



# ACTRIS

## CiGas

*NO<sub>x</sub>/VOC QA workshop 2023*

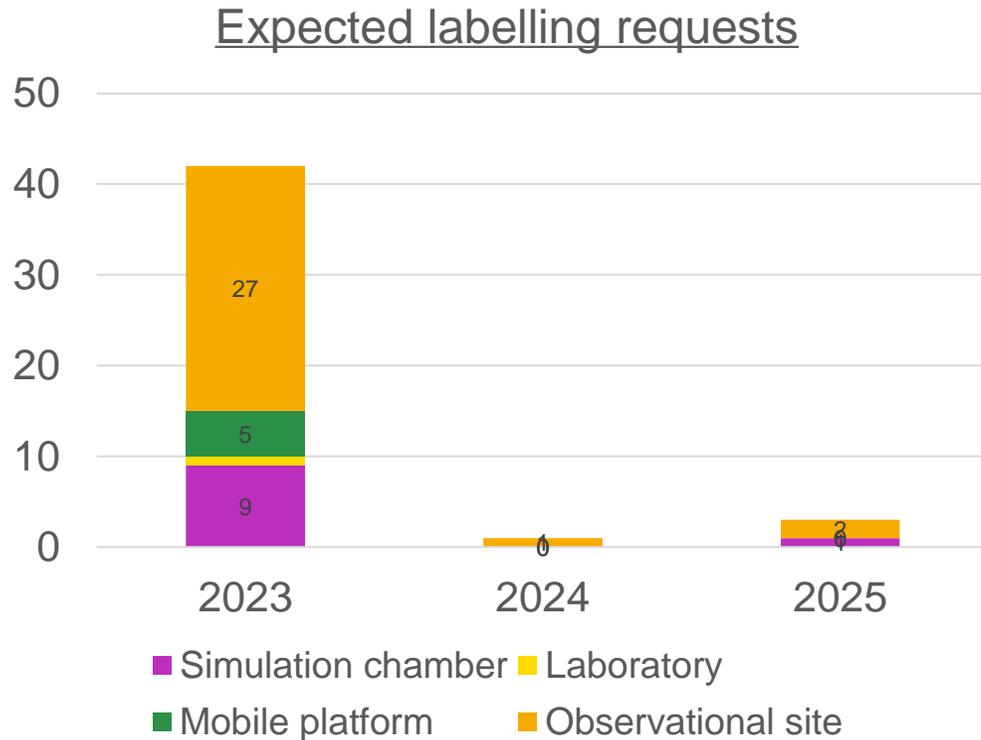


*NO<sub>x</sub>/VOC QA workshop 2023; Online – April, 17<sup>th</sup> - 19<sup>th</sup> 2023*



This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreements No 654109 and 739530

# Labelling (CiGas)



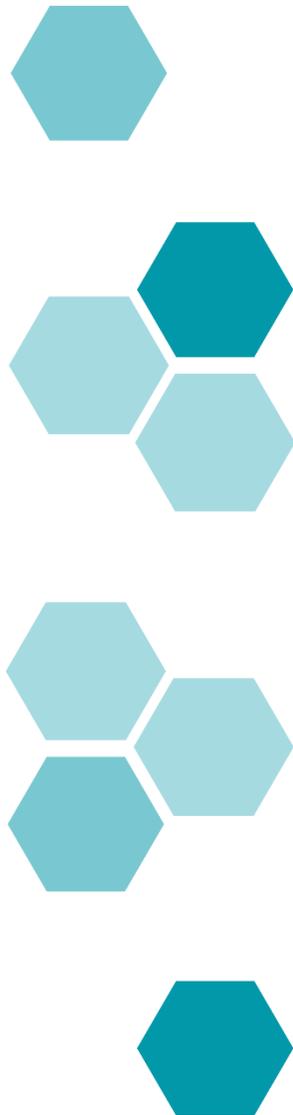
## Pilot sites:

SMEAR II, Pallas, Kosetice, Jungfraujoch, Zeppelin

→ Aim: Labelling step 1a approval by the RI Committee: End of May/ early June 2023

