

## **Supplementary material**

---

# **CLEPS 1.0: A NEW PROTOCOL FOR CLOUD AQUEOUS PHASE OXIDATION OF VOC MECHANISMS**

## SM1: Computational method

---

All geometries [1] have been optimized and characterized by vibrational analysis at the DFT level [2] with the M06-2X[3] functional and the 6-311+G(d,p) basis set. [4] Then energies have been recalculated by single-point calculation with the 6-311++G(3df,2pd) [4,5] basis set. Finally, these values are combined with the enthalpy and entropy contributions calculated at room temperature with the 6-311+G(d,p) basis set to get the final reaction energies and free energies. The latter have been converted from the gas phase to the 1M standard state at 1 atm and 298.15 K.[6] Solvent effects were introduced both in geometry optimization -and single point calculation- by the Polarized Continuum Method (PCM) [7] within the universal Solvation Model Density (SMD). [8] All calculations have been performed by program Gaussian 09. [9]

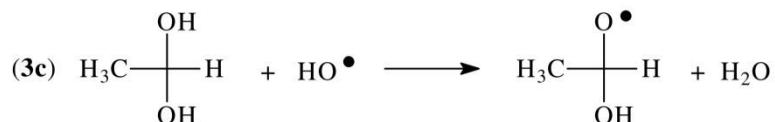
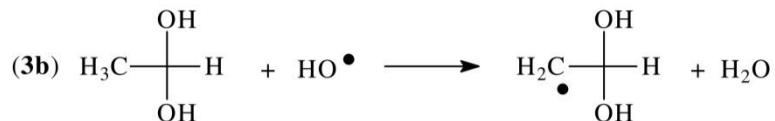
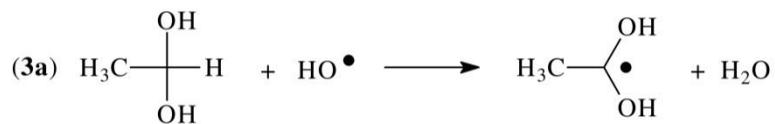
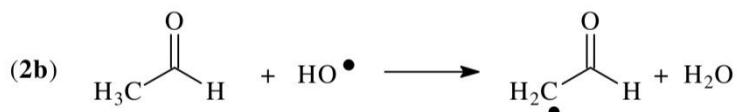
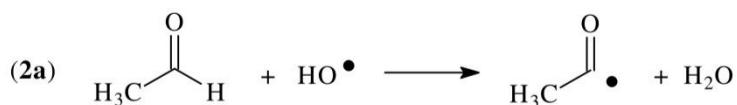
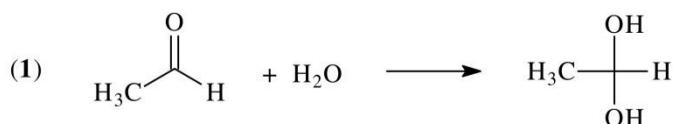
- [1] Reaction enthalpies and free energies were computed as outlined, for instance, in: (a) J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian, Inc., Pittsburgh, PA (USA), 1996, p. 166-168. (b) D. A. McQuarrie, Statistical Thermodynamics, Harper and Row, New York, 1973.
- [2] Jensen W. Introduction to Computational Chemistry, Wiley; Chichester, 1999, Chap. 6 ISBN 0-471-98425-6.
- [3] Y. Zhao, DG. Truhlar, Theor. Chem. Account 2008; 120: 215. (b) Y. Zhao, DG. Truhlar, Acc. Chem. Res. 2008; 41: 157.
- [4] A. D. McLean, G. S. Chandler, J. Chem. Phys. 1980, 72, 5639; (b) T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. v. R. Schleyer, J. Comp. Chem. 1983, 4, 294.
- [5] M. J. Frisch, J. A. Pople, J. S. Binkley, J. Chem. Phys. 1984, 80, 3265.
- [6] R. F. Ribeiro, A. V. Marenich, C. J. Cramer, D. G. Truhlar, J. Phys. Chem. B 2011, 115, 14556.
- [7] (a) V. Barone, M. Cossi, J. Phys. Chem. A1998, 102, 1995; (b) M. Cossi, N. Rega, G. Scalmani, V. Barone, J. Chem. Phys. 2001, 114, 5691; (c) M. T. Cancas, B. Mennucci, J. Tomasi, J. Chem. Phys. 1997, 107, 3032; (d) M. Cossi, V. Barone, B. Mennucci, J. Tomasi; Chem. Phys. Lett. 1998, 286, 253; (e) B. Mennucci, J. Tomasi, J. Chem. Phys. 1997, 106, 5151.
- [8] (a) A. V. Marenich, C. J. Cramer, D. G. TruhlarJ. Phys. Chem. B2009, 113, 6378. (b) A. V. Marenich, C. J. Cramer, D. G. TruhlarJ. Phys. Chem. B 2009, 113, 4538.
- [9] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, et al. Gaussian, Inc., Wallingford CT, 2009.

## SM2: Calculated Reaction Enthalpies & Free Energies (298 K, 1 atm)

---

### Acetaldehyde

---

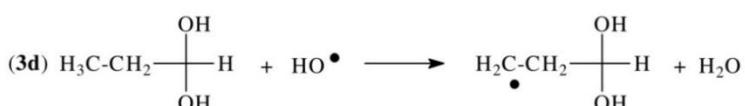
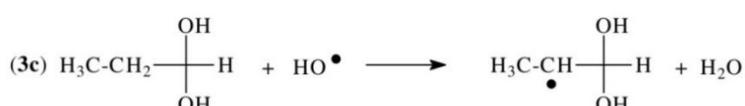
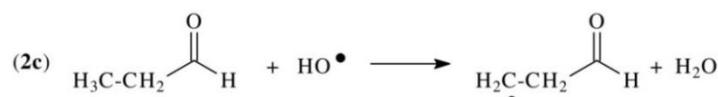
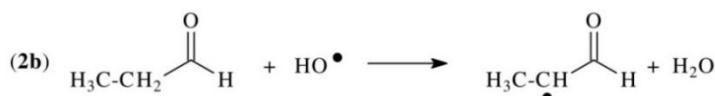
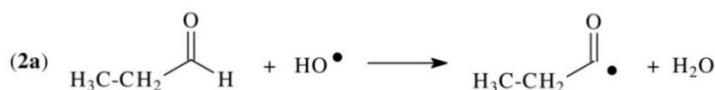
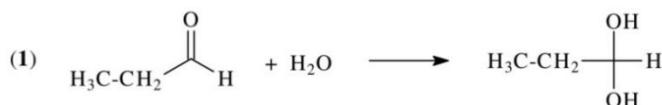


