

# AEROCLO-sA PEGASUS PTR-MS volatile organic compounds

## General information

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Dataset name: AEROCLO-sA PEGASUS PTR-MS volatile organic compounds  
Dataset DOI: 10.6096/AEROCLO.1773  
Created on: 2018-07-20

## Contact(s)

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## Period

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Date begin (yyyy-mm-jj): 2017-08-21  
Date end (yyyy-mm-jj): 2017-09-12

## Project(s)

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AEROCLO

## Data description

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### Abstract

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The concentration of volatile organic compounds was measured by a proton transfer reaction time-of-flight mass spectrometer (PTR-ToF-MS) Kore Inc? (second generation) operated in the PEGASUS mobile lab. Air was taken into the instrument through a 1.5 m long Silcosteel® coated stainless steel tube (2.1 mm inner diameter), at a constant flow rate of about 3 cm<sup>3</sup>/s . Instrumental settings were: glow discharge region P=2.00 mbar, proton transfer reaction tube P=1.69 mbar, T=60 °C and E=390 V, leading to an E/N of 112 Td (1 Td=10<sup>21</sup> V cm<sup>2</sup>).

List of gas standard mixtures used for calibration:

- (i) built-in GCU gas standard containing formaldehyde, methanol, acetonitrile, acetaldehyde, ethanol, acrolein, acetone, isoprene, crotonaldehyde, 2-butanone, benzene, toluene, o-xylene, chlorobenzene,  $\alpha$ -pinene, 1,2-dichlorobenzene, and 1,2,4-trichlorobenzene at a nominal concentration of 1 ppm;
- (ii) NPL primary reference gas mixture containing ethane, ethene, propane, propene, 2-methylpropane, butane, ethyne, trans-but-2-ene, but-1-ene, cis-but-2-ene, 2-methylbutane, pentane, 1,3-butadiene, trans-pent-2-ene, pent-1-ene, 2-methylpentane, hexane, isoprene, heptane, benzene, 2,2,4-trimethylpentane, octane, toluene, ethylbenzene, m-xylene, p-xylene, o-xylene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, and 1,2,3-trimethylbenzene at a nominal concentration of 4 ppb;
- (iii) standard mixture made in-house containing dimethyl sulphide (DMS, 1.39 ppm), dimethyl sulfoxide (DMSO, 1.34 ppm), diethyl sulphide (DES, 2.03 ppm), dimethyl disulphide (DMDS, 1.7 ppm) and dimethyl sulphate (DMSO<sub>4</sub>, 1.79 ppm).

## Observing strategy

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Data acquisition was done with 5-min resolution and blank spectra were recorded three-times per day using zero-air. Calibration of instrumental signals was performed every three days using three different gas standard mixtures containing hydrocarbons, oxygenated hydrocarbons and sulphurated hydrocarbons in the concentration range between 0.3 ppb and 1 ppm at 70% RH and 25 °C.

## References

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References for quantification formulas and k used are:

Bohme, D.K., Mackay, G.I., Tanner, S.D., 1979. An experimental study of the gas-phase kinetics of reactions with hydrated hydronium(1+) ions(n = 1-3) at 298 K. *J. Am. Chem. Soc.* 101, 3724-3730. <https://doi.org/10.1021/ja00508a003>

Ellis, A.M., Mayhew, C.A., 2014. *Proton Transfer Reaction Mass Spectrometry: Principles and Applications*. John Wiley & Sons, Ltd., Chichester, England.

Zhao, J., Zhang, R., 2004. Proton transfer reaction rate constants between hydronium ion (H<sub>3</sub>O<sup>+</sup>) and volatile organic compounds. *Atmos. Environ.* 38, 2177-2185. <https://doi.org/10.1016/j.atmosenv.2004.01.019>

## Instrument information

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### Sensor

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Instrument type:	Samplers
Manufacturer:	Kore

### Sensor resolution

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Observation frequency:	5 minutes
Horizontal coverage:	Point measurement

### Sensor location

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Longitude (°):	-22.1
Latitude (°):	14.5
Height above ground (m):	2

## Geographic information

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### Henties Bay

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Location name:	Henties Bay
Platform type:	GROUND STATIONS

## Measured parameter

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### Non-methane Hydrocarbons/Volatile Organic Compounds

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Parameter keyword: Atmosphere > Atmospheric Chemistry > Carbon and Hydrocarbon Compounds > Non-methane Hydrocarbons/Volatile Organic Compounds

Unit: part per billion - ppb

Acquisition methodology and quality: The concentration of volatile organic compounds was measured by a proton transfer reaction time-of-flight mass spectrometer (PTR-ToF-MS) Kore Inc? (second generation) operated in the PEGASUS mobile lab. Air was taken into the instrument through a 1.5 m long Teflon tubing to a 6-port manifold common for all gaz phase measurements. From the manifold, a Silcosteel® coated stainless steel tube (2.1 mm inner diameter) was connected to the instrument and brought air at a constant flow rate of about 3 cm<sup>3</sup>/s . Instrumental settings were: glow discharge region P=2.00 mbar, proton transfer reaction tube P=1.69 mbar, T=60 °C and E=390 V, leading to an E/N of 112 Td (1 Td=10<sup>17</sup> V cm<sup>2</sup>). Data acquisition was done with 5-min resolution and blank spectra were recorded three-times per day using zero-air. Calibration of instrumental signals was performed every three days using three different gas standard mixtures containing hydrocarbons, oxygenated hydrocarbons and sulphurated hydrocarbons in the concentration range between 0.3 ppb and 1 ppm at 70% RH and 25 °C.

List of gas standard mixtures used for calibration:

(i) built-in GCU gas standard containing formaldehyde, methanol, acetonitrile, acetaldehyde, ethanol, acrolein, acetone, isoprene, crotonaldehyde, 2-butanone, benzene, toluene, o-xylene, chlorobenzene,  $\alpha$ -pinene, 1,2-dichlorobenzene, and 1,2,4-trichlorobenzene at a nominal concentration of 1 ppm;

(ii) NPL primary reference gas mixture containing ethane, ethene, propane, propene, 2-methylpropane, butane, ethyne, trans-but-2-ene, but-1-ene, cis-but-2-ene, 2-methylbutane, pentane, 1,3-butadiene, trans-pent-2-ene, pent-1-ene, 2-methylpentane, hexane, isoprene, heptane, benzene, 2,2,4-trimethylpentane, octane, toluene, ethylbenzene, m-xylene, p-xylene, o-xylene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, and 1,2,3-trimethylbenzene at a nominal concentration of 4 ppb;

(iii) standard mixture made in-house containing dimethyl sulphide (DMS, 1.39 ppm), dimethyl sulfoxide (DMSO, 1.34 ppm), diethyl sulphide (DES, 2.03 ppm), dimethyl disulphide (DMDS, 1.7 ppm) and dimethyl sulphate (DMSO<sub>4</sub>, 1.79 ppm).

Sensor precision: see excel file

Date begin (yyyy-mm-jj): 2017-08-21

Date end (yyyy-mm-jj): 2017-09-12

## Derived parameter

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### Atmosphere

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Parameter keyword:	Atmosphere
Unit:	cm-3

## Data use information

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Use constraints: The Principal Investigator(s) of the PTR-MS data for the AEROCLO-sA campaign are Chiara Giorio ([chiara.giorio@atm.ch.cam.ac.uk](mailto:chiara.giorio@atm.ch.cam.ac.uk)) and Jean-François Doussin ([jean-francois.doussin@lisa.ipsl.fr](mailto:jean-francois.doussin@lisa.ipsl.fr)). Please contact the PIs whenever using the data for publications or presentations.

Data were acquired with the support of Mathieu Cazaunau (LISA) and of the Technical Department of the LISA. The LISA ([www.lisa.u-pec.fr](http://www.lisa.u-pec.fr)) is a joint research unit of the CNRS, University Paris-Est Créteil and University of Paris).

Data policy: AEROCLO data policy

Database: AEROCLO-sA on BAOBAB

Original data format(s): Excel