## Remaining observational platforms:

→ Start labelling step 1a: July 2023



# Labelling Workflow

## Responsible partners

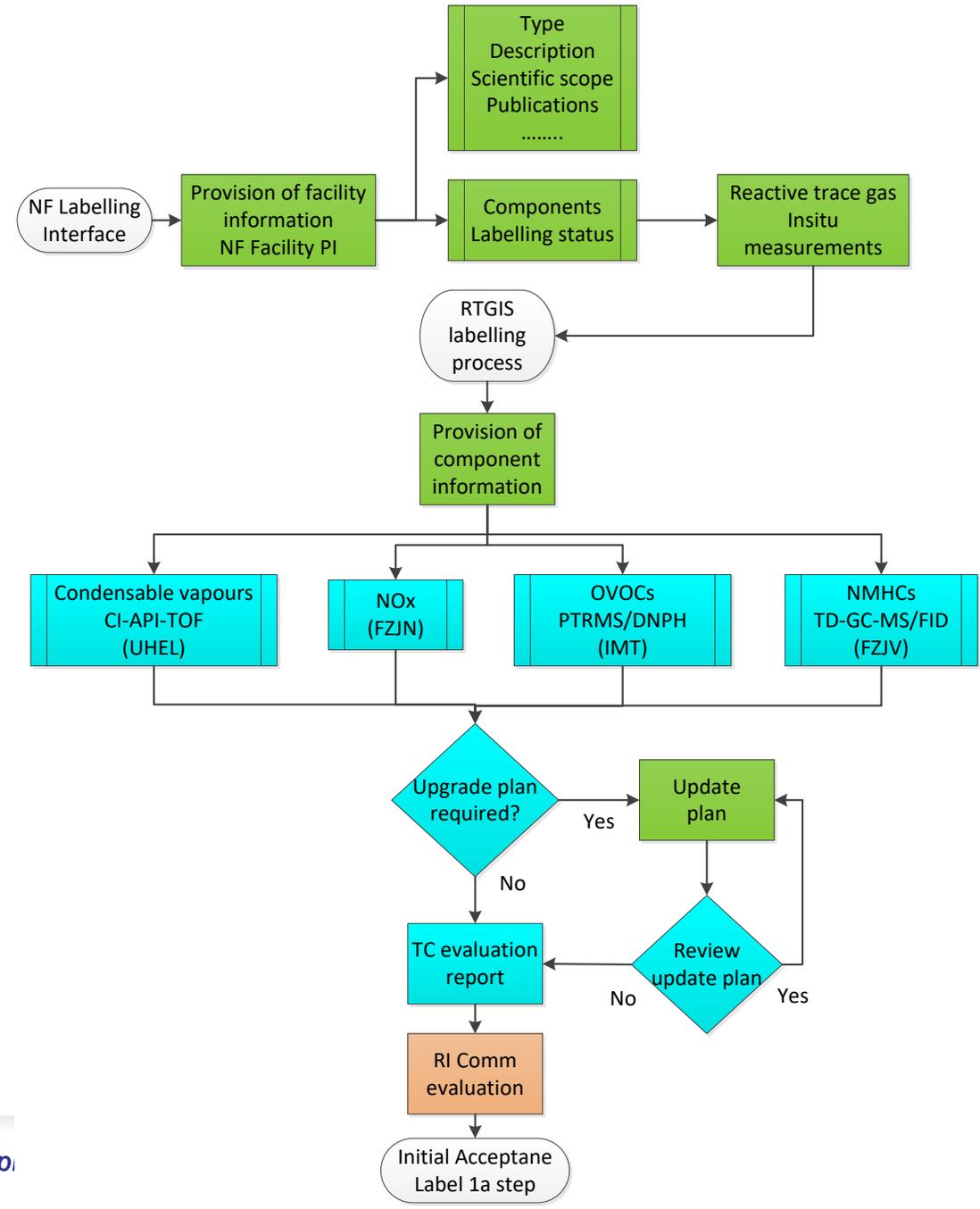
NF

TC

RI Comm



## NF Labelling process: Step 1a



# Start labelling process

## SMEAR II (Hyytiälä)

[View details](#)