	$\Delta H$	$\Delta G$
<b>1 Idratation</b>	-7.0	2.99
<b>2a RHT from CHO</b>	-28.1	-28.7
<b>2b RHT from CH<sub>3</sub></b>	-25.5	-25.5
<b>3a RHT from CH</b>	-24.5	-26.0
<b>3b RHT from CH<sub>3</sub></b>	-16.5	-17.9
<b>3c RHT from OH</b>	-13.7	-14.7

For hydration (reaction 1), the calculated  $K_h$  is 0.36. The “preferred value” <sup>a</sup> is 1.2. The estimated error in the calculated  $\Delta G$  is +0.7 Kcal mol<sup>-1</sup>.

## Propionaldehyde

---

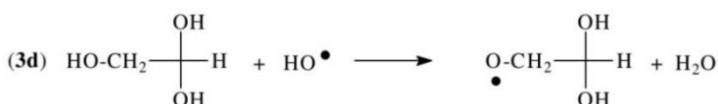
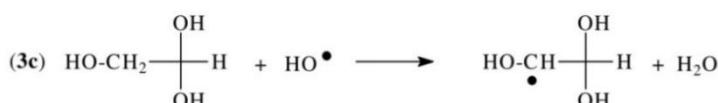
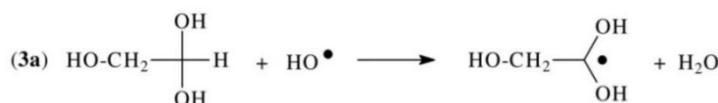
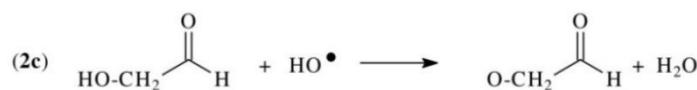
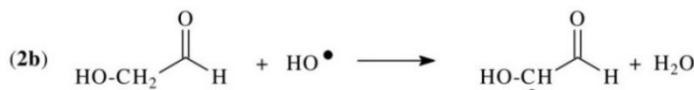
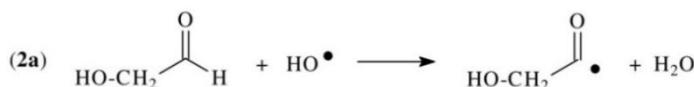
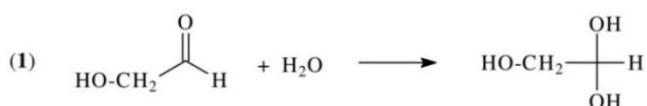


	$\Delta H$	$\Delta G$
<b>1 Hydration<sup>a</sup></b>	-7.6	2.1
<b>2a RHT from CHO</b>	-28.8	-30.0
<b>2b RHT from CH<sub>2</sub></b>	-33.1	-33.8
<b>2c RHT from CH<sub>3</sub></b>	-18.8	-20.1
<b>3a RHT from CH</b>	-25.1	-27.0
<b>3b RHT from OH</b>	-14.2	-15.1
<b>3c RHT from CH<sub>2</sub></b>	-20.7	-23.0
<b>3d RHT from CH<sub>3</sub></b>	-19.2	-20.9

<sup>a</sup> For hydration (reaction 1), the calculated  $K_h$  is 1.8. The “preferred value”<sup>1</sup> is 0.9. The estimated error in the calculated  $\Delta G$  is -0.5 Kcal mol<sup>-1</sup>.

## Glyceraldehyde

---

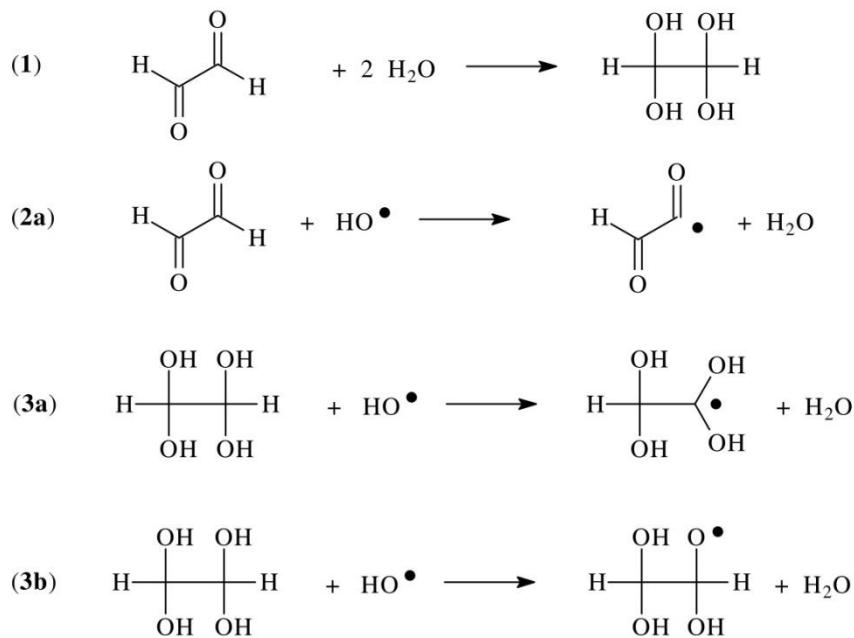


	$\Delta H$	$\Delta G$
<b>1 Hydration<sup>a</sup></b>	-8.9	0.6
<b>2a RHT from CHO</b>	-28.5	-29.2
<b>2b RHT from CH<sub>2</sub></b>	-41.6	-41.6
<b>2c RHT from w-OH</b>	-13.7	-14.2
<b>3a RHT from CH</b>	-25.5	-26.5
<b>3b RHT from OH</b>	-15.4	-16.1
<b>3c RHT from CH<sub>2</sub></b>	-25.3	-26.2
<b>3d RHT from w-OH</b>	-14.9	-15.5

<sup>a</sup> For hydration (reaction 1), the calculated  $K_h$  is 20. The “preferred value”<sup>1</sup> is 16. The estimated error in the calculated  $\Delta G$  is -0.1 Kcal mol<sup>-1</sup>.

