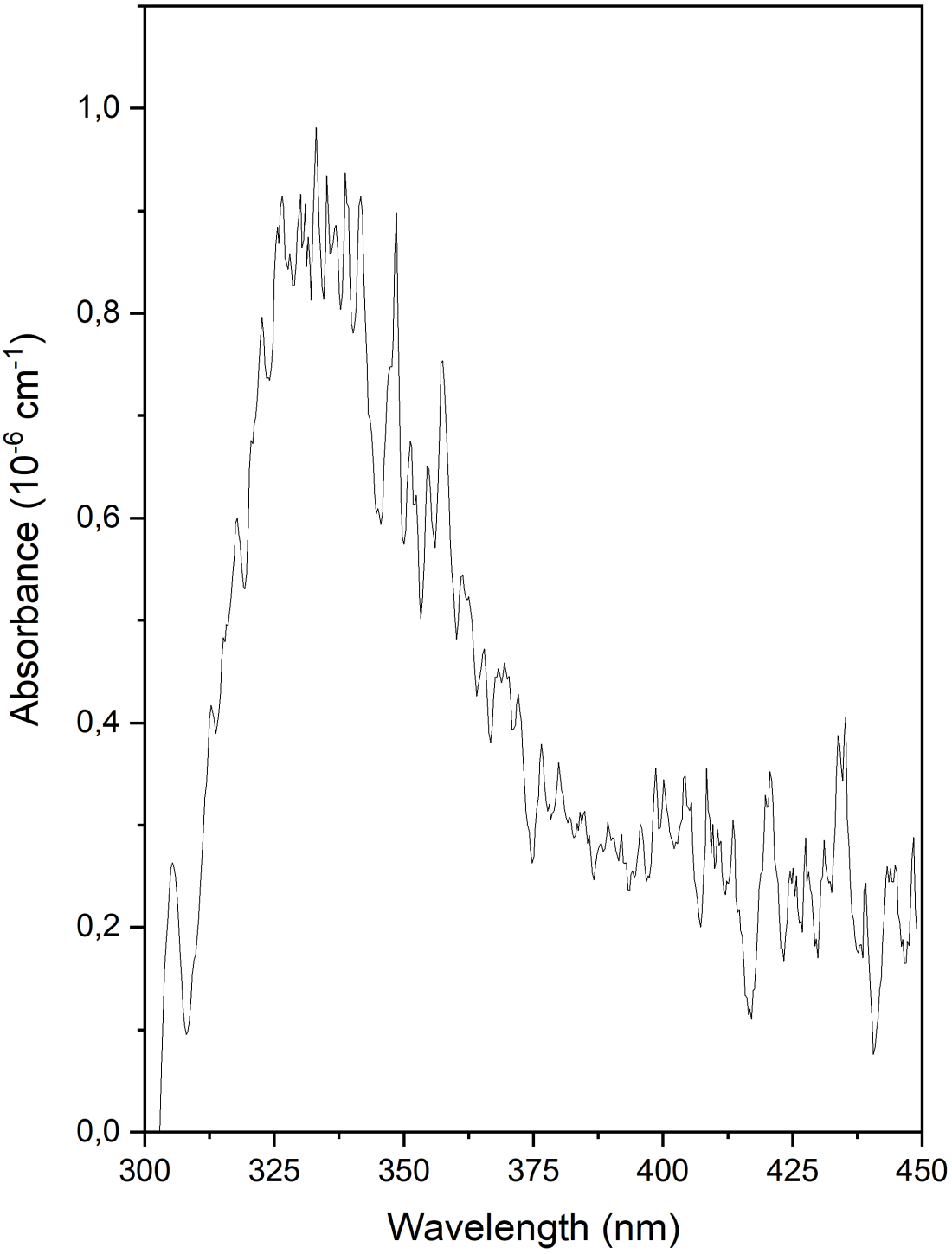

Figure S5. Measured absorbance between 300 and 450 nm wavelength region in $(CH_3)_2ClBr$ / 213 nm / O_2 / N_2 environment. A dip around 347 nm and the sharp decline at the short wavelengths, *i.e.* ≤ 320 nm, are due to poor light transmission trough the optical cavity mirrors. The spectrum was recorded at 296 K temperature and 10 torr pressure. The spectrum was averaged over t = 0 – 1 ms.

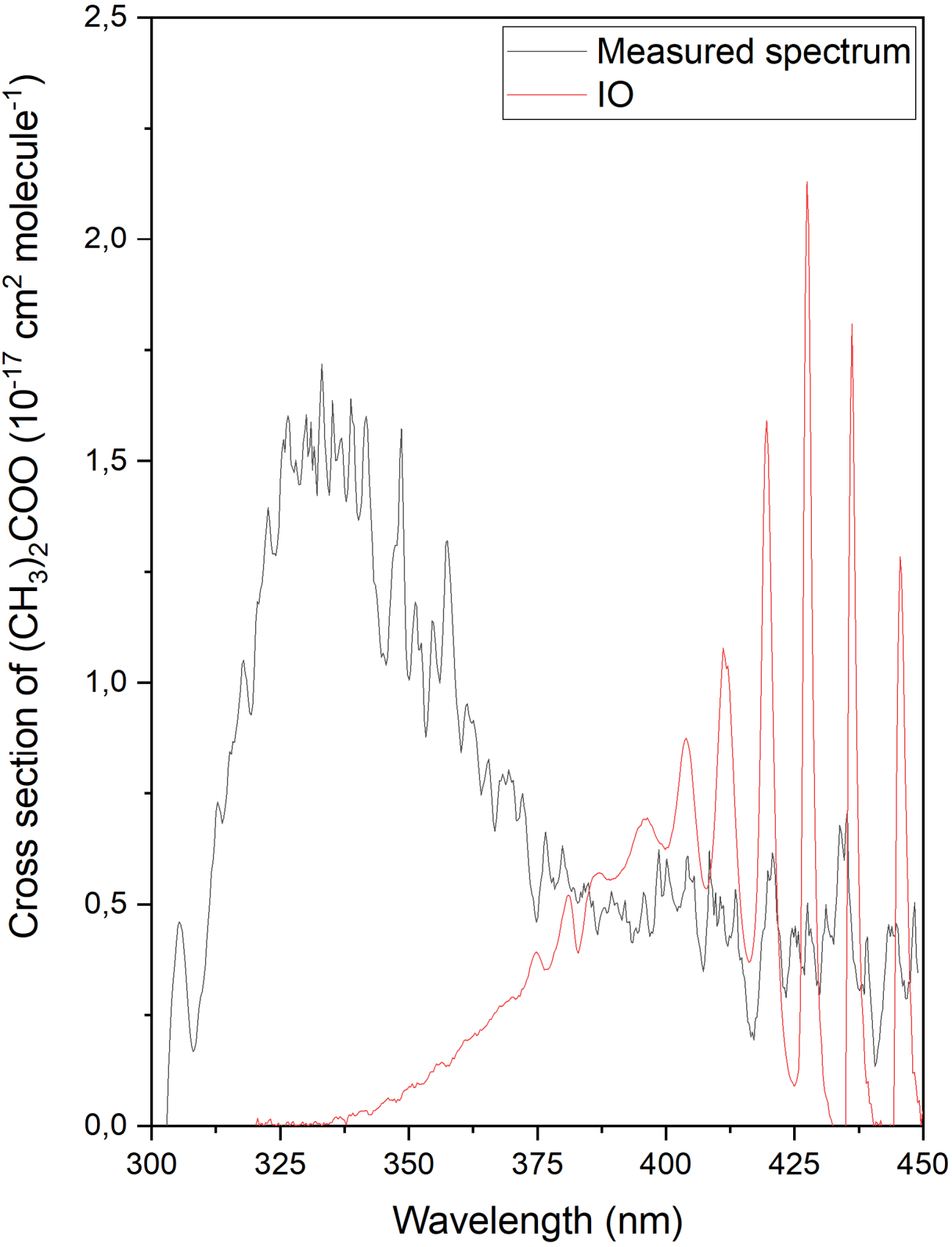

Figure S6. Measured "raw" cross section of acetone oxide $(CH_3)_2COO$ (black), with contribution from iodine oxide IO at longer wavelengths, obtained from the measured absorbance shown in Figure S5 using $[(CH_3)_2COO] = 5.5 \times 10^{10}$ molecule cm^{-3} (determined at 340 nm), and iodine oxide IO (red) cross section.[9] The spectrum was recorded at 296 K temperature and 10 torr pressure in $(CH_3)_2ClBr$ / 213 nm / O_2 / N_2 environment. The spectrum was averaged over t = 0 – 1 ms.