**Type**  
Observational platform

**Country**  
Finland

**Hosting institute**  
University of Helsinki (UH)

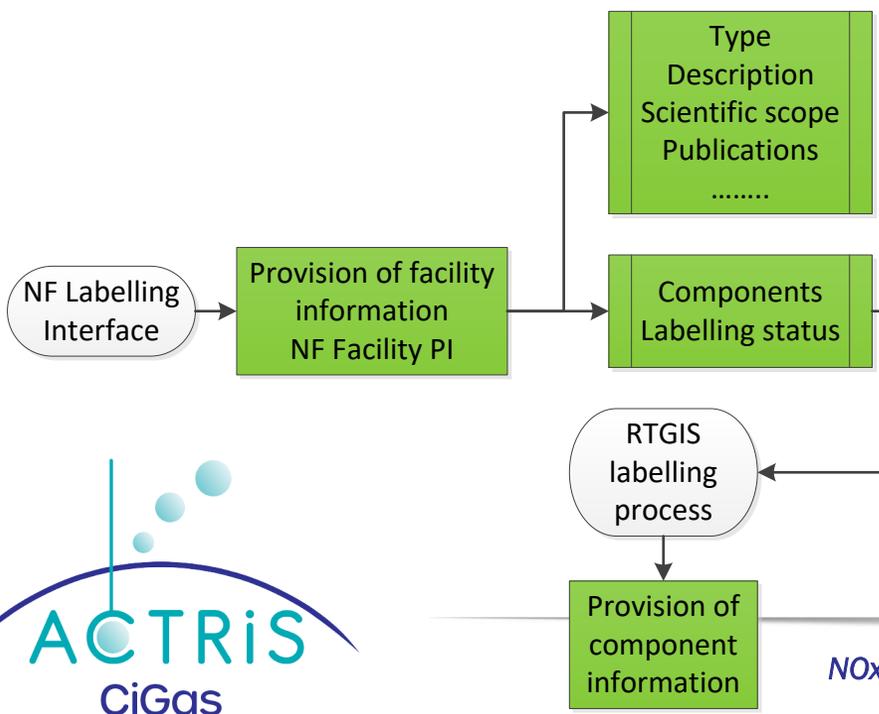
**Website**  
<https://www.atm.helsinki.fi/SMEAR/index.php/smea-ii>

**Contacts**  
Tuukka Petäjä  
Facility PI

**Description**  
The SMEAR II (Station for Measuring Ecosystem-Atmosphere Relations) is a ground-based fixed, observational platform and background site. SMEAR II started its operation in 1995, with an extensive range of measurements. The station is situated in a 60-year-old (in 2022) rather homogenous Scots pine forest in Hyytiälä. The station represents a boreal coniferous forest that covers 8% of the Earth's surface and stores about 10% of the total carbon in the terrestrial ecosystem.



Main site: 61.850°N 24.283°E 181 m a.s.l.  
Tower: 61.850°N 24.283°E 216 m a.s.l.



# ACTRIS Labelling step 1a for 'Reactive trace gases in situ measurements'

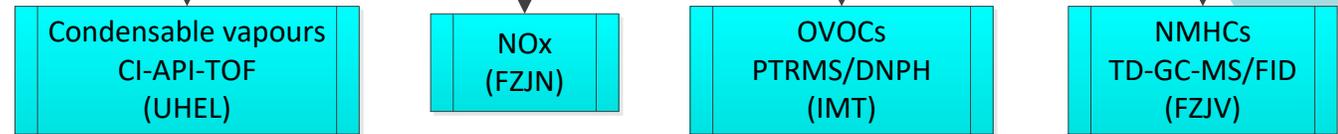


NF PIs receive an Email from CiGas with request for instrument information provision



- NFs fill in questionnaire with detailed instrument information
- Provide upgrade plan (if applicable)
- Provide copies of calibration standard certificates

Provision of component information



NATIONAL PHYSICAL LABORATORY  
Teddington Middlesex UK TW11 0LW Telephone +44 20 8977 3222

Certificate of Calibration

NPL PRIMARY REFERENCE MATERIAL

Cylinder Number: D93529

This certificate is issued in accordance with the laboratory accreditation requirements of the United Kingdom Accreditation Service. It provides traceability of measurement to the SI system of units and/or to units of measurement realized at the National Physical Laboratory or other recognized national metrology institutes. This certificate may not be reproduced other than in full, except with the prior written approval of the issuing laboratory.