## Glyoxal

---

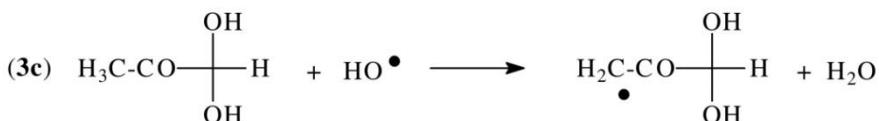
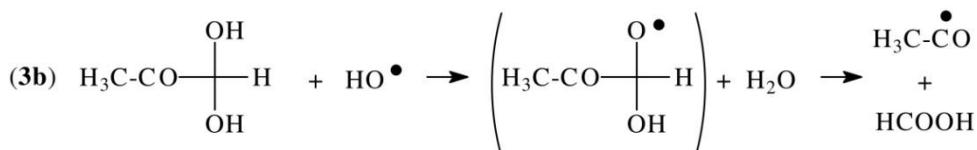
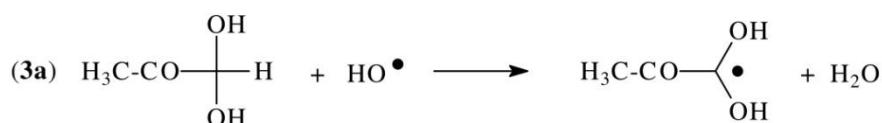
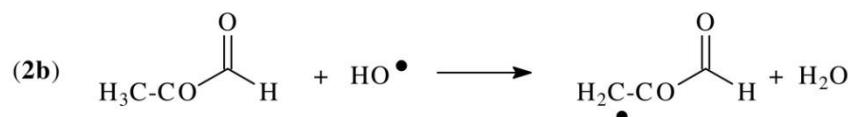
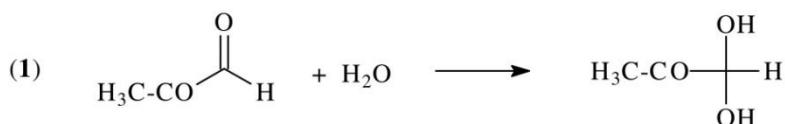


	$\Delta H$	$\Delta G$
<b>1 Hydration<sup>a</sup></b>	-22.8	-5.0
<b>2a RHT from CHO</b>	-26.6	-27.3
<b>3a RHT from CH</b>	-25.2	-26.5
<b>3b RHT from OH</b>	-13.5	-15.1

<sup>a</sup> For hydration (reaction 1), the calculated  $K_h$  is  $2 \cdot 10^5$ . The “preferred value”<sup>1</sup> is  $4 \cdot 10^6$ . The estimated error in the calculated  $\Delta G$  is  $+1.6$  Kcal mol<sup>-1</sup>.

## Methylglyoxal

---

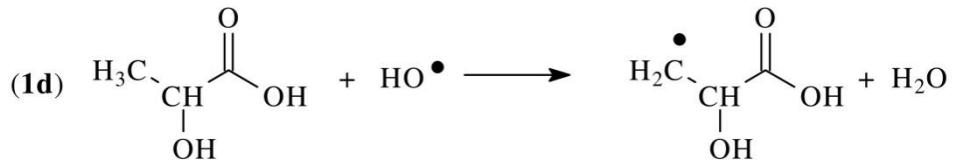
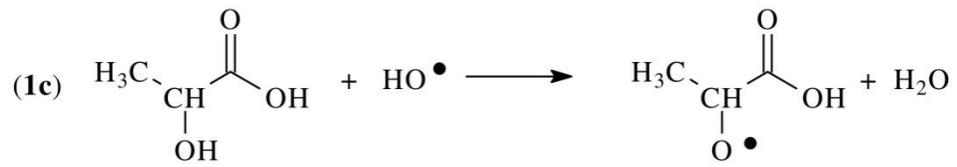
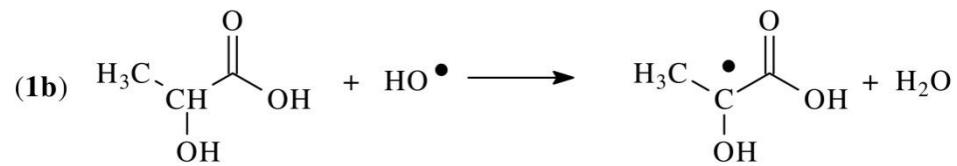
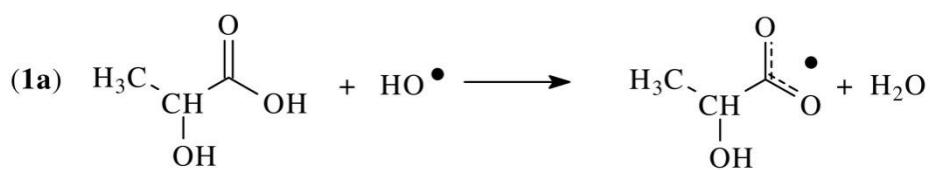


	$\Delta H$	$\Delta G$
<b>1 Hydration<sup>a</sup></b>	-10.2	-1.1
<b>2a RHT from CHO</b>	-32.6	-33.4
<b>2b RHT from CH<sub>3</sub></b>	-25.9	-26.1
<b>3a RHT from CH</b>	-47.3	-47.2
<b>3b RHT from OH<sup>b</sup></b>	-27.2	-31.3
<b>3c RHT from CH<sub>3</sub></b>	-25.2	-25.9

<sup>a</sup> For hydration (reaction 1), the calculated  $K_h$  is  $4 \cdot 10^2$ . The “preferred value” <sup>1</sup> is  $2 \cdot 10^3$ . The estimated error in the calculated  $\Delta G$  is +1.0 Kcal mol-1. <sup>b</sup> Radical  $\text{CH}_3\text{-CO-CH(OH)O}^\bullet$  is not stable and spontaneously breaks in formic acid and acetyl radical. Data are referred to the complex between these two species.