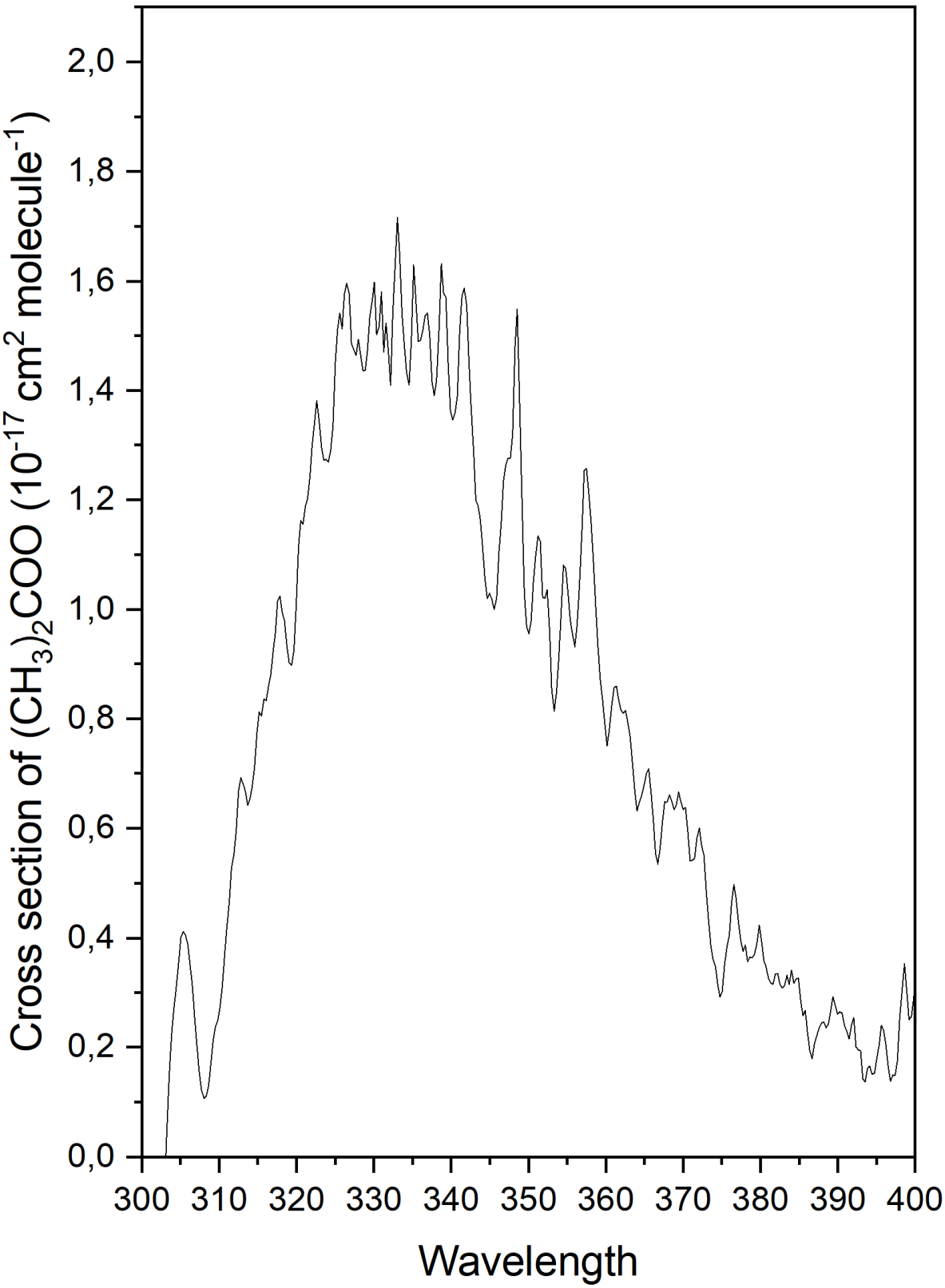

Figure S7. The measured cross section of acetone oxide $(CH_3)_2COO$ obtained from absorption spectrum shown in Figure S5 after subtracting the absorbance of iodine oxide IO contribution. The concentrations used for the calculations were 5.5×10^{10} molecule cm^{-3} for $(CH_3)_2COO$ and 2×10^{10} molecule cm^{-3} for IO. The IO concentration was calculated from the IO peaks centered at 419, 427, and 436 nm.[9] The spectrum was recorded at 296 K temperature and 10 torr pressure in $(CH_3)_2CIBr$ / 213 nm / O_2 / N_2 environment.

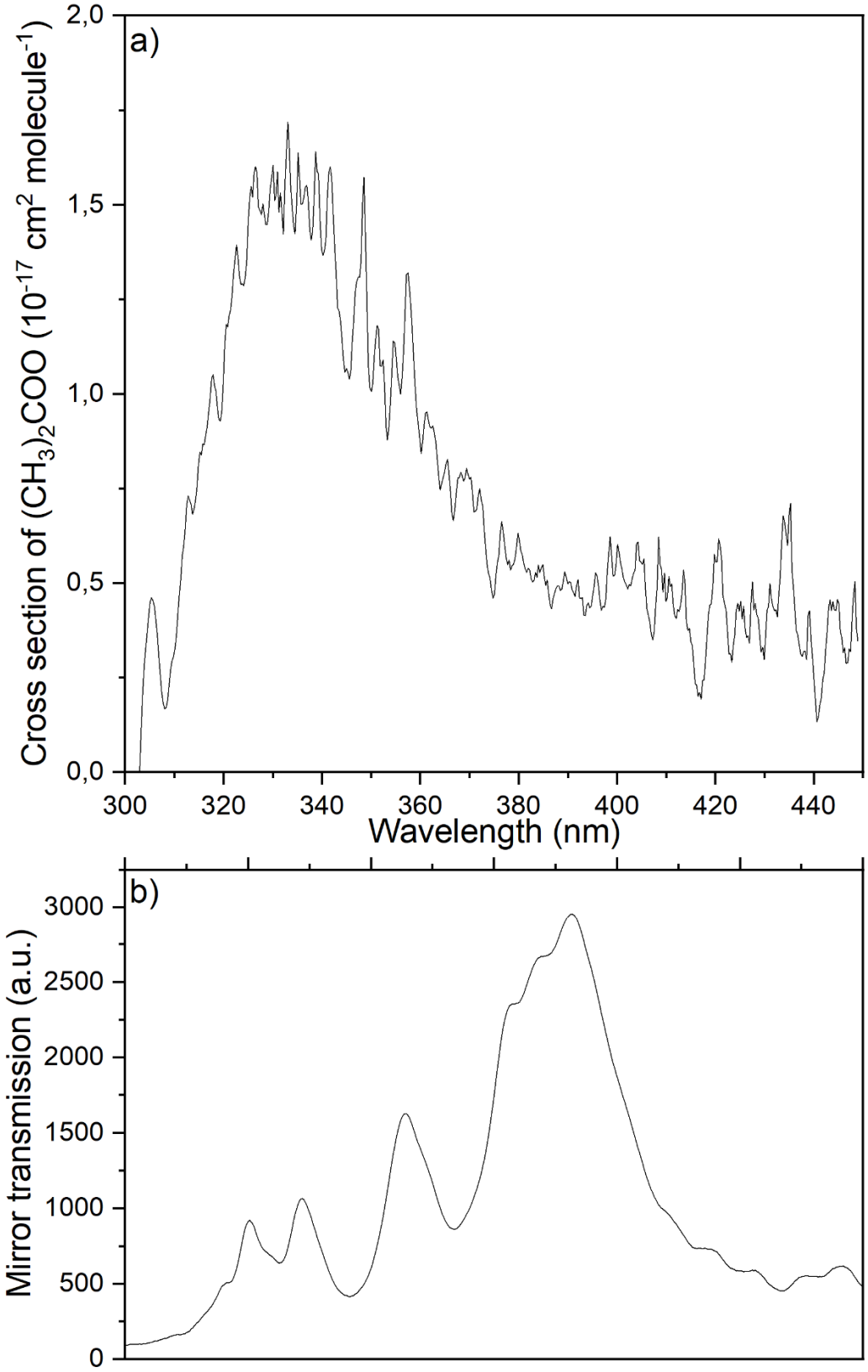

Figure S8. Measured "raw" cross section of $(CH_3)_2COO$ with contribution from iodine oxide IO at longer wavelengths (a, from Figure S6 where $[(CH_3)_2COO] = 5.5 \times 10^{10}$ molecule cm^{-3}) and the transmission of the mirrors used for the optical cavity (b) from 300 to 450 nm wavelength. A dip around 347 nm and the sharp decline at the short wavelength end of the spectrum are due to poor transmission of light trough the cavity mirrors. The spectrum was recorded at 296 K temperature and 10 torr pressure in $(CH_3)_2ClBr$ / 213 nm / O_2 / N_2 environment. The spectrum was averaged over t = 0 – 1 ms after photolysis initiation.

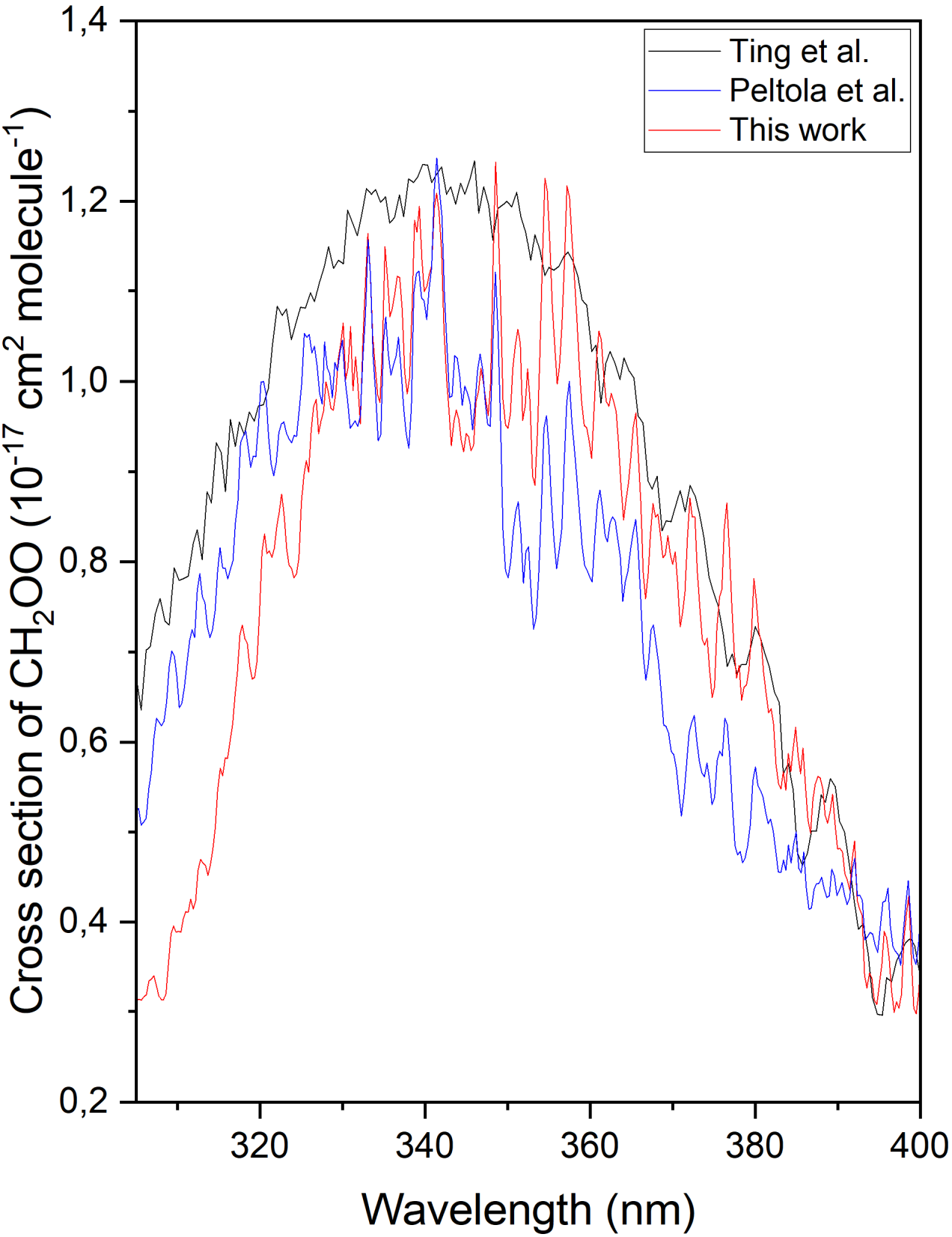

Figure S9. A comparison of the CH_2OO spectra measured during this work to those reported earlier by our group and Ting et al.[3,10] The differences between the spectra measured by our group before[3] and in this work are caused by different set of mirrors used to construct optical cavity for the two measurements. The spectrum of this work was recorded at 296 K temperature and 10 torr pressure in CH_2IBr / 213 nm / O_2 / N_2 environment, where [CH_2OO] was 3.1 × 10^{11} molecule cm^{-3}. The spectrum was averaged over t = 0 – 1 ms.