CUSTOMER: Forschungszentrum Jülich GmbH  
ADDRESS: Institut IEK-8, Troppstraße, Wilhelm-Johnen-Strasse, 52425 Jülich, Germany

CALIBRATION DATE: 08 December 2020

AMOUNT FRACTIONS:

Component	Amount fraction (molefraction)	Component	Amount fraction (nmol/mol)
Ethane	4.24 ± 0.13	2-methylpentane	4.39 ± 0.09
Ethene	4.15 ± 0.09	n-butane	4.39 ± 0.09
Propane	4.18 ± 0.09	Isoprene	4.37 ± 0.09
Propene	4.15 ± 0.09	n-Butene	4.40 ± 0.09
2-methylpropane	4.26 ± 0.11	Benzene	3.72 ± 0.08
n-butane	4.22 ± 0.09	2,2,4-trimethylpentane	4.13 ± 0.09
Ethylacetylene	4.37 ± 0.22	n-octane	4.14 ± 0.09
trans-but-2-ene	4.23 ± 0.09	Toluene	3.41 ± 0.10
But-1-ene	4.21 ± 0.09	Ethylbenzene	3.91 ± 0.10
cis-but-2-ene	4.22 ± 0.09	m-xylene + p-xylene	7.60 ± 0.20
2-methylbutane	4.16 ± 0.09	n-xylene	3.74 ± 0.10
n-pentane	4.18 ± 0.09	1,3,5-trimethylbenzene	3.80 ± 0.10
1,3-butadiene	4.27 ± 0.09	1,4-dimethylbenzene	3.83 ± 0.10
trans-pent-2-ene	4.20 ± 0.09	1,2,3-trimethylbenzene	3.80 ± 0.10
Pent-1-ene	4.27 ± 0.09	Nitrogen	Balance

The reported expanded uncertainties are based on standard uncertainties multiplied by a coverage factor  $k=2$ , providing a coverage probability of approximately 95%. The uncertainty evaluation has been carried out in accordance with UKAS requirements.

METHODS: Preparation: gravimetry; Analysis: gas chromatography (FID)

TRACEABILITY: The values on this certificate are traceable to NPL Primary Standards

EXPIRY: Certificate valid for 5 years from the date of issue

PRESSURE: Fill pressure: 100 bar, Minimum utilisation pressure: 10 bar

STORAGE: No special precautions are required

HANDLING: Refer to ISO 10664

OUTLET: DIN 477 No. 1 valve

INTENDED USE: Calibration standard

Reference: 2021030009-1 Date of issue: 22 March 2021

Signed: *[Signature]* (Authorised Signatory)

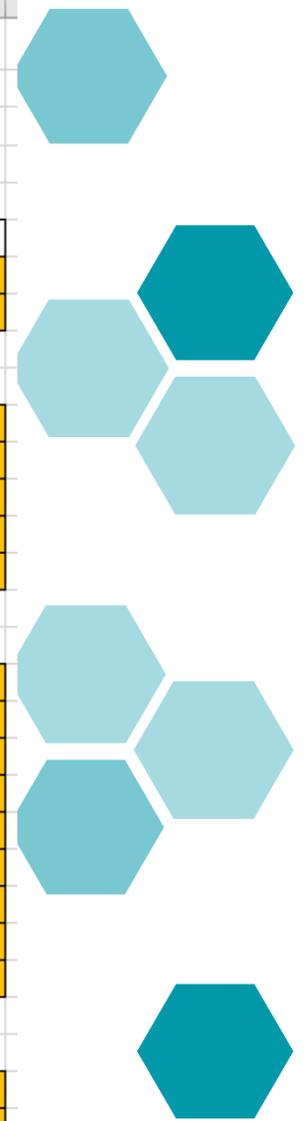
Name: Dr D R Worton (on behalf of NPLML)