## L-Lactic Acid

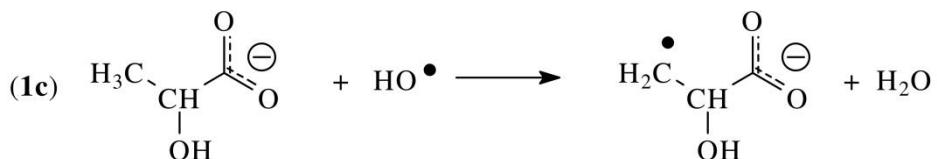
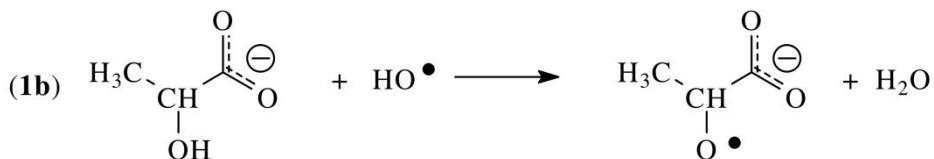
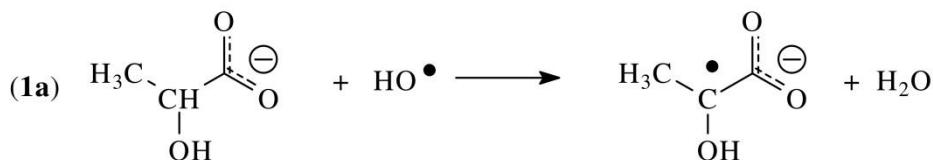
---



	$\Delta H$	$\Delta G$
<b>1a RHT from COOH</b>	-24.3	-28.8
<b>1b RHT from CH</b>	-39.5	-40.5
<b>1c RHT from OH</b>	-11.9	-12.9

## L-Lactate

---

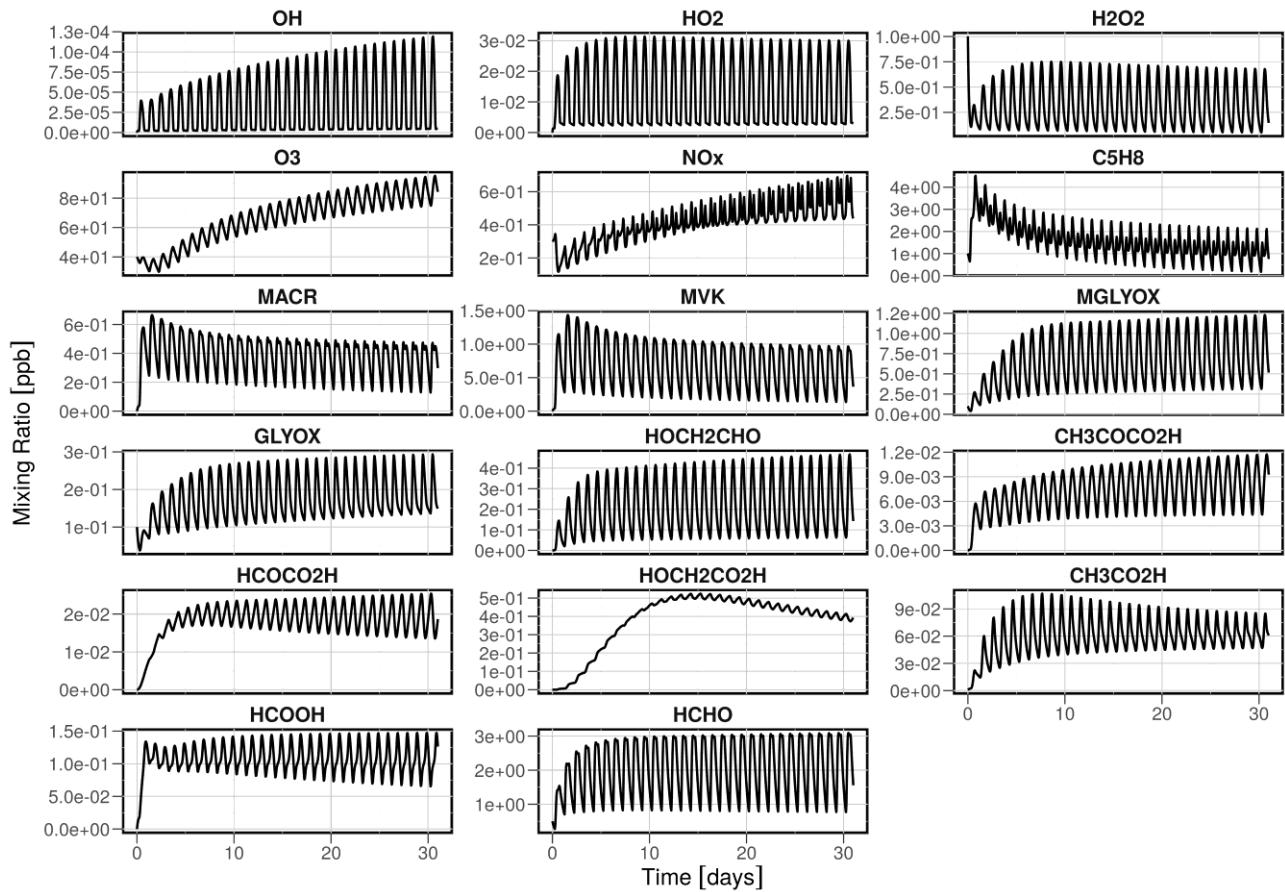


	$\Delta H$	$\Delta G$
<b>1a RHT from CH</b>	-35.3	-36.5
<b>1b RHT from OH</b>	-17.4	-19.0
<b>1c RHT from CH<sub>3</sub></b>	-18.5	-20.2

<sup>a</sup> Doussin, J.-F. and Monod, A.: Structure–activity relationship for the estimation of OH-oxidation rate constants of carbonyl compounds in the aqueous phase, Atmos. Chem. Phys., 13, 11625-11641, doi:10.5194/acp-13-11625-2013, 2013.