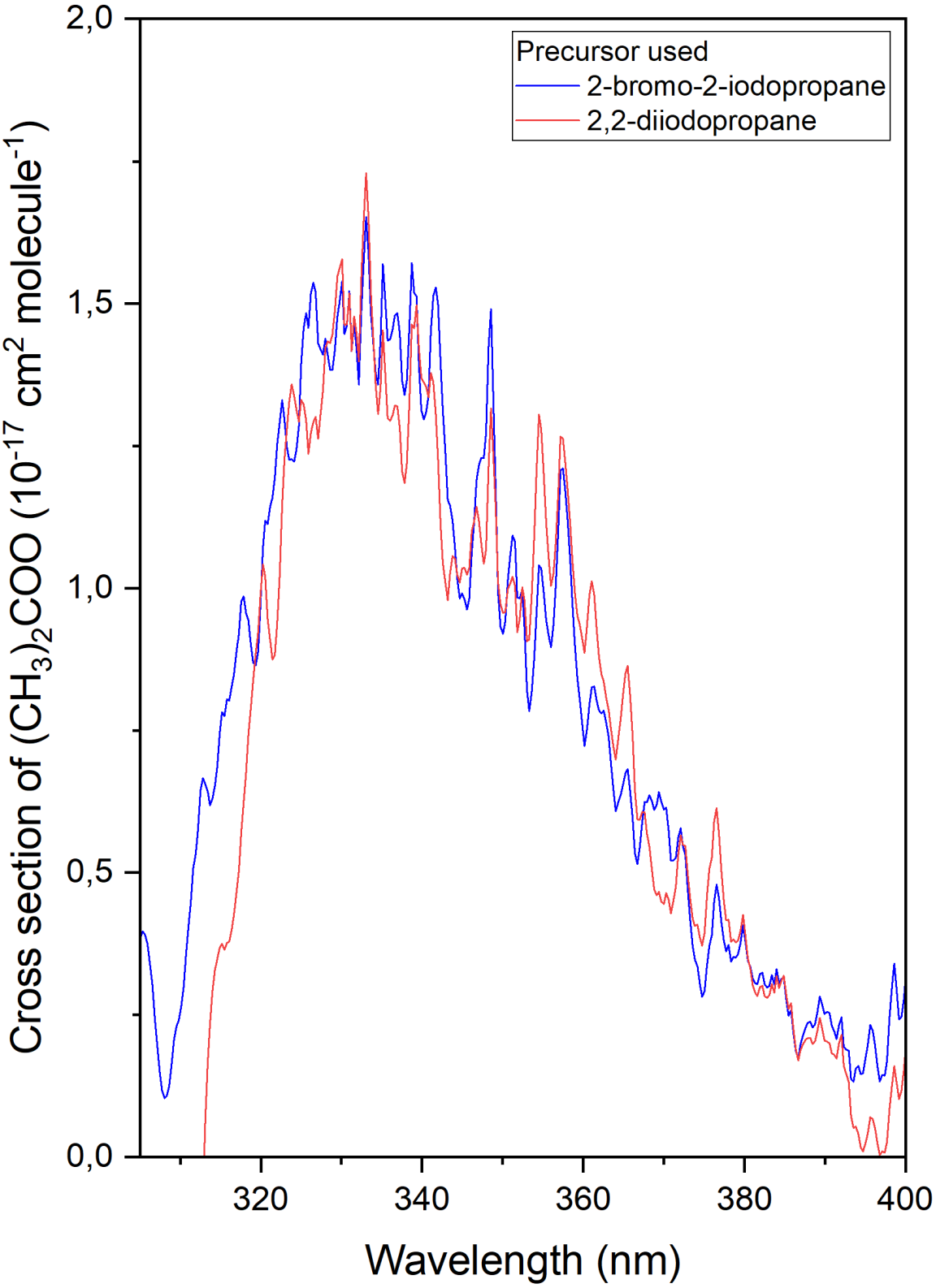

Figure S10. A comparison of the absorption cross sections of acetone oxide determined in this work using 2,2-bromoiodopropane ($(CH_3)_2ClBr$ / 213 nm / O_2 / N_2 environment) and 2,2-diiodopropane ($(CH_3)_2I_2$ / 266 nm / O_2 / N_2 environment). Small differences between the two determinations are likely due to changes made to the experimental setup to accommodate the different precursor molecules (i.e, changing the wavelength of the laser and adjusting the mirror system for the measurements). The spectra were recorded at 296 K temperature and 10 torr pressure, the $(CH_3)_2COO$ concentrations were 5.5×10^{10} molecule cm^{-3} for $(CH_3)_2ClBr$ and 5.4×10^{10} molecule cm^{-3} for $(CH_3)_2I_2$. The spectra were averaged over t = 0 – 1 ms.

Comparison with the previous k_{uni} kinetic simulations and current branching ratios of the methyl-vinyl hydroperoxide and methyl-vinoxy + OH products

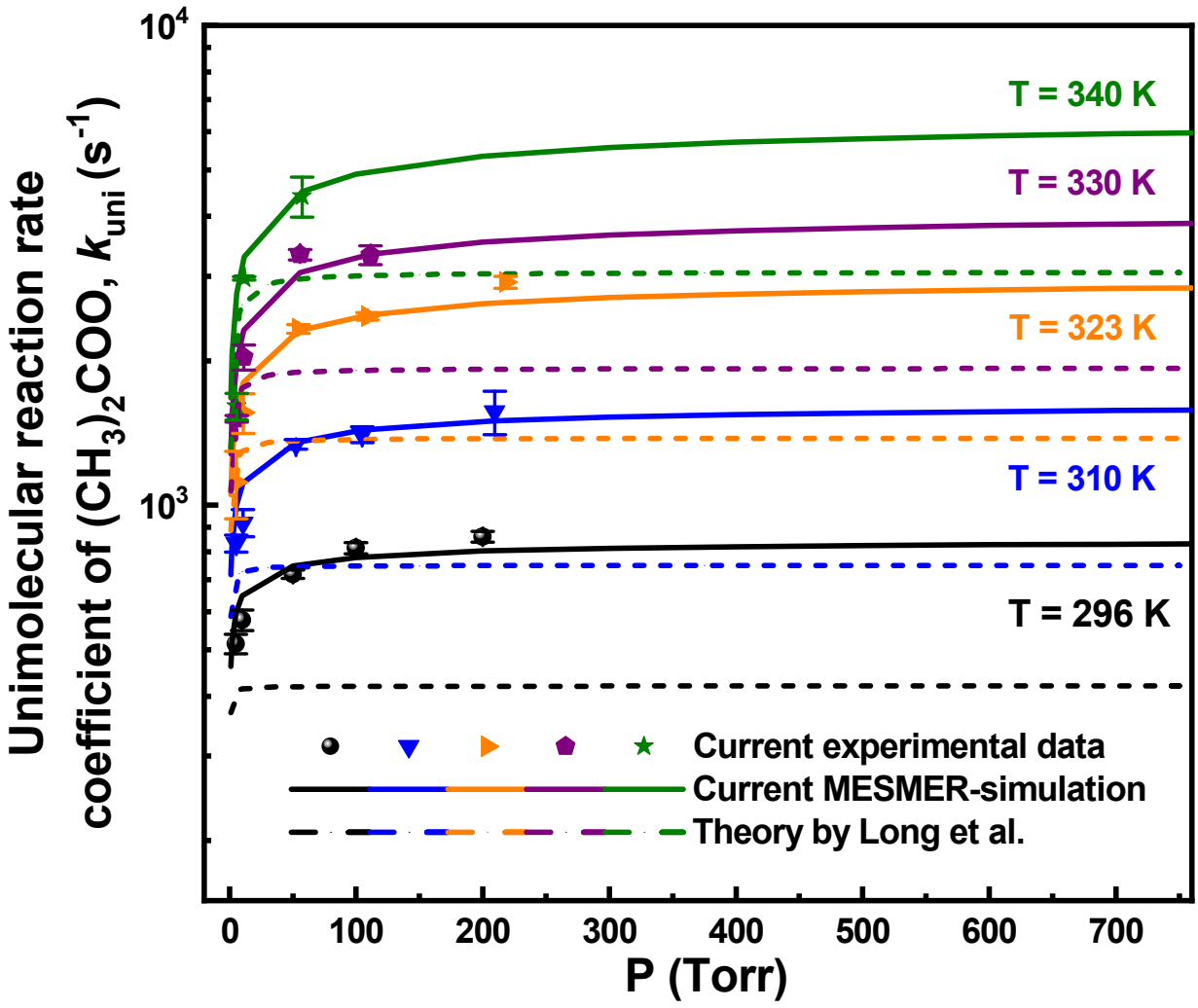

Figure S11. A comparison of the high-pressure limiting rate coefficients between the present work and that of Long et al.[11] The points are the experimental data whereas solid lines are the MESMER simulated results. The dashed lines are taken from ref.[8]

Table S3 Branching ratios (BRs) at 1 sec (in %) after reaction initiation based on the PES with only TS1 and TS2 channel. Values in parentheses are BRs at 500 secs.