Checked by: *[Signature]* Page 1 of 1

# Instrument Questionnaire



	A	B	C
1	<b>NOx</b>		
2			
3	<b>CiGas PI for NOx:</b>	<b>Robert Wegener</b>	<a href="mailto:r.wegener@fz-juelich.de">r.wegener@fz-juelich.de</a>
4			
5	<b>Component group specific contact:</b>		
6	<b>Firstname(s), Lastname(s)</b>	<b>Expertise level</b>	<b>Contact (Email address)</b>
7	Please fill out	Please select...	Please fill out
8	Please fill out	Please select...	Please fill out
9			
10	<b>Instruments for NO and NO<sub>2</sub> respectively:</b>		
11	Status:	Please select...	
12	Date of full operation:	Please specify [ month & year ]	
13	Instrument type:	Please select...	
14	Instrument manufacturer:	Please select...	
15	Instrument model:	Please select...	
16			
17	<b>Inlet:</b>		
18	Measurement height above ground level:	Please specify [ m ]	
19	Distance from VOC inlet:	Please specify [ m ]	
20	Distance from condensables inlet (if applicable):	Please specify [ m ]	
21	Distance from ozone inlet:	Please specify [ m ]	
22	Inlet tube material:	Please select...	
23	Residence time from entry inlet line to entry of converter:	Please specify [ s ]	
24	Humidity/temperature control:	Please select...	
25	Inlet line temperature:	Please specify [ °C ]	
26	Inlet filter:	Please select...	
27			
28	<b>Converter (If CLD is used for NO<sub>2</sub> measurements):</b>		
29	Converter type:	Please select...	
30	Converter manufacturer:	Please select...	
31	Converter model:	Please select...	
32	Duration of stay in converter or bypass line:	Please specify [ s ]	
33	Duration of stay in converter:	Please specify [ s ]	
34	Converter temperature:	Please specify [ K ]	
35			
36	<b>Zeroing (If CAPS is used for NO<sub>2</sub> measurements):</b>		



## Component information

submitted 23 Sep 2022, 10:19 UTC

The facility PI fills information on the component-specific contacts and instrumentation in the forms below. After that he / she submits the information, and it will be automatically directed to the respective Topical Centre and Data Centre unit for further elaboration and contact with the facility PI and staff.

### Contacts

6 contacts

### Instruments

6 instruments

Condensable vapours  
CI-API-TOF  
(UHEL)

NO<sub>x</sub>  
(FZJN)

OVOCs  
PTRMS/DNPH  
(IMT)

NMHCs  
TD-GC-MS/FID  
(FZJV)

## Upgrade plan

The facility PI is to provide a plan how and when the facility will reach full technical compliance with ACTRIS requirements. If the facility is already in line with ACTRIS requirements, the PI is to upload a document stating that.

This should be uploaded only after contact with the respective TC.

### Upgrade plan

Not uploaded yet

## Commitment letter

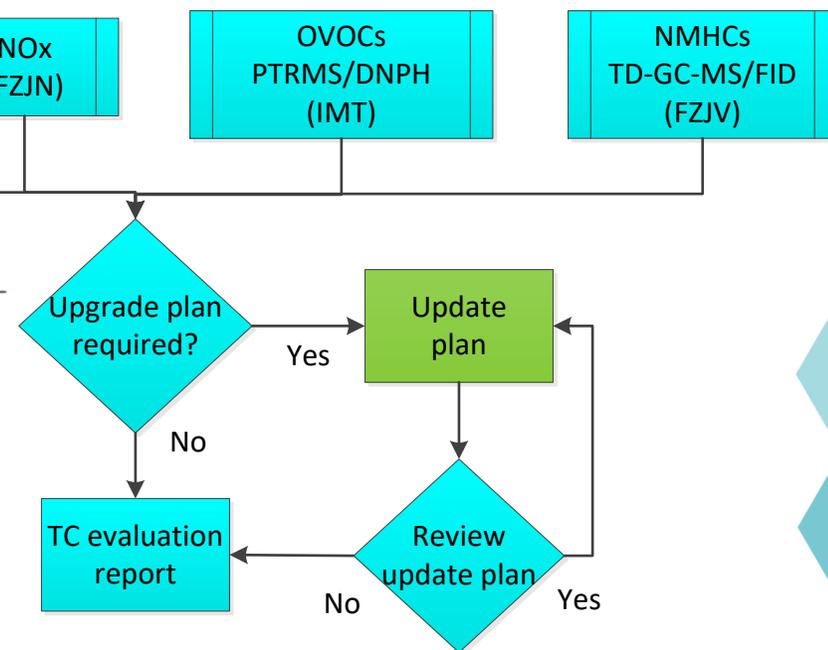
submitted 23 Sep 2022, 10:26 UTC

The organization hosting the facility has to commit to providing the needed resources for the facility for at least 5 years, and to approve the relevant ACTRIS policies. This commitment has to be signed by a legal signatory of the organization.