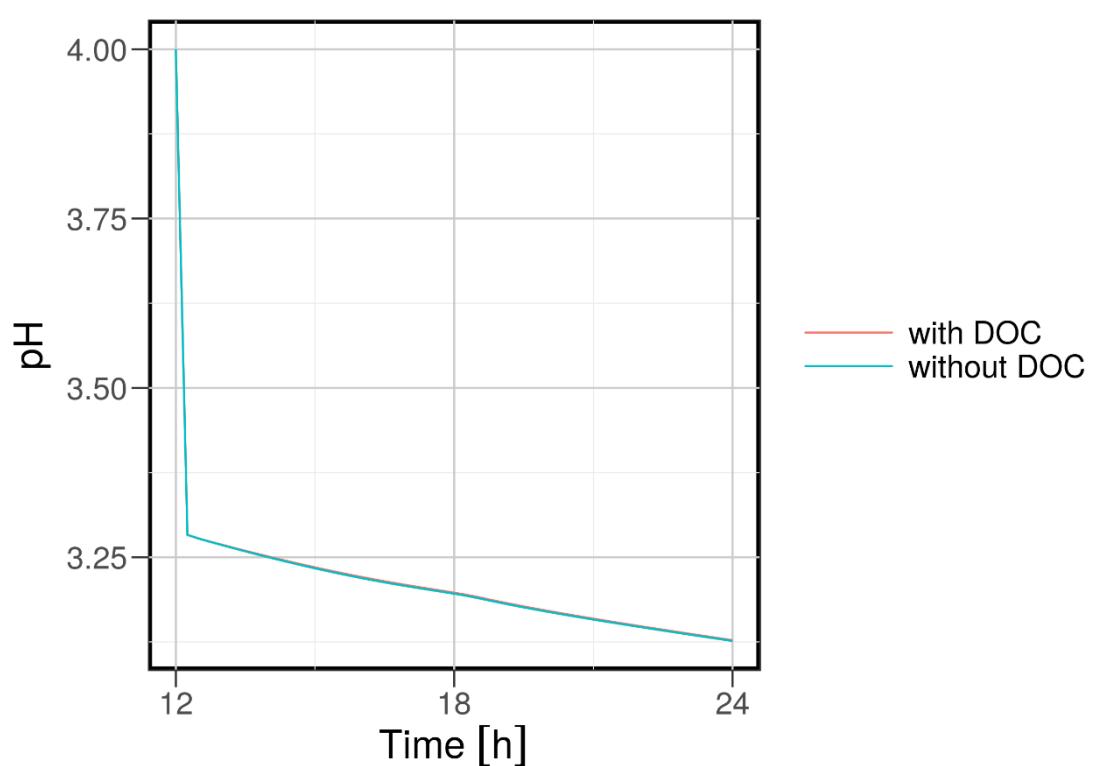
## SM3: Gas chemistry simulation (31 days)

The model was run with initial and environmental conditions adapted from the low- $\text{NO}_x$  situation described by McNeill et al. (2012). Information about emissions, deposition and initial concentrations of chemical species are provided in Table 4. Temperature is constant (290K) during the simulations. Under these chemical conditions, a gas chemistry simulation has been run for 31 days starting 21<sup>st</sup> June 2000. The figure below shows the time evolution of targeted gas species in MCM V3.3.1.



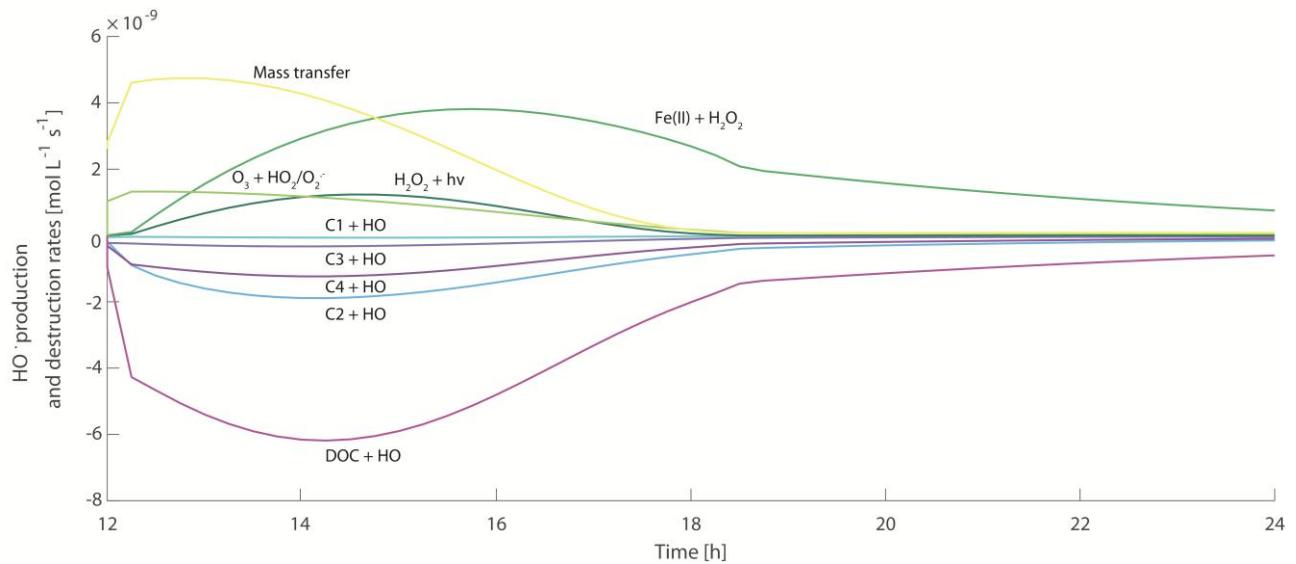
## SM4: pH time evolution

---



## SM5: Time evolution of sources and sinks of HO<sup>·</sup> radicals over the cloud period

---



Average relative contributions of the main production and destruction pathways of HO<sup>·</sup> over the cloud period

	Relative contributions (%)
<b>Destruction pathways</b>	
C <sub>1</sub> + HO <sup>·</sup>	1%
C <sub>2</sub> + HO <sup>·</sup>	18%
C <sub>3</sub> + HO <sup>·</sup>	4%
C <sub>4</sub> + HO <sup>·</sup>	12%
DOC + HO <sup>·</sup>	64%
<b>Production pathways</b>	
H <sub>2</sub> O <sub>2</sub> + Fe(II) (Fenton)	63%
Mass transfer	22%
O <sub>3</sub> + HO <sub>2</sub> /O <sub>2</sub> <sup>·-</sup> / H <sub>2</sub> O <sub>2</sub> + hv	13%

## SM6: List of 267 dissolved MCM species without a reactive equivalent in CLEPS

---

CH <sub>3</sub> COCH(OOH)CH <sub>2</sub> (OOH)	CH <sub>3</sub> COCO(OONO <sub>2</sub> )
CH <sub>2</sub> (OH)CH(ONO <sub>2</sub> )C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CHO	CH <sub>3</sub> C(CH <sub>2</sub> (OH))=CHCO(OOH)
CH <sub>3</sub> CH(OOH)CH <sub>2</sub> (OH)	CH <sub>3</sub> C(OOH)(CH <sub>2</sub> (OOH))CHO
CH <sub>2</sub> (ONO <sub>2</sub> )CH(OH)C(ONO <sub>2</sub> )(CH <sub>3</sub> )CO(OOH)	CH <sub>3</sub> COCH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>3</sub> C(OH)(CO(OONO <sub>2</sub> ))CHO	CH <sub>3</sub> CH(OH)CO(OONO <sub>2</sub> )
CH <sub>2</sub> (OH)CH <sub>2</sub> CO(OONO <sub>2</sub> )	CH <sub>3</sub> C(CH <sub>2</sub> (ONO <sub>2</sub> ))=CHCH <sub>2</sub> (OOH)
CH <sub>3</sub> CH(ONO <sub>2</sub> )CH <sub>3</sub>	CH <sub>2</sub> (OH)COCH(OH)CH <sub>2</sub> (OOH)
CH <sub>3</sub> C(OOH)(CH <sub>2</sub> (OH))CH <sub>2</sub> CHO	CH <sub>3</sub> C(OOH)(CO(OH))CH(OH)CH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH=CH <sub>2</sub>	CH <sub>2</sub> (OH)CH(OH)C(ONO <sub>2</sub> )(CH <sub>3</sub> )CO(OONO <sub>2</sub> )
CH <sub>3</sub> C(ONO <sub>2</sub> )(CO(OH))CH(OH)CHO	CO(OOH)CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>
CH <sub>3</sub> C(OH)(CH <sub>2</sub> (ONO <sub>2</sub> ))COCHO	CH <sub>2</sub> (OOH)CH(OH)CHO
CH <sub>2</sub> (OH)CH(ONO <sub>2</sub> )C(OOH)(CH <sub>3</sub> )CO(OONO <sub>2</sub> )	CO(OONO <sub>2</sub> )CH=C(CH <sub>3</sub> )CHO
CH <sub>2</sub> (OH)CH(OH)C(CH <sub>2</sub> (OH))=CH <sub>2</sub>	CO(OOH)CH=CH <sub>2</sub>
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OH)CO(OH)	CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OOH)CO(OOH)
CH <sub>3</sub> C(OOH)(CH <sub>2</sub> (OH))CH=CH <sub>2</sub>	CH <sub>3</sub> C(CH <sub>2</sub> (OH))=CHCO(OH)
CO(OOH)CHO	CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(ONO <sub>2</sub> )CHO
CO(OH)CH=CH <sub>2</sub>	CH <sub>3</sub> C(CH <sub>2</sub> (OH))=CHCO(OONO <sub>2</sub> )
CH <sub>3</sub> C(ONO <sub>2</sub> )(CO(OOH))CH(OH)CHO	CH <sub>3</sub> COCH(ONO <sub>2</sub> )CO(OOH)
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OOH)CH <sub>2</sub> (OH)	CH <sub>2</sub> (OH)COC(OOH)(CH <sub>3</sub> )CHO
CH <sub>3</sub> CH(ONO <sub>2</sub> )CO(OOH)	CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OOH)CO(OONO <sub>2</sub> )
CH <sub>3</sub> CH <sub>3</sub>	CH <sub>3</sub> C(OH)(CHO)CH(OH)CHO
CH <sub>3</sub> COCOCH <sub>2</sub> (OOH)	CH <sub>2</sub> (OH)CH(ONO <sub>2</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub>
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(ONO <sub>2</sub> )CO(OONO <sub>2</sub> )	CH <sub>2</sub> (OH)CH <sub>2</sub> (OOH)
CO(OH)CH=C(CH <sub>3</sub> )CH <sub>2</sub> (ONO <sub>2</sub> )	CH <sub>3</sub> C(CH <sub>2</sub> (ONO <sub>2</sub> ))=CHCH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CHO	CH <sub>2</sub> (OH)CH(OOH)C(CH <sub>3</sub> )=CH <sub>2</sub>
CH <sub>2</sub> (OH)C(OH)(CH <sub>2</sub> (OH))CHO	CH <sub>2</sub> (ONO <sub>2</sub> )CH(OH)C(OOH)(CH <sub>3</sub> )CHO
CH <sub>3</sub> C(OOH)(CH <sub>2</sub> (OH))CH(OH)CHO	CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OH)CH <sub>2</sub> (OH)
CH <sub>3</sub> C(CH <sub>2</sub> (OOH))=CHCHO	CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CO(OH)
CH <sub>2</sub> (OH)CH=CH <sub>2</sub>	CH <sub>3</sub> COCH(ONO <sub>2</sub> )CO(OONO <sub>2</sub> )
CH <sub>2</sub> (OH)C(OOH)(CH <sub>2</sub> (OH))CHO	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>
CH <sub>2</sub> (OH)COC(OOH)(CH <sub>2</sub> (OH))CH <sub>2</sub> (OH)	CH <sub>2</sub> (OH)CH(OOH)C(OH)(CH <sub>3</sub> )CH <sub>2</sub> (ONO <sub>2</sub> )
CO(OONO <sub>2</sub> )CH(OH)CHO	CH <sub>2</sub> (ONO <sub>2</sub> )COC(ONO <sub>2</sub> )(CH <sub>3</sub> )CO(OONO <sub>2</sub> )
CH <sub>3</sub> C(ONO <sub>2</sub> )(CH <sub>2</sub> (OH))CH(OH)CHO	CH <sub>2</sub> (OH)CH=C(CH <sub>3</sub> )CH <sub>2</sub> (OOH)
CH <sub>2</sub> (OH)CH <sub>2</sub> CH <sub>2</sub> (OOH)	CH <sub>3</sub> C(OOH)(CH <sub>2</sub> (OOH))CH(OH)CO(OOH)
CH <sub>2</sub> (OH)CH(OOH)CHO	CH <sub>2</sub> =CHC(CH <sub>3</sub> )=CH <sub>2</sub>
CH <sub>2</sub> (OOH)CH=CH <sub>2</sub>	CH <sub>3</sub> C(OH)(CO(OH))CH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>2</sub> (ONO <sub>2</sub> )COCHO	CH <sub>2</sub> (OH)COCH(OH)CO(OONO <sub>2</sub> )
CH <sub>3</sub> C(OH)(CH <sub>2</sub> (ONO <sub>2</sub> ))CH(ONO <sub>2</sub> )CHO	CH <sub>2</sub> (OH)COC(CH <sub>3</sub> )=CH <sub>2</sub>
CH <sub>2</sub> (ONO <sub>2</sub> )CO(OOH)	CH <sub>3</sub> C(CO(OONO <sub>2</sub> ))=CHCHO
CH <sub>3</sub> CH=CH <sub>2</sub>	CH <sub>2</sub> (OH)CH(OOH)C(OOH)(CH <sub>3</sub> )CHO
CH <sub>3</sub> COCH <sub>2</sub> CH(OH)CH <sub>2</sub> (OH)	CH <sub>3</sub> C(OH)(CH <sub>2</sub> (OH))CHO
CH <sub>2</sub> (ONO <sub>2</sub> )CH(OH)C(OOH)(CH <sub>3</sub> )CO(OONO <sub>2</sub> )	CH <sub>3</sub> C(OH)(CO(OH))CH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>3</sub> CH(OH)CH <sub>2</sub> (ONO <sub>2</sub> )	CH <sub>2</sub> (OH)CH(OH)CO(OONO <sub>2</sub> )
CH <sub>3</sub> CH(OOH)CH <sub>2</sub> (ONO <sub>2</sub> )	CH <sub>3</sub> COCH <sub>2</sub> CH=CH <sub>2</sub>
CH <sub>2</sub> (OH)CH(OH)C(ONO <sub>2</sub> )(CH <sub>3</sub> )CHO	CH <sub>2</sub> (ONO <sub>2</sub> )CH(OH)CHO
CH <sub>3</sub> C(CH <sub>2</sub> (OH))=CHCHO	CH <sub>3</sub> COCOCH <sub>2</sub> (ONO <sub>2</sub> )
CH <sub>3</sub> COCH <sub>2</sub> CH(ONO <sub>2</sub> )CH <sub>2</sub> (OH)	CH <sub>3</sub> C(ONO <sub>2</sub> )(CHO)CHO
CH <sub>3</sub> C(OH)(CH <sub>2</sub> (OH))CH=CH <sub>2</sub>	CH <sub>3</sub> C(OH)(CH <sub>2</sub> (ONO <sub>2</sub> ))CHO
CH <sub>3</sub> C(ONO <sub>2</sub> )(CO(OH))CHO	CH <sub>3</sub> C(ONO <sub>2</sub> )(CO(OH))CH(OH)CH <sub>2</sub> (ONO <sub>2</sub> )