T (K)	P (Torr)	BR(Methyl-VHP)	BR(Methyl-vinoxy + OH)
		He bath gas	
296	5.0	33.4 (0.0)	66.6 (100.0)
	10.0	39.0 (0.0)	61.0 (100.0)
	50.0	55.8 (0.0)	44.2 (100.0)
	100.0	63.9 (0.0)	36.1 (100.0)
	200.0	72.0 (0.0)	28.0 (100.0)
310	5.23	24.7 (0.0)	75.3 (100.0)
	10.47	28.9 (0.0)	71.1 (100.0)
	52.3	42.1 (0.0)	57.9 (100.0)
	104.8	49.1 (0.0)	50.9 (100.0)
	209.5	56.4 (0.0)	43.6 (100.0)
323	5.45	15.6 (0.0)	84.4 (100.0)
	10.9	17.5 (0.0)	82.5 (100.0)
	54.5	23.9 (0.0)	76.1 (100.0)
	109	27.6 (0.0)	72.4 (100.0)
330	5.57	10.3 (0.0)	89.7 (100.0)
	11.15	10.9 (0.0)	89.1 (100.0)
	55.6	13.2 (0.0)	86.8 (100.0)
	111.5	14.8 (0.0)	85.2 (100.0)
340	5.75	3.8 (0.0)	96.2 (100.0)
	11.74	3.3 (0.0)	96.7 (100.0)
	57.5	2.8 (0.0)	97.2 (100.0)
		N_2 bath gas	
243	4.1	79.8 (78.0)	20.2 (22.0)
	8.2	85.1 (83.2)	14.9 (16.8)
	41.0	94.4 (92.1)	5.6 (7.9)
	82.0	96.8 (94.4)	3.2 (5.6)
253	4.26	73.1 (66.1)	26.9 (33.9)
	8.53	79.4 (71.4)	20.6 (28.6)
	42.6	91.3 (81.5)	8.7 (18.5)
	85.3	94.7 (84.4)	5.3 (15.6)
263	4.43	66.0 (44.1)	34.0 (55.9)
	8.87	73.1 (47.5)	26.9 (52.5)
	44.3	87.5 (55.0)	12.5 (45.0)
	88.7	92.0 (57.4)	8.0 (42.6)
273	4.6	58.8 (13.7)	41.2 (86.3)
	9.21	66.3 (13.8)	33.7 (86.2)
	46.0	82.9 (14.9)	17.1 (85.1)
	92.1	88.5 (15.4)	11.5 (84.6)
283	4.78	51.7 (0.4)	48.3 (99.6)

	9.55	59.3 (0.3)	40.7 (99.7)
	47.8	77.5 (0.2)	22.5 (99.8)
	95.5	84.2 (0.2)	15.8 (99.8)
296	5.0	42.4 (0.0)	57.6 (100.0)
	10.0	49.6 (0.0)	50.4 (100.0)
	50.0	68.4 (0.0)	31.6 (100.0)
	200.0	82.5 (0.0)	17.5 (100.0)
310	10.47	36.8 (0.0)	63.2 (100.0)
	52.3	52.8 (0.0)	47.2 (100.0)

References

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MESMER input files

He bath gas

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</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 372.51 has been eliminated in favour of a 1 dimensional hindered rotor. 2-4 Dihedral rotation -->

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</me:ExtraDOSCMethod>

</molecule>

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<atom id="a2" elementType="C" x3="0.581386" y3="0.294677" z3="-1.511105" />

<atom id="a3" elementType="O" x3="-0.205025" y3="-0.550839" z3="-2.260355" />

<atom id="a4" elementType="O" x3="-1.118524" y3="-1.238050" z3="-1.412596" />

<atom id="a5" elementType="H" x3="-0.935999" y3="-2.158799" z3="-1.650821" />

<atom id="a6" elementType="C" x3="0.964317" y3="1.424289" z3="-2.095127" />

<atom id="a7" elementType="H" x3="1.408704" y3="-1.194846" z3="-0.223044" />

<atom id="a8" elementType="H" x3="0.154251" y3="-0.212273" z3="0.524041" />

<atom id="a9" elementType="H" x3="1.758898" y3="0.484382" z3="0.238211" />

<atom id="a10" elementType="H" x3="1.686148" y3="2.067042" z3="-1.613136" />

<atom id="a11" elementType="H" x3="0.584989" y3="1.698077" z3="-3.069557" />

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</property>
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</property>
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      <property title="Rotational Constants" dictRef="me:rotConsts">
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     </propertyList>

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                    <!--  Frequency 221.84 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2
Dihedral Me rotation -->
                    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
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UseSineTerms="yes">
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</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 90.10 has been eliminated in favour of a 1 dimensional hindered rotor. 2-3 Dihedral rotation -->

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</me:HinderedRotorPotential>

</me:ExtraDOSCMethod>

<!-- Frequency 182.72 has been eliminated in favour of a 1 dimensional hindered rotor. 3-4 Dihedral rotation -->

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<me:PotentialPoint angle="210" potential=" 0.5513550"/>

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                                 </me:HinderedRotorPotential>
    </me:ExtraDOSCMethod>

    <me:DistributionCalcMethod name="Boltzmann" />
    <me:energyTransferModel xsi:type="me:ExponentialDown">
     <me:deltaEDown units="cm-1" referenceTemperature="298.0" >91.422</me:deltaEDown>
     <me:deltaEDownTExponent referenceTemperature="298.0" >0.995832</me:deltaEDownTExponent>
    </me:energyTransferModel>
   </molecule>

   <molecule id="Me2COO" spinMultiplicity="1" >
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     <atom id="a2" elementType="C" spinMultiplicity="2" x3="0.431297" y3="-0.097242" z3="0.077740" />
     <atom id="a3" elementType="O" spinMultiplicity="2" x3="-1.694385" y3="0.420841" z3="-0.371211"
/>
     <atom id="a4" elementType="O" x3="-0.659943" y3="0.353551" z3="0.512236" />
     <atom id="a5" elementType="C" x3="1.553234" y3="-0.168112" z3="1.043778" />
     <atom id="a6" elementType="H" x3="0.222831" y3="0.334188" z3="-1.955976" />
     <atom id="a7" elementType="H" x3="-0.260557" y3="-1.263359" z3="-1.511936" />
     <atom id="a8" elementType="H" x3="1.504744" y3="-0.883405" z3="-1.582214" />
     <atom id="a9" elementType="H" x3="2.394878" y3="0.426040" z3="0.680803" />
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 <atom id="a10" elementType="H" x3="1.240334" y3="0.197314" z3="2.018853" />
 <atom id="a11" elementType="H" x3="1.903553" y3="-1.198934" z3="1.132145" />
</atomArray>
<bondArray>
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 <bond id="b2" atomRefs2="a8 a1" order="1" />
 <bond id="b3" atomRefs2="a7 a1" order="1" />
 <bond id="b4" atomRefs2="a1 a2" order="1" />
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 <bond id="b6" atomRefs2="a2 a4" order="1" />
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 <bond id="b10" atomRefs2="a5 a10" order="1" />
</bondArray>
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  <scalar>Gaussian 16, Revision B.01</scalar>
 </property>
 <property title="basis">
  <scalar>def2TZVP (5D, 7F)</scalar>
 </property>
 <property title="method">
  <scalar>mn15</scalar>
 </property>
 <property title="File Format">
  <scalar>g03</scalar>
 </property>
 <property title="Energy" dictRef="me:ZPE">
  <scalar units="kJ/mol" >0</scalar>
 </property>
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<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">285.98 319.85 347.62 481.07 599.97 824.08 911.44 949.81 972.69 1069.13 1081.19 1304.79 1376.88 1397.45 1415.37 1448.25 1452.94 1472.80 1628.10 3059.86 3068.96 3114.37 3131.24 3190.16 3191.84</array>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.299 0.146 0.102</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

<property dictRef="me:sigma" >

<scalar>4.46</scalar>

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<property dictRef="me:frequenciesScaleFactor">

<scalar>0.993</scalar>

</property>

</propertyList>

<me:DOSCMethod name="QMRotors" />

<!-- Frequency 162.06 has been eliminated in favour of a 1 dimensional hindered rotor. 2-5 Dihedral Me rotation -->

<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">

<me:bondRef>b7</me:bondRef>

<me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="10" UseSineTerms="yes">

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<me:PotentialPoint angle="5" potential=" 0.1050200"/>

<me:PotentialPoint angle="10" potential=" 0.3938250"/>

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<me:PotentialPoint angle="20" potential=" 1.4440250"/>

<me:PotentialPoint angle="25" potential=" 2.1529100"/>

<me:PotentialPoint angle="30" potential=" 2.9668150"/>

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<me:PotentialPoint angle="40" potential=" 4.6733900"/>

<me:PotentialPoint angle="45" potential=" 5.4347850"/>

<me:PotentialPoint angle="50" potential=" 6.0911600"/>

<me:PotentialPoint angle="55" potential=" 6.5374950"/>

<me:PotentialPoint angle="60" potential=" 6.7737900"/>

<me:PotentialPoint angle="65" potential=" 6.7475350"/>

<me:PotentialPoint angle="70" potential=" 6.4587300"/>

<me:PotentialPoint angle="75" potential=" 5.9598850"/>

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<me:PotentialPoint angle="100" potential=" 1.8115950"/>

<me:PotentialPoint angle="105" potential=" 1.1027100"/>

<me:PotentialPoint angle="110" potential=" 0.5513550"/>

<me:PotentialPoint angle="115" potential=" 0.1837850"/>

<me:PotentialPoint angle="120" potential=" 0.0000000"/>

<me:PotentialPoint angle="125" potential=" 0.0787650"/>

<me:PotentialPoint angle="130" potential=" 0.3413150"/>

<me:PotentialPoint angle="135" potential=" 0.8139050"/>

<me:PotentialPoint angle="140" potential=" 1.4440250"/>

<me:PotentialPoint angle="145" potential=" 2.2316750"/>

<me:PotentialPoint angle="150" potential=" 3.0980900"/>

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<me:PotentialPoint angle="160" potential=" 4.8571750"/>

<me:PotentialPoint angle="165" potential=" 5.6448250"/>

<me:PotentialPoint angle="170" potential=" 6.2486900"/>

<me:PotentialPoint angle="175" potential=" 6.6425150"/>

<me:PotentialPoint angle="180" potential=" 6.8000450"/>

<me:PotentialPoint angle="185" potential=" 6.6687700"/>

<me:PotentialPoint angle="190" potential=" 6.3274550"/>

<me:PotentialPoint angle="195" potential=" 5.7761000"/>

<me:PotentialPoint angle="200" potential=" 5.0409600"/>

<me:PotentialPoint angle="205" potential=" 4.2270550"/>

<me:PotentialPoint angle="210" potential=" 3.3868950"/>

<me:PotentialPoint angle="215" potential=" 2.5467350"/>

<me:PotentialPoint angle="220" potential=" 1.7590850"/>

<me:PotentialPoint angle="225" potential=" 1.1027100"/>

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<me:PotentialPoint angle="235" potential=" 0.2100400"/>

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<me:PotentialPoint angle="265" potential=" 1.8641050"/>

<me:PotentialPoint angle="270" potential=" 2.6780100"/>

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<me:PotentialPoint angle="305" potential=" 6.6950250"/>

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<me:PotentialPoint angle="320" potential=" 4.9096850"/>

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<me:PotentialPoint angle="335" potential=" 2.2579300"/>