For commitment letter template and more information, press the button below.

### Commitment letter

Document uploaded



## Evaluation

In this stage the Director General of ACTRIS initially approves or refuses the facility to be an ACTRIS National Facility. The decision is communicated to the facility PI, the hosting organization and the hosting country. In case the facility is initially accepted, the status will also be visible in ACTRIS maps and documents.

### TC evaluation

The Topical Centre in charge of the applied measurement component evaluates the readiness of the facility and feasibility of its upgrade plan.

#### TC evaluation report

Not uploaded yet

### RI committee evaluation

The RI committee evaluates the facility in a broader context and gives recommendation whether the initial acceptance should be granted.

#### RI com evaluation report

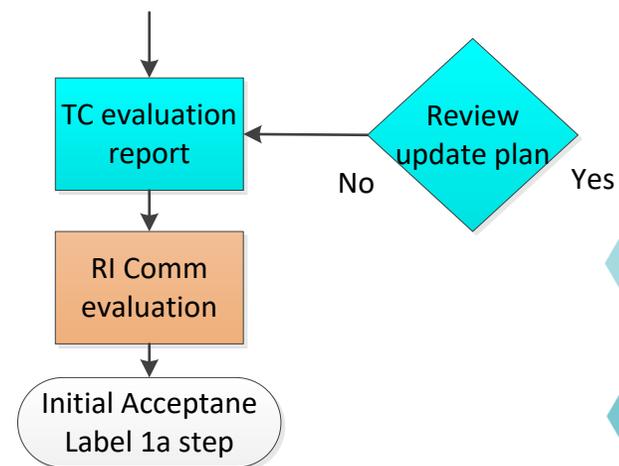
Not uploaded yet

1a

## Initial acceptance

1b

## Performance evaluation



Thank you!



# General Requirements for CiGas-NFs

- Collocated measurements of at least **6 different VOCs and NO<sub>x</sub>**
- Accompanied measurements of **meteorological parameters** in high time resolution near the place of the air intake port for the analysers. (wind speed, wind direction, air temperature, and air pressure)
- Use of a **standard traceable** to the CiGas Measurements
- The performance of the measurement instrument has to be checked against a target gas in regular intervals (e.g., monthly).
- Reported data include the measured amount fractions, precisions and uncertainties as specified in SOP-VOC (2014) and SOP-NO<sub>x</sub> (2014), as well as flags
- Data have to be regularly (e.g., monthly) reviewed for consistency with existing data from the same measurement site and against similar European measurement sites → @VOC@-Tool
- Data are submitted with metadata and data flagging at least yearly (by end of March).
- Data is reviewed by CiGas and will be discussed at an annual data quality meeting
- Participation in round-robin exercises
- Accept and organize performance audits by CiGas.

**Specific requirements for cluster compounds and data submission → Following presentations**



Reference: ACTRIS-PPP-Deliverable D5.1: Documentation on technical concepts and requirements for ACTRIS Observational Platforms



# Measurement Requirements for NMHCs

- At least 6 different VOCs have to be measured
- Atmospheric NMHCs have to be preconcentrated, subsequently separated by gas chromatography and finally analysed by mass spectrometry (GC-MS) or flame ionization detection (GC-FID).
- Analysis can be performed on-line (at the site) or off-line (i.e., sampling at the site and analysis remotely in the lab).
  - Off-line sampling intervals have to be **at least twice a week** and sampling has to follow a station-specific protocol, where station-characteristic air masses are sampled with little contamination due to local sources.
  - On-line sampling has to be performed continuously, with an interval of **at least twice daily** but preferably in hourly intervals.
- Alternatively, unsaturated NMