TNA User Report

The completed and signed form below should be returned by email to
eurochamp2020@lisa.u-pec.fr

Project title	EUROCHAMP PTR-MS Intercomparison Campaign
Name of the accessed chamber	HELIOS
Number of users in the project	5
Project objectives (max 100 words)	The project objective was to participate in the PTR-MS intercomparison campaign that was carried out at the HELIOS simulation chamber in Orléans (France) in the period from May 6 to May 24, 2019. The main scientific goal of the comparison exercise was to ensure comparability of results generated by different PTR-MS instruments and by different instrument operators. The objective of the joint University of Oslo/Ionicon Analytik team was to test a new high-resolution PTR-ToF-MS instrument that is soon to be launched on the market. The University of Utrecht team wanted to further explore the use of its newly developed PTR-MS calibration device.
Description of work (max 100 words):	The two instrument teams installed and de-installed two PTR-MS analyzers and a calibration unit for common use. Alexander Håland, PhD student at the University of Oslo, operated and overlooked all three devices during the whole campaign. He participated in the on-site team discussions, was responsible for common calibrations and delivered preliminary data.

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[1] Physics; Chemistry; Earth Sciences & Environment; Engineering & Technology; Mathematics; Information & Communication Technologies; Material Sciences; Energy; Social sciences; Humanities.
[2] UNI= University and Other Higher Education Organisation;
RES= Public Research Organisation (including international research organisations and private research organisations controlled by public authority);
SME= Small and Medium Enterprise;
PRV= Other Industrial and/or Profit Private Organisation;
OTH= Other type of organization.
[3] UND= Undergraduate; PGR= Post graduate; PDOC= Post-doctoral researcher; RES= Researcher ENG= Engineer; ACA= Academic; TEC= Technician.

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Trans-National Access (TNA) Scientific Report

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Name of the PI: Armin Wisthaler
Chamber name and location: HELIOS, Orléans (France)
Campaign name and period: EUROCHAMP PTR-MS Intercomparison Campaign, May 6-24, 2019

Introduction and motivation

Proton-Transfer-Reaction Mass Spectrometry (PTR-MS; *Hansel et al., 1995*; *Yuan et al., 2017*) is nowadays widely used by the atmospheric community for measuring organic trace gases, both in ambient air and in atmosphere simulation chambers. Despite its analytical maturity, PTR-MS remains a challenging technique where the experience of the user is central for obtaining high-quality results. Transfer of knowledge and best practices (*e.g.,* optimization of instrument parameters, inlet lines, and data analysis procedures) are essential for generating reliable and traceable results. A measurement comparison campaign is thus a very useful event for training young and/or unexperienced PTR-MS users.

Scientific objectives

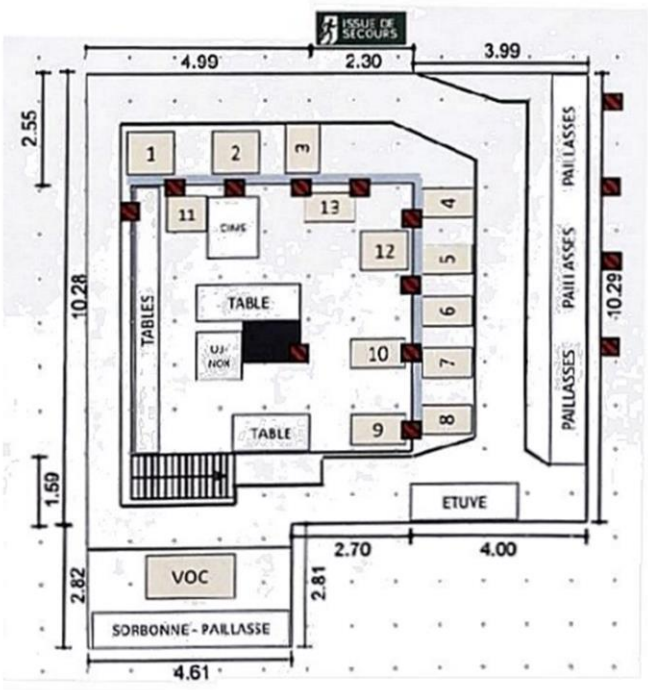
In the frame of EUROCHAMP 2020, a PTR-MS intercomparison campaign was performed during a three week period at HELIOS simulation chamber in Orléans, France (http://helios-cnrs.org/). The objectives of the measurement campaign were to determine advantages and drawbacks of different PTR-MS instrument types and operation practices, to characterize reliability and uncertainties, and to develop recommendations for best practices. The objective of the joint University of Oslo/Ionicon Analytik team was to test a new high-resolution PTR-ToF-MS instrument that is soon to be launched on the market. The University of Utrecht team wanted to further explore the use of its newly developed PTR-MS calibration device. The group from the University of York which was originally included in the TNA proposal did not participate in the campaign for logistical reasons.

Reason for choosing the simulation chamber/ calibration facility

The HELIOS facility is one of the few large chamber facilities that can accommodate a large number of PTR-MS instruments in their laboratory (staffing, logistics, space, power, cooling, etc.).

• Method and experimental set-up

13 PTR-MS instruments participated in the measurement intercomparison exercise. A list of the deployed instruments (including model type) and their location in the HELIOS laboratory is shown in Figure 1. The joint University of Oslo/Ionicon Analytik team deployed a prototype of a new instrument including a high mass resolution time-of-flight mass spectrometer (here named PTR-nG, nG standing for next generation). The Utrecht University team deployed a PTR-TOF 1000 analyzer although the main scope was to test and provide a newly developed PTR-MS calibration device. Figure 2 is a photograph of the experimental set-up in the laboratory. Figure 3 shows the glass manifold to which the instrument sampling lines were connected.



#	Groupe	Instrument
1	EPOC	Kore v2
2	LISA	Kore v2
3	UEF	PTR-ToF-8000
4	INRA	PTR-Qi-ToF
5	LSCE	PTR-ToF-1000
6	CEAM	PTR-MS SRI
7	UEA	PTR-QMS
8	IMT	PTR-Qi-ToF
9	ICARE	PTR-ToF-8000
10	TROPOS	PTR-ToF-8000
11	Wuppertal	PTR-ToF-1000
12	UiO/Ionicon	PTR-nG
13	UTRECHT	PTR-ToF-1000

Figure 1: List of PTR-MS instruments and their location in the HELIOS laboratory

Figure 2: Alexander Håland (University of Oslo) with an orchestra of PTR-MS instruments

Figure 3: The glass sampling manifold skeptically inspected by Dr. Markus Müller (Ionicon Analytik)

• Data description

The following experiments were carried out at the HELIOS facility:

1. Hydrocarbon calibration under different RH (0-80%)
2. OVOC calibration under different RH (0-80%)
3. Hydrocarbon ozonolysis under high RH (50%) and photolysis
4. Hydrocarbon ozonolysis under dry conditions and photolysis
5. OVOC ozonolysis under different RH (0-60%)
6. OVOC ozonolysis under dry conditions
7. Calibration of all instruments through manifold
8. isoprene + OH
9. α-pinene + ozone

The PTR-ng instrument was fully operational during all experiments. The data to be delivered will consist of time series of volume mixing ratios of selected organic traces gases, still to be defined by the campaign organizers.

• Preliminary results and conclusions

Preliminary data processed during the campaign showed very large discrepancies between the different instruments. Given the very preliminary character of the data, no conclusions should be

drawn apart from the fact that it was indeed important to carry out this intercomparison exercise. The data are currently being analyzed and quality-controlled by the individual groups. The deadline for data submission is July 31, 2019, after which the first conclusions can be drawn.

• **Outcome and future studies**

Both the instrument prototype produced by Ionicon and the calibration unit provided by the University of Utrecht were fully operational during the entire campaign. The work funded through the TNA was thus successfully carried out. After delivery of the quality-assured data, it will be the responsibility of the campaign organizers to summarize the results and to produce a manuscript for publication.

• **References**

Hansel, A.; Jordan, A.; Holzinger, R.; Prazeller, P.; Vogel, W.; Lindinger, W. Proton Transfer Reaction Mass Spectrometry: On-Line Trace Gas Analysis at the Ppb Level. International Journal of Mass Spectrometry and Ion Processes 1995, 149–150, 609–619. https://doi.org/10.1016/0168-1176(95)04294-U.

Yuan, B.; Koss, A. R.; Warneke, C.; Coggon, M.; Sekimoto, K.; de Gouw, J. A. Proton-Transfer-Reaction Mass Spec-trometry: Applications in Atmospheric Sciences. Chem. Rev. 2017, 117 (21), 13187–13229. https://doi.org/10.1021/acs.chemrev.7b00325