<me:PotentialPoint angle="340" potential=" 1.4965350"/>

<me:PotentialPoint angle="345" potential=" 0.8664150"/>

<me:PotentialPoint angle="350" potential=" 0.3938250"/>

<me:PotentialPoint angle="355" potential=" 0.1050200"/>

</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 216.14 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->

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<me:PotentialPoint angle="10" potential=" 0.6563750"/>

<me:PotentialPoint angle="15" potential=" 1.3915150"/>

<me:PotentialPoint angle="20" potential=" 2.3629500"/>

<me:PotentialPoint angle="25" potential=" 3.4919150"/>

<me:PotentialPoint angle="30" potential=" 4.6996450"/>

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<me:PotentialPoint angle="40" potential=" 7.1151050"/>

<me:PotentialPoint angle="45" potential=" 8.1915600"/>

<me:PotentialPoint angle="50" potential=" 9.1104850"/>

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<me:PotentialPoint angle="60" potential="10.2657050"/>

<me:PotentialPoint angle="65" potential="10.4232350"/>

<me:PotentialPoint angle="70" potential="10.2919600"/>

<me:PotentialPoint angle="75" potential=" 9.8193700"/>

<me:PotentialPoint angle="80" potential=" 9.0579750"/>

<me:PotentialPoint angle="85" potential=" 7.9815200"/>

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<me:PotentialPoint angle="100" potential=" 3.8594850"/>

<me:PotentialPoint angle="105" potential=" 2.5467350"/>

<me:PotentialPoint angle="110" potential=" 1.4177700"/>

<me:PotentialPoint angle="115" potential=" 0.5776100"/>

<me:PotentialPoint angle="120" potential=" 0.1050200"/>

<me:PotentialPoint angle="125" potential=" 0.0262550"/>

<me:PotentialPoint angle="130" potential=" 0.3150600"/>

<me:PotentialPoint angle="135" potential=" 0.9714350"/>

<me:PotentialPoint angle="140" potential=" 1.9428700"/>

<me:PotentialPoint angle="145" potential=" 3.2031100"/>

<me:PotentialPoint angle="150" potential=" 4.5946250"/>

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<me:PotentialPoint angle="190" potential="10.0556650"/>

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<me:PotentialPoint angle="200" potential=" 8.6641500"/>

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<me:PotentialPoint angle="225" potential=" 2.8880500"/>

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<me:PotentialPoint angle="235" potential=" 0.9976900"/>

<me:PotentialPoint angle="240" potential=" 0.3675700"/>

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<me:PotentialPoint angle="325" potential=" 6.9575750"/>

<me:PotentialPoint angle="330" potential=" 5.4872950"/>

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<me:PotentialPoint angle="340" potential=" 2.6780100"/>

<me:PotentialPoint angle="345" potential=" 1.5227900"/>

<me:PotentialPoint angle="350" potential=" 0.6826300"/>

<me:PotentialPoint angle="355" potential=" 0.1837850"/>

</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<me:DistributionCalcMethod name="Boltzmann" />

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 <me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1" referenceTemperature="298.0" >91.422</me:deltaEDown>
  <me:deltaEDownTExponent referenceTemperature="298.0" >0.995832</me:deltaEDownTExponent>
 </me:energyTransferModel>
</molecule>

<molecule id="TS1" spinMultiplicity="1">
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  <atom id="a2" elementType="C" spinMultiplicity="2" x3="0.045791" y3="0.123850" z3="0.195019" />
  <atom id="a3" elementType="O" x3="1.014966" y3="0.502187" z3="0.964041" />
  <atom id="a4" elementType="O" spinMultiplicity="2" x3="1.337155" y3="1.825212" z3="0.705651" />
  <atom id="a5" elementType="H" x3="0.124868" y3="1.993062" z3="0.109444" />
  <atom id="a6" elementType="C" x3="-0.430606" y3="1.105136" z3="-0.693445" />
  <atom id="a7" elementType="H" x3="-0.319179" y3="-1.906486" z3="-0.294081" />
  <atom id="a8" elementType="H" x3="-1.617030" y3="-1.115003" z3="0.588676" />
  <atom id="a9" elementType="H" x3="-0.127080" y3="-1.586957" z3="1.446695" />
  <atom id="a10" elementType="H" x3="-1.427735" y3="0.951650" z3="-1.087740" />
  <atom id="a11" elementType="H" x3="0.289665" y3="1.453258" z3="-1.434613" />
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  <bond id="b3" atomRefs2="a6 a5" order="1" />
  <bond id="b4" atomRefs2="a6 a2" order="1" />
  <bond id="b5" atomRefs2="a7 a1" order="1" />
  <bond id="b6" atomRefs2="a2 a1" order="1" />
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  <bond id="b8" atomRefs2="a1 a8" order="1" />
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 <property title="basis">
  <scalar>def2TZVP (5D, 7F)</scalar>
 </property>
 <property title="method">
  <scalar>mn15</scalar>
 </property>
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  <scalar>g03</scalar>
 </property>
 <property title="Energy" dictRef="me:ZPE">
                <scalar units="kJ/mol">64.52</scalar>
 </property>
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  <array units="cm-1">276.84 350.89 512.21 540.50 666.78 752.37 853.07 942.55 976.46 990.73
1046.09 1080.57 1329.04 1374.07 1412.86 1449.53 1455.90 1524.29 1564.70 1882.56 3080.58 3119.60
3152.24 3186.63 3227.71</array>
 </property>
 <property title="ImaginaryFrequency" dictRef="me:imFreqs">
  <scalar units="cm-1">1582.87</scalar>
 </property>
 <property title="Rotational Constants" dictRef="me:rotConsts">
  <array units="cm-1">0.328 0.148 0.106</array>
 </property>
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  <scalar>1</scalar>
 </property>
 <property dictRef="me:frequenciesScaleFactor">
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        <scalar>0.993</scalar>
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                <!--  Frequency 120.02 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation  -->
                <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
      <me:bondRef>b6</me:bondRef>
      <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="10" UseSineTerms="yes">
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 <me:PotentialPoint angle="10"  potential=" 0.2100400"/>
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 <me:PotentialPoint angle="30"  potential=" 1.6015550"/>
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 <me:PotentialPoint angle="50"  potential=" 3.1768550"/>
 <me:PotentialPoint angle="60"  potential=" 3.4919150"/>
 <me:PotentialPoint angle="70"  potential=" 3.3081300"/>
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 <me:PotentialPoint angle="90"  potential=" 1.8378500"/>
 <me:PotentialPoint angle="100"  potential=" 0.9451800"/>
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 <me:PotentialPoint angle="120"  potential=" 0.0000000"/>
 <me:PotentialPoint angle="130"  potential=" 0.1837850"/>
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</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

</molecule>

<molecule id="TS2" spinMultiplicity="1">

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<atom id="a2" elementType="C" x3="0.989507" y3="0.453877" z3="-2.008828" />

<atom id="a3" elementType="O" x3="0.934339" y3="-0.717029" z3="-2.485448" />

<atom id="a4" elementType="O" spinMultiplicity="2" x3="-1.029996" y3="-0.439044" z3="-2.477970" />

<atom id="a5" elementType="H" x3="-1.800648" y3="-1.042528" z3="-2.500191" />

<atom id="a6" elementType="C" spinMultiplicity="2" x3="0.405873" y3="1.448269" z3="-2.788379" />

<atom id="a7" elementType="H" x3="2.320258" y3="0.154847" z3="-0.365336" />

<atom id="a8" elementType="H" x3="0.607767" y3="0.219126" z3="0.056652" />

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  <atom id="a9" elementType="H" x3="1.479033" y3="1.718941" z3="-0.331667" />
  <atom id="a10" elementType="H" x3="0.223755" y3="2.444437" z3="-2.404682" />
  <atom id="a11" elementType="H" x3="0.136577" y3="1.211227" z3="-3.806334" />
 </atomArray>
 <bondArray>
  <bond id="b1" atomRefs2="a11 a6" order="1" />
  <bond id="b2" atomRefs2="a6 a10" order="1" />
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  <bond id="b4" atomRefs2="a5 a4" order="1" />
  <bond id="b5" atomRefs2="a3 a2" order="2" />
  <bond id="b6" atomRefs2="a2 a1" order="1" />
  <bond id="b7" atomRefs2="a1 a7" order="1" />
  <bond id="b8" atomRefs2="a1 a9" order="1" />
  <bond id="b9" atomRefs2="a1 a8" order="1" />
 </bondArray>
 <propertyList>
  <property title="program">
   <scalar>Gaussian 16, Revision C.01</scalar>
  </property>
  <property title="basis">
   <scalar>def2TZVP (5D, 7F)</scalar>
  </property>
  <property title="method">
   <scalar>mn15</scalar>
  </property>
  <property title="File Format">
   <scalar>g03</scalar>
  </property>
  <property title="Energy" dictRef="me:ZPE">
   <scalar units="kJ/mol" >17.57</scalar>
  </property>
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<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">135.36 357.21 377.81 391.75 492.75 537.51 621.01 864.48 896.78 969.01 980.34 1033.74 1060.89 1339.40 1386.60 1453.24 1465.70 1490.97 1535.58 3076.87 3157.11 3173.01 3200.16 3324.62 3696.20</array>

</property>

<property title="ImaginaryFrequency" dictRef="me:imFreqs">

<scalar units="cm-1">587.55</scalar>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.241 0.138 0.119</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

<property dictRef="me:frequenciesScaleFactor">

<scalar>0.993</scalar>

</property>

</propertyList>

<me:DOSCMethod name="QMRotors" />

<!-- Frequency 116.19 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->

<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">

<me:bondRef>b6</me:bondRef>

<me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="10" UseSineTerms="yes">

<me:PotentialPoint angle="0" potential=" 0.0000000"/>

<me:PotentialPoint angle="5" potential="-0.6826300"/>

<me:PotentialPoint angle="10" potential="-1.1814750"/>

<me:PotentialPoint angle="15" potential="-1.5227900"/>

<me:PotentialPoint angle="20" potential="-1.6803200"/>

<me:PotentialPoint angle="25" potential="-1.6278100"/>

<me:PotentialPoint angle="30" potential="-1.4177700"/>

<me:PotentialPoint angle="35" potential="-0.9976900"/>

<me:PotentialPoint angle="40" potential="-0.4463350"/>

<me:PotentialPoint angle="45" potential=" 0.2888050"/>

<me:PotentialPoint angle="50" potential=" 1.1027100"/>

<me:PotentialPoint angle="55" potential=" 1.9953800"/>

<me:PotentialPoint angle="60" potential=" 2.9143050"/>

<me:PotentialPoint angle="65" potential=" 3.7807200"/>

<me:PotentialPoint angle="70" potential=" 4.4896050"/>

<me:PotentialPoint angle="75" potential=" 5.0147050"/>

<me:PotentialPoint angle="80" potential=" 5.2510000"/>

<me:PotentialPoint angle="85" potential=" 5.1984900"/>

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<me:PotentialPoint angle="100" potential=" 3.5444250"/>