CH3C(CH2(ONO2))=CHCO(OOH)	CH3C(CO(OH))=CHCHO
CH3CH(ONO2)CO(OONO2)	CO(OOH)CH(OH)CHO
CH3C(OH)(CH2(OH))CH(OH)CH2(ONO2)	CH2(ONO2)CH(OH)C(OOH)(CH3)CO(OOH)
CH3COCO(OOH)	CH3COCH2COCH2(OH)
CH2(OH)COC(OH)(CH3)CH2(ONO2)	CH3C(CO(OOH))=CH2
CH3C(ONO2)(CH2(OH))CO(OOH)	CH2(ONO2)CO(OONO2)
CH2(ONO2)CH(OH)C(ONO2)(CH3)CHO	CH2(OH)COCH(OOH)CH2(OH)
CO(OOH)CH(OH)C(CH3)=CH2	CH3C(OOH)(CH2(ONO2))CH(OH)CHO
CH3CO(OONO2)	CH3COCH(OH)CO(OONO2)
CH3C(OH)(CH3)CO(OOH)	CH3C(ONO2)(CH2(OH))CH(OOH)CO(OH)
CH2(OH)CH(OH)CH2(OOH)	CH3CH(ONO2)CHO
CO(OOH)CH(OH)C(ONO2)(CH3)CHO	CH3C(OOH)(CH2(OH))CHO
CH2(ONO2)CH2(OOH)	CH2(OOH)CHO
CH2(OH)CH(OOH)C(CH2(OH))=CH2	CH2(OH)C(CO(OONO2))=CH2
CH3C(OH)(CHO)CHO	CH3C(ONO2)(CH2(OH))CH(OH)CO(OONO2)
CH3COCH2COCHO	CH3C(OOH)(CH2(OOH))CH(OH)CHO
CH3C(CO(OOH))=CHCHO	CH2(OH)CH(ONO2)C(OH)(CH3)CH2(ONO2)
CH3C(ONO2)(CO(OOH))CHO	CH3C(OH)(CH2(OOH))CHO
CO(OONO2)CH=CH2	CH2(OOH)CH=C(CH3)CHO
CH2(OOH)CH(OH)C(CH3)=CH2	CH3COCH2CH(OOH)CH2(OH)
CH3C(ONO2)(CO(OH))COCH2(ONO2)	CH3C(ONO2)(CH2(OH))CO(OONO2)
CH3C(OH)(CO(OOH))CHO	CH3CH(ONO2)CH2(OH)
CH2(OH)CH(ONO2)C(ONO2)(CH3)CO(OH)	CH2(OH)COCH(ONO2)CH2(OH)
CH3C(ONO2)(CH2(OH))CH(ONO2)CH2(OH)	CH3C(OH)(CO(OONO2))CHO
CH2(OH)CH2CO(OOH)	CH3C(OOH)(CH2(OH))CH(ONO2)CH2(OH)
CH2(OH)CH(OH)C(CH3)=CH2	CH3CH2CO(OOH)
CH2(OH)COC(CH2(OH))=CH2	CH2(ONO2)COC(ONO2)(CH3)CHO
CH3C(ONO2)(CH2(OH))CH(OH)CO(OOH)	CH3C(OOH)(CH2(OH))CH(OH)CH2(ONO2)
CH2(OH)CH(ONO2)C(ONO2)(CH3)CO(OOH)	CH2(OH)CH=C(CH3)CO(OONO2)
CH2(OH)C(CO(OH))=CH2	CH2(OH)CH(ONO2)C(OH)(CH3)CO(OOH)
CH3C(OH)(CH3)CO(OONO2)	CH3COCH2CHO
CO(OONO2)CH(OH)C(ONO2)(CH3)CHO	CH3C(OH)(CH2(ONO2))CH(OH)CHO
CH2(OH)CH(ONO2)C(ONO2)(CH3)CO(OONOO2)	CH3C(CHO)=CH(OH)
CH3C(OH)(CH2(ONO2))CH(ONO2)CO(OONO2)	CH3CH(ONO2)CO(OH)
CH3COCH2(OOH)	CH2(OH)CH2CH2(OH)
CH3C(OOH)(CH2(OH))COCH2(OH)	CH3COCH2CO(OONO2)
CO(OH)CH(OH)C(ONO2)(CH3)CHO	CH3C(CH2(OH))=CHCH2(OOH)
CH2(OH)COCH(OH)CO(OOH)	CH2(ONO2)COC(ONO2)(CH3)CO(OOH)
CO(OOH)CH(OH)C(OOH)(CH3)CHO	CH3C(ONO2)(CH2(OH))CH(OH)CH2(ONO2)
CH3C(OOH)(CHO)CHO	CH3C(ONO2)(CH2(OH))COCHO
CH3C(ONO2)(CH2(OH))CH(ONO2)CO(OH)	CO(OH)CH2(ONO2)
CH3COCH2CO(OH)	CH2(OH)CO(OONO2)
CH3C(OH)(CH2(OH))CH(ONO2)CH2(OH)	CH3C(ONO2)(CH2(OH))COCH2(ONO2)
CH2(OH)CH(ONO2)C(OH)(CH3)CHO	CH2(OH)CH(ONO2)C(OH)(CH3)CO(OONO2)
CH3COCH(OH)CH2(ONO2)	CH3C(OH)(CO(OOH))CHO
CH2(OH)CH(OH)C(OH)(CH3)CHO	CH3C(OOH)(CH2(OH))CH(OOH)CHO
CH3C(OH)(CH3)CHO	CH3CH(OOH)CH3
CH3C(ONO2)(CH2(OH))CH(ONO2)CO(OOH)	CH3C(OH)(CH2(OH))CH(OH)CHO
CH2(OH)C(CO(OOH))=CH2	CH3COCH=CH(OH)
CO(OOH)CH=C(CH3)CHO	CH3COCH(ONO2)CH2(OH)
CH3COCH(OOH)CH2(OH)	CH3C(OH)(CO(OH))CH(OH)CH2(ONO2)
	CH2(OH)CH(ONO2)C(ONO2)(CH3)CHO

CH2(OH)CH(OH)C(ONO2)(CH3)CO(OH)	CH2(OH)CH(OH)C(ONO2)(CH3)CO(OOH)
CH2(OH)CH(OH)C(OH)(CH3)CH2(ONO2)	CH2(OH)CH=C(CH3)CH2(ONO2)
CH3C(CH2(OH))=CHCH2(OH)	CH3C(CH2(OH))=CHCH2(ONO2)
CH2(OH)C(OH)(CH2(OH))CH(OOH)CHO	CH3C(CH2(ONO2))=CHCHO
CHOCH(OH)C(CH3)=CH2	CH2(OOH)COCH=CH2
CH2(OH)CH(OH)C(OOH)(CH3)CHO	CH2(OH)CH=C(CH3)CHO
CH3C(CH2(ONO2))=CHCO(OONO2)	CH2(OH)CH(ONO2)C(OOH)(CH3)CO(OOH)
CH2(OH)CH(OH)C(OOH)(CH2(OH))CHO	CH2(OH)CH(ONO2)C(ONO2)(CH2(OH))CH2(OH)
CH2(OH)CH(ONO2)C(OH)(CH2(OH))CHO	CH3C(ONO2)(CO(OONO2))CH(OH)CHO
CH2=CH2	CH2(OH)COCH(OH)CH2(ONO2)
CH2(ONO2)CHO	CH3C(ONO2)(CHO)CH(OH)CHO
CH2(ONO2)CH(OH)C(OH)(CH3)CO(OONO2)	CH3C(ONO2)(CH2(OH))CH(OH)CH2(OOH)
CH3COCH(OH)CO(OOH)	CH3C(CO(OONO2))=CH2
CH2(OH)CH(OOH)C(OH)(CH3)CHO	CH2(OH)CH(OH)CO(OOH)
CH2(ONO2)CH(OH)C(OH)(CH3)CO(OOH)	CH3CH2CH2(OOH)
CH2(OH)CH(ONO2)C(OOH)(CH2(OH))CHO	CH3CH2CH2(ONO2)
CH3C(OOH)(CH2(OOH))CH(OOH)CHO	CH3C(ONO2)(CH2(OH))CH(OOH)CHO
CH3C(CHO)=CHCHO	CH3COCH2CO(OOH)
CH2(OH)CH=C(CH3)CO(OH)	CO(OH)CH(ONO2)C(OH)(CH3)CH2(ONO2)
CH3CH(OH)CO(OOH)	CH3C(ONO2)(CH2(OH))COCH2(OH)
CH3C(OH)(CH2(OH))CH(OOH)CHO	CHOCOCH=CH2
CH2(OH)CH(ONO2)C(OOH)(CH2(OH))CH2(OH)	CHOCH2C(CH3)=CH2
CH2(OH)CH(ONO2)C(CH2(OH))=CH2	CH3C(OH)(CH2(ONO2))CH(ONO2)CO(OOH)
CH3CH(OH)CH2(OOH)	CH3CH(ONO2)CH2(OOH)
CH3COCH(ONO2)CHO	CH3COCH(OOH)CHO
CH3CH2CO(OONO2)	CH3C(OH)(CH2(ONO2))CO(OONO2)
CH2(OH)CH2CH2(ONO2)	CH2(OH)CH=C(CH3)CO(OOH)
CH2(ONO2)CH(OH)C(OH)(CH3)CHO	CH2(OH)CH(ONO2)COCHO
CH3C(OH)(CH3)CO(OH)	CH3C(OOH)(CHO)CH(OH)CHO
CH2(OH)CH(ONO2)C(OH)(CH2(OH))CH2(OH)	CH2(ONO2)CH(OH)C(ONO2)(CH3)CO(OONO2)
CH2(OH)CH(ONO2)C(OOH)(CH3)CHO	CH3C(ONO2)(CO(OONO2))CHO
CH3C(CH2(OOH))=CH2	CH2(OOH)CH(OOH)C(OOH)(CH3)CHO
CH3C(OOH)(CO(OOH))CH(OH)CHO	

---

## SM7: Time evolution of the sum of organic acids in the gas and the aqueous phase during the cloud event

---