<me:PotentialPoint angle="105" potential=" 2.6517550"/>

<me:PotentialPoint angle="110" potential=" 1.7590850"/>

<me:PotentialPoint angle="115" potential=" 0.8664150"/>

<me:PotentialPoint angle="120" potential=" 0.0787650"/>

<me:PotentialPoint angle="125" potential="-0.6038650"/>

<me:PotentialPoint angle="130" potential="-1.1289650"/>

<me:PotentialPoint angle="135" potential="-1.4965350"/>

<me:PotentialPoint angle="140" potential="-1.6540650"/>

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<me:PotentialPoint angle="155" potential="-1.0239450"/>

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<me:PotentialPoint angle="175" potential=" 1.9691250"/>

<me:PotentialPoint angle="180" potential=" 2.8880500"/>

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<me:PotentialPoint angle="190" potential=" 4.4633500"/>

<me:PotentialPoint angle="195" potential=" 4.9884500"/>

<me:PotentialPoint angle="200" potential=" 5.2510000"/>

<me:PotentialPoint angle="205" potential=" 5.2247450"/>

<me:PotentialPoint angle="210" potential=" 4.9096850"/>

<me:PotentialPoint angle="215" potential=" 4.3320750"/>

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<me:PotentialPoint angle="230" potential=" 1.8115950"/>

<me:PotentialPoint angle="235" potential=" 0.9189250"/>

<me:PotentialPoint angle="240" potential=" 0.1312750"/>

<me:PotentialPoint angle="245" potential="-0.5513550"/>

<me:PotentialPoint angle="250" potential="-1.1027100"/>

<me:PotentialPoint angle="255" potential="-1.4702800"/>

<me:PotentialPoint angle="260" potential="-1.6540650"/>

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<me:PotentialPoint angle="270" potential="-1.4702800"/>

<me:PotentialPoint angle="275" potential="-1.1027100"/>

<me:PotentialPoint angle="280" potential="-0.5513550"/>

<me:PotentialPoint angle="285" potential=" 0.1312750"/>

<me:PotentialPoint angle="290" potential=" 0.9451800"/>

<me:PotentialPoint angle="295" potential=" 1.8641050"/>

<me:PotentialPoint angle="300" potential=" 2.7830300"/>

<me:PotentialPoint angle="305" potential=" 3.6757000"/>

<me:PotentialPoint angle="310" potential=" 4.4108400"/>

<me:PotentialPoint angle="315" potential=" 4.9621950"/>

<me:PotentialPoint angle="320" potential=" 5.2510000"/>

<me:PotentialPoint angle="325" potential=" 5.1984900"/>

<me:PotentialPoint angle="330" potential=" 4.8834300"/>

<me:PotentialPoint angle="335" potential=" 4.2795650"/>

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<me:PotentialPoint angle="340"  potential=" 3.4919150"/>
<me:PotentialPoint angle="345"  potential=" 2.5992450"/>
<me:PotentialPoint angle="350"  potential=" 1.6803200"/>
<me:PotentialPoint angle="355"  potential=" 0.7876500"/>
                                </me:HinderedRotorPotential>
                                 <me:periodicity>3</me:periodicity>
   </me:ExtraDOSCMethod>

  </molecule>

 </moleculeList>

 <reactionList>

  <reaction id="R1" reversible="true">
   <reactantList>
    <reactant>
     <molecule ref="Me2COO" role="modelled" />
    </reactant>
   </reactantList>
   <productList>
    <product>
     <molecule ref="Methyl-VHP" role="modelled" />
    </product>
   </productList>
   <me:transitionState>
    <molecule ref="TS1" role="transitionState" />
   </me:transitionState>
                  <me:tunneling name="Eckart" />
   <me:MCRCMethod name="RRKM" />
  </reaction>
```

```
                <reaction id="R2">
  <reactantList>
   <reactant>
    <molecule ref="Methyl-VHP" role="modelled" />
   </reactant>
  </reactantList>
  <productList>
   <product>
    <molecule ref="Methyl-vinoxy" role="sink" />
   </product>
   <product>
    <molecule ref="OH" role="sink" />
   </product>
  </productList>
  <me:transitionState>
   <molecule ref="TS2" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="RRKM" />
 </reaction>

</reactionList>

<me:conditions>

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

 <me:PTs>

      <me:PTpair units="Torr" P="5.0" T="296" precision="qd" bathGas="He" >
      <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="12">466</me:experimentalRate>
```

```
</me:PTpair>
<me:PTpair units="Torr" P="10.0" T="296" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="14">546</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="50.0" T="296" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="7">704</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="100.0" T="296" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="11">802</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="200.0" T="296" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="11">851</me:experimentalRate>
</me:PTpair>

<me:PTpair units="Torr" P="5.23" T="310" precision="qd" bathGas="He" >
        <me:experimentalRate ref1="Me2COO" ref2="Me2COO"
error="17">784</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="10.47" T="310" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="30">889</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="52.3" T="310" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="15">1325</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="104.8" T="310" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="27">1392</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="209.5" T="310" precision="qd" bathGas="He" >
 <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="81">1556</me:experimentalRate>
</me:PTpair>
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<me:PTpair units="Torr" P="5.45" T="323" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="90">1068</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="10.9" T="323" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="74">1529</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="54.5" T="323" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="25">2317</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="109.0" T="323" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="22">2465</me:experimentalRate>
</me:PTpair>

<me:PTpair units="Torr" P="5.57" T="330" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="12">1466</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="11.15" T="330" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="61">2004</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="55.6" T="330" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="42">3315</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="111.5" T="330" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="75">3309</me:experimentalRate>
</me:PTpair>

<me:PTpair units="Torr" P="5.75" T="340" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="52">1560</me:experimentalRate>
</me:PTpair>
<me:PTpair units="Torr" P="11.74" T="340" precision="qd" bathGas="He" >
<me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="13">2941</me:experimentalRate>

```
      </me:PTpair>
                                  <me:PTpair units="Torr" P="57.5" T="340" precision="qd" bathGas="He" >
       <me:experimentalRate ref1="Me2COO" ref2="Me2COO" error="211">4394</me:experimentalRate>
      </me:PTpair>

  </me:PTs>

  <me:InitialPopulation>
    <me:molecule ref="Me2COO" me:population="1.0" />
  </me:InitialPopulation>

</me:conditions>

<me:modelParameters>
  <me:grainSize units="cm-1">60</me:grainSize>
  <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
</me:modelParameters>

<me:control>
  <me:printSpeciesProfile />
  <me:eigenvalues>3</me:eigenvalues>
  <me:calcMethod name="simpleCalc" />
  <!--<me:calcMethod xsi:type="me:marquardt">
    <me:MarquardtIterations>20</me:MarquardtIterations>
    <me:MarquardtTolerance>0.01</me:MarquardtTolerance>
    <me:MarquardtDerivDelta>1.e-03</me:MarquardtDerivDelta>
  </me:calcMethod>-->
</me:control>

<metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
  <dc:title>Project name</dc:title>
```

```
    <dc:source>CH32COO-test.xml</dc:source>
    <dc:creator>Mesmer v5.2</dc:creator>
    <dc:date>20200118_112216</dc:date>
    <dc:contributor>praseal</dc:contributor>
  </metadataList>
</me:mesmer>
```

N_2 bath gas

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
```

```
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer" xmlns:xsi="http://www.w3.org/2001/XMLSchema-
instance">
 <me:title>Project name</me:title>
 <moleculeList convention="">

    <molecule id="N2">
  <atomArray>
   <atom id="a1" elementType="N" />
   <atom id="a2" elementType="N" />
  </atomArray>
  <bondArray>
   <bond atomRefs2="a2 a1" order="3"/>
  </bondArray>
  <propertyList>
   <property dictRef="me:epsilon">
    <scalar>48.0</scalar>
   </property>
   <property dictRef="me:sigma">
    <scalar>3.90</scalar>
   </property>
   <property dictRef="me:MW">
    <scalar units="amu">28.0</scalar>
   </property>
  </propertyList>
 </molecule>

            <molecule id="OH" spinMultiplicity="2">
   <atomArray>
    <atom id="a1" elementType="O" spinMultiplicity="2" x3="0.772188" y3="-1.028683" z3="-1.079052"
/>
    <atom id="a2" elementType="H" x3="1.058651" y3="-1.784301" z3="-1.627078" />
```

```
</atomArray>
<bondArray>
 <bond atomRefs2="a2 a1" order="1" />
</bondArray>
<propertyList>
 <property title="program">
  <scalar>Gaussian 16, Revision C.01</scalar>
 </property>
 <property title="basis">
  <scalar>def2TZVP (5D, 7F)</scalar>
 </property>
 <property title="method">
  <scalar>mn15</scalar>
 </property>
 <property title="File Format">
  <scalar>g03</scalar>
 </property>
 <property title="Energy" dictRef="me:ZPE">
  <scalar units="kJ/mol" >0</scalar>
 </property>
 <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
  <scalar>2.00</scalar>
 </property>
 <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
  <array units="cm-1">3762.87</array>
 </property>
 <property title="Rotational Constants" dictRef="me:rotConsts">
  <array units="cm-1">18.638</array>
 </property>
 <property title="Symmetry Number" dictRef="me:symmetryNumber">
  <scalar>1</scalar>
```

```
  </property>
                                <property dictRef="me:frequenciesScaleFactor">
    <scalar>0.993</scalar>
  </property>
 </propertyList>
                 <me:DOSCMethod name="QMRotors" />
</molecule>

                <molecule id="Methyl-vinoxy" spinMultiplicity="2">
 <atomArray>
  <atom id="a1" elementType="C" x3="1.377768" y3="0.656098" z3="-0.588781" />
  <atom id="a2" elementType="C" x3="1.050787" y3="0.416179" z3="-2.043330" />
  <atom id="a3" elementType="O" x3="1.430425" y3="-0.596608" z3="-2.628385" />
  <atom id="a4" elementType="C" spinMultiplicity="2" x3="0.278079" y3="1.407261" z3="-2.737943" />
  <atom id="a5" elementType="H" x3="1.960840" y3="-0.177513" z3="-0.206049" />
  <atom id="a6" elementType="H" x3="0.461158" y3="0.760829" z3="-0.005239" />
  <atom id="a7" elementType="H" x3="1.944099" y3="1.582331" z3="-0.474469" />
  <atom id="a8" elementType="H" x3="-0.067716" y3="2.305648" z3="-2.247202" />
  <atom id="a9" elementType="H" x3="0.041377" y3="1.241371" z3="-3.778023" />
 </atomArray>
 <bondArray>
  <bond id="b1" atomRefs2="a9 a4" order="1" />
  <bond id="b2" atomRefs2="a4 a8" order="1" />
  <bond id="b3" atomRefs2="a4 a2" order="1" />
  <bond id="b4" atomRefs2="a3 a2" order="2" />
  <bond id="b5" atomRefs2="a2 a1" order="1" />
  <bond id="b6" atomRefs2="a1 a7" order="1" />
  <bond id="b7" atomRefs2="a1 a5" order="1" />
  <bond id="b8" atomRefs2="a1 a6" order="1" />
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<property title="program">
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</property>
<property title="basis">
<scalar>def2TZVP (5D, 7F)</scalar>
</property>
<property title="method">
<scalar>mn15</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kJ/mol" >11.83</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">366.32 506.50 515.00 761.64 835.02 921.67 1015.23 1051.99 1278.18 1383.00 1445.47 1460.13 1462.34 1647.86 3072.68 3141.58 3192.41 3194.24 3312.48</array>
</property>
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</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
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<property dictRef="me:frequenciesScaleFactor">
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</property>

</propertyList>

<me:DOSCMethod name="QMRotors" />

<!-- Frequency 61.67 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->

<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">

<me:bondRef>b5</me:bondRef>

<me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="10" UseSineTerms="yes">

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<me:PotentialPoint angle="25" potential=" 0.3150600"/>

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<me:PotentialPoint angle="35" potential=" 0.4988450"/>

<me:PotentialPoint angle="40" potential=" 0.6038650"/>

<me:PotentialPoint angle="45" potential=" 0.6563750"/>

<me:PotentialPoint angle="50" potential=" 0.7088850"/>

<me:PotentialPoint angle="55" potential=" 0.7351400"/>

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<me:PotentialPoint angle="65" potential=" 0.7351400"/>

<me:PotentialPoint angle="70" potential=" 0.6826300"/>

<me:PotentialPoint angle="75" potential=" 0.6301200"/>

<me:PotentialPoint angle="80" potential=" 0.5513550"/>

<me:PotentialPoint angle="85" potential=" 0.4725900"/>

<me:PotentialPoint angle="90" potential=" 0.3675700"/>

<me:PotentialPoint angle="95" potential=" 0.2888050"/>

<me:PotentialPoint angle="100" potential=" 0.1837850"/>

<me:PotentialPoint angle="105" potential=" 0.1050200"/>

<me:PotentialPoint angle="110" potential=" 0.0525100"/>

<me:PotentialPoint angle="115" potential=" 0.0000000"/>

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<me:PotentialPoint angle="125" potential=" 0.0000000"/>

<me:PotentialPoint angle="130" potential=" 0.0262550"/>

<me:PotentialPoint angle="135" potential=" 0.1050200"/>

<me:PotentialPoint angle="140" potential=" 0.1837850"/>

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<me:PotentialPoint angle="150" potential=" 0.3675700"/>

<me:PotentialPoint angle="155" potential=" 0.4725900"/>

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<me:PotentialPoint angle="165" potential=" 0.6301200"/>

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<me:PotentialPoint angle="190" potential=" 0.7088850"/>

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<me:PotentialPoint angle="200" potential=" 0.5513550"/>

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<me:PotentialPoint angle="210" potential=" 0.3675700"/>

<me:PotentialPoint angle="215" potential=" 0.2625500"/>

<me:PotentialPoint angle="220" potential=" 0.1837850"/>

<me:PotentialPoint angle="225" potential=" 0.1050200"/>

<me:PotentialPoint angle="230" potential=" 0.0262550"/>

<me:PotentialPoint angle="235" potential=" 0.0000000"/>

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<me:PotentialPoint angle="245" potential=" 0.0000000"/>

<me:PotentialPoint angle="250" potential=" 0.0525100"/>

<me:PotentialPoint angle="255" potential=" 0.1050200"/>

<me:PotentialPoint angle="260" potential=" 0.1837850"/>

<me:PotentialPoint angle="265" potential=" 0.2888050"/>

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<me:PotentialPoint angle="280" potential=" 0.5513550"/>

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<me:PotentialPoint angle="290" potential=" 0.6826300"/>

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<me:PotentialPoint angle="305" potential=" 0.7351400"/>

<me:PotentialPoint angle="310" potential=" 0.7088850"/>

<me:PotentialPoint angle="315" potential=" 0.6563750"/>

<me:PotentialPoint angle="320" potential=" 0.6038650"/>

<me:PotentialPoint angle="325" potential=" 0.5251000"/>

<me:PotentialPoint angle="330" potential=" 0.4200800"/>

<me:PotentialPoint angle="335" potential=" 0.3150600"/>

<me:PotentialPoint angle="340" potential=" 0.2100400"/>

<me:PotentialPoint angle="345" potential=" 0.1312750"/>

<me:PotentialPoint angle="350" potential=" 0.0525100"/>

<me:PotentialPoint angle="355" potential=" 0.0000000"/>

</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 372.51 has been eliminated in favour of a 1 dimensional hindered rotor. 2-4 Dihedral rotation -->

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<me:PotentialPoint angle="50" potential="17.1445150"/>

<me:PotentialPoint angle="55" potential="20.2951150"/>

<me:PotentialPoint angle="60" potential="23.5769900"/>

<me:PotentialPoint angle="65" potential="26.8851200"/>

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<me:PotentialPoint angle="75" potential="33.3963600"/>

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</me:HinderedRotorPotential>

<me:periodicity>2</me:periodicity>

</me:ExtraDOSCMethod>

</molecule>

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<atom id="a2" elementType="C" x3="0.581386" y3="0.294677" z3="-1.511105" />

<atom id="a3" elementType="O" x3="-0.205025" y3="-0.550839" z3="-2.260355" />

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<atom id="a5" elementType="H" x3="-0.935999" y3="-2.158799" z3="-1.650821" />

<atom id="a6" elementType="C" x3="0.964317" y3="1.424289" z3="-2.095127" />

<atom id="a7" elementType="H" x3="1.408704" y3="-1.194846" z3="-0.223044" />

<atom id="a8" elementType="H" x3="0.154251" y3="-0.212273" z3="0.524041" />

<atom id="a9" elementType="H" x3="1.758898" y3="0.484382" z3="0.238211" />

<atom id="a10" elementType="H" x3="1.686148" y3="2.067042" z3="-1.613136" />

<atom id="a11" elementType="H" x3="0.584989" y3="1.698077" z3="-3.069557" />

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<bond id="b3" atomRefs2="a3 a4" order="1" />

<bond id="b4" atomRefs2="a6 a10" order="1" />

<bond id="b5" atomRefs2="a6 a2" order="2" />

<bond id="b6" atomRefs2="a5 a4" order="1" />

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<scalar>Gaussian 16, Revision B.01</scalar>

</property>

<property title="basis">

<scalar>def2TZVP (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>mn15</scalar>

</property>

<property title="File Format">

<scalar>g03</scalar>

</property>

<property title="Energy" dictRef="me:ZPE">

<scalar units="kJ/mol">-59.75</scalar>

</property>

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">320.84 405.42 473.58 563.31 734.32 851.24 884.42 932.61 1011.07 1039.60 1057.79 1293.11 1384.43 1395.31 1421.69 1455.80 1471.65 1742.32 3076.48 3149.68 3179.16 3201.43 3299.93 3831.03</array>

</property>

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<array units="cm-1">0.285 0.148 0.103</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

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    <property dictRef="me:sigma" >
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    </property>
    <property dictRef="me:epsilon" >
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    </property>
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  </propertyList>

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            <!--  Frequency 221.84 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->
            <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
    <me:bondRef>b7</me:bondRef>
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<me:PotentialPoint angle="5"  potential=" 0.1837850"/>
<me:PotentialPoint angle="10"  potential=" 0.7088850"/>
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<me:PotentialPoint angle="45"  potential=" 8.2178150"/>
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<me:PotentialPoint angle="65" potential=" 9.9769000"/>

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<me:PotentialPoint angle="125" potential=" 0.1837850"/>

<me:PotentialPoint angle="130" potential=" 0.7088850"/>

<me:PotentialPoint angle="135" potential=" 1.5227900"/>

<me:PotentialPoint angle="140" potential=" 2.5729900"/>

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<me:PotentialPoint angle="200" potential=" 7.9027550"/>

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<me:PotentialPoint angle="255" potential=" 1.4440250"/>

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<me:PotentialPoint angle="355" potential=" 0.1837850"/>

</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 90.10 has been eliminated in favour of a 1 dimensional hindered rotor. 2-3 Dihedral rotation -->

<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">

<me:bondRef>b2</me:bondRef>

<me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="10" UseSineTerms="yes">

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<me:PotentialPoint angle="25" potential=" 3.203110"/>

<me:PotentialPoint angle="30" potential=" 4.647135"/>

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<me:PotentialPoint angle="55" potential=" 13.862640"/>

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<me:PotentialPoint angle="70" potential=" 16.934475"/>

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<me:PotentialPoint angle="115" potential=" -1.864105"/>

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</me:ExtraDOSCMethod>

<!-- Frequency 182.72 has been eliminated in favour of a 1 dimensional hindered rotor. 3-4 Dihedral rotation -->

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</me:HinderedRotorPotential>
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<me:energyTransferModel xsi:type="me:ExponentialDown">
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<me:deltaEDownTExponent referenceTemperature="298.0" >0.704807</me:deltaEDownTExponent>
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</molecule>

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      <property title="Rotational Constants" dictRef="me:rotConsts">
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      <property dictRef="me:epsilon" >
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       <scalar>0.993</scalar>
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    </propertyList>
    <me:DOSCMethod name="QMRotors" />


                <!--  Frequency 162.06 has been eliminated in favour of a 1 dimensional hindered rotor. 2-5 Dihedral Me rotation -->
                <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
      <me:bondRef>b7</me:bondRef>
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</me:HinderedRotorPotential>

<me:periodicity>3</me:periodicity>

</me:ExtraDOSCMethod>

<!-- Frequency 216.14 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->

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  <atom id="a4" elementType="O" spinMultiplicity="2" x3="1.337155" y3="1.825212" z3="0.705651" />
  <atom id="a5" elementType="H" x3="0.124868" y3="1.993062" z3="0.109444" />
  <atom id="a6" elementType="C" x3="-0.430606" y3="1.105136" z3="-0.693445" />
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  </property>

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</property>

<property title="method">

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</property>

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</property>

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<array units="cm-1">0.328 0.148 0.106</array>

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<!-- Frequency 120.02 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation -->

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<me:bondRef>b6</me:bondRef>

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</molecule>

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<atom id="a3" elementType="O" x3="0.934339" y3="-0.717029" z3="-2.485448" />

<atom id="a4" elementType="O" spinMultiplicity="2" x3="-1.029996" y3="-0.439044" z3="-2.477970" />

<atom id="a5" elementType="H" x3="-1.800648" y3="-1.042528" z3="-2.500191" />

<atom id="a6" elementType="C" spinMultiplicity="2" x3="0.405873" y3="1.448269" z3="-2.788379" />

<atom id="a7" elementType="H" x3="2.320258" y3="0.154847" z3="-0.365336" />

<atom id="a8" elementType="H" x3="0.607767" y3="0.219126" z3="0.056652" />

<atom id="a9" elementType="H" x3="1.479033" y3="1.718941" z3="-0.331667" />

<atom id="a10" elementType="H" x3="0.223755" y3="2.444437" z3="-2.404682" />

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                <!--  Frequency 116.19 has been eliminated in favour of a 1 dimensional hindered rotor. 1-2 Dihedral Me rotation  -->
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    <dc:contributor>praseal</dc:contributor>
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ChemKin PLOG format

! 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)

He bath gas

Me2COO => Methyl-VHP 1.34139e+16 -4.21585 5004.3

PLOG/ 0.001 1.34139e+16 -4.21585 5004.3/

PLOG/ 0.005 1.05703e+10 -1.75141 4641.58/

PLOG/ 0.01 1.90908e+06 -0.292097 4310.91/

PLOG/ 0.025 1.04144 2.09736 3644.08/

PLOG/ 0.05 1.47193e-06 4.28895 2931.11/

PLOG/ 0.1 2.37602e-13 6.80045 2026.37/

PLOG/ 0.25 1.98802e-23 10.4798 570.716/

PLOG/ 0.5 2.00894e-31 13.3666 -666.32/

PLOG/ 0.75 4.78107e-36 15.0239 -1413.22/

PLOG/ 1 3.13034e-39 16.1603 -1940.75/

PLOG/ 2.5 2.42703e-48 19.3915 -3507.35/

PLOG/ 5 1.06523e-53 21.2785 -4466.05/

PLOG/ 7.5 4.07813e-56 22.1267 -4907.15/

PLOG/ 10 1.61291e-57 22.6182 -5165.57/

PLOG/ 50 1.02528e-61 24.085 -5949.18/

PLOG/ 100 2.31685e-62 24.3103 -6071.22/

Me2COO => Methyl-vinoxy + OH 9.39794e+12 -1.95556 7599.86

PLOG/ 0.001 9.39794e+12 -1.95556 7599.86/

PLOG/ 0.005 4.60003e+11 -1.16505 8386.74/

PLOG/ 0.01 7.50547e+10 -0.74563 8722.24/

PLOG/ 0.025 4.35219e+09 -0.123527 9165.43/

PLOG/ 0.05 2.89594e+08 0.427507 9477.44/

PLOG/ 0.1 7.73846e+06 1.10809 9722.15/

PLOG/ 0.25 5592.46 2.35208 9825.28/

PLOG/ 0.5 1.67385 3.66265 9640.68/

PLOG/ 0.75 0.00438269 4.59493 9404.8/

PLOG/ 1 3.87425e-05 5.32576 9179.34/

PLOG/ 2.5 1.45169e-12 7.91679 8193.1/

PLOG/ 5 2.155e-18 9.90753 7306.33/

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PLOG/ 10 1.39726e-23 11.6469 6470.8/

PLOG/ 50 4.34206e-31 14.0474 5248.27/

PLOG/ 100 1.2357e-32 14.484 5018.74/

Methyl-VHP => Me2COO 4.92036e+18 -5.3312 19690

PLOG/ 0.001 4.92036e+18 -5.3312 19690/

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PLOG/ 1 1.14824e-36 15.045 12745/

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PLOG/ 5 3.90735e-51 20.1631 10219.7/

PLOG/ 7.5 1.4959e-53 21.0114 9778.58/

PLOG/ 10 5.91631e-55 21.5029 9520.16/

PLOG/ 50 3.76083e-59 22.9697 8736.54/

PLOG/ 100 8.49845e-60 23.1949 8614.5/

Methyl-VHP => Methyl-vinoxy + OH 1.05191e+37 -8.99153 22441.2

PLOG/ 0.001 1.05191e+37 -8.99153 22441.2/

PLOG/ 0.005 3.82531e+33 -7.58615 22166.9/

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PLOG/ 0.5 4.89222e+16 -1.43763 19547.5/

PLOG/ 0.75 4.56654e+15 -1.07609 19358.3/

PLOG/ 1 1.11036e+15 -0.860912 19244.5/

PLOG/ 2.5 4.69299e+13 -0.380578 18986.8/

PLOG/ 5 1.23675e+13 -0.178572 18876.9/

PLOG/ 7.5 7.55493e+12 -0.103985 18836.1/

PLOG/ 10 5.83872e+12 -0.0650061 18814.8/

PLOG/ 50 3.03407e+12 0.0339598 18760.3/

PLOG/ 100 2.78426e+12 0.0469437 18753.1/

N_2 bath gas

Me2COO => Methyl-VHP 71.0087 0.90556 2607.8

PLOG/ 0.001 71.0087 0.90556 2607.8/

PLOG/ 0.005 3.51122e-12 5.88097 902.083/

PLOG/ 0.01 9.02343e-20 8.67211 -169.514/

PLOG/ 0.025 1.51446e-31 12.9596 -1925.71/

PLOG/ 0.05 1.91056e-41 16.5354 -3467.25/

PLOG/ 0.1 1.46349e-51 20.1696 -5088.91/

PLOG/ 0.25 7.6112e-64 24.5615 -7108.84/

PLOG/ 0.5 2.51598e-71 27.2264 -8362.67/

PLOG/ 0.75 8.70225e-75 28.457 -8948.53/

PLOG/ 1 7.89198e-77 29.1825 -9295.96/

PLOG/ 2.5 2.56133e-81 30.7753 -10064.1/

PLOG/ 5 3.66278e-83 31.429 -10381.6/

PLOG/ 7.5 7.80107e-84 31.667 -10497.6/

PLOG/ 10 3.49647e-84 31.7904 -10557.8/

PLOG/ 50 4.65508e-85 32.1005 -10709.3/

PLOG/ 100 3.5824e-85 32.1408 -10729/

Me2COO => Methyl-vinoxy + OH 186506 0.92452 6756.38

PLOG/ 0.001 186506 0.92452 6756.38/

PLOG/ 0.005 6.8268 2.80079 7023.32/

PLOG/ 0.01 0.0292793 3.76781 7092.91/

PLOG/ 0.025 2.85473e-06 5.34554 7042.41/

PLOG/ 0.05 2.82614e-10 6.86374 6821.29/

PLOG/ 0.1 2.62684e-15 8.71979 6383.97/

PLOG/ 0.25 2.05704e-23 11.6356 5457.2/

PLOG/ 0.5 4.4624e-30 13.9857 4574.26/

PLOG/ 0.75 7.37427e-34 15.3029 4042.42/

PLOG/ 1 2.21459e-36 16.1742 3678.81/

PLOG/ 2.5 4.98261e-43 18.4315 2699.66/

PLOG/ 5 1.85641e-46 19.5548 2194.97/

PLOG/ 7.5 6.8663e-48 20.0048 1989.84/

PLOG/ 10 1.07182e-48 20.2488 1877.93/

PLOG/ 50 3.25393e-51 20.8989 1577.4/

PLOG/ 100 9.17379e-52 20.9878 1536.07/

Methyl-VHP => Me2COO 4091.57 0.0667793 17130.6

PLOG/ 0.001 4091.57 0.0667793 17130.6/

PLOG/ 0.005 2.02319e-10 5.04219 15424.9/

PLOG/ 0.01 5.19937e-18 7.83333 14353.3/

PLOG/ 0.025 8.72643e-30 12.1209 12597.1/

PLOG/ 0.05 1.10088e-39 15.6966 11055.5/

PLOG/ 0.1 8.43272e-50 19.3308 9433.85/

PLOG/ 0.25 4.38563e-62 23.7227 7413.93/

PLOG/ 0.5 1.44973e-69 26.3876 6160.09/

PLOG/ 0.75 5.0143e-73 27.6182 5574.24/

PLOG/ 1 4.54742e-75 28.3438 5226.81/

PLOG/ 2.5 1.47586e-79 29.9365 4458.69/

PLOG/ 5 2.11052e-81 30.5903 4141.12/

PLOG/ 7.5 4.49504e-82 30.8282 4025.19/

PLOG/ 10 2.01469e-82 30.9516 3964.97/

PLOG/ 50 2.68229e-83 31.2617 3813.46/

PLOG/ 100 2.06421e-83 31.302 3793.76/

Methyl-VHP => Methyl-vinoxy + OH 3.78237e+30 -6.64781 21324.3

PLOG/ 0.001 3.78237e+30 -6.64781 21324.3/

PLOG/ 0.005 1.33321e+25 -4.56699 20669.3/

PLOG/ 0.01 2.46373e+22 -3.55655 20284.7/

PLOG/ 0.025 7.80268e+18 -2.28032 19758.8/

PLOG/ 0.05 4.17526e+16 -1.45961 19401.7/

PLOG/ 0.1 6.91613e+14 -0.81968 19114.2/

PLOG/ 0.25 1.87336e+13 -0.258826 18856.2/

PLOG/ 0.5 3.79078e+12 -0.0111992 18740.3/

PLOG/ 0.75 2.06505e+12 0.0828245 18696.1/

PLOG/ 1 1.49629e+12 0.132666 18672.5/

PLOG/ 2.5 8.06889e+11 0.22815 18627.2/

PLOG/ 5 6.48483e+11 0.261923 18611.1/

PLOG/ 7.5 6.01937e+11 0.273431 18605.6/

PLOG/ 10 5.79744e+11 0.279235 18602.9/

PLOG/ 50 5.29275e+11 0.293304 18596.2/

PLOG/ 100 5.23234e+11 0.295077 18595.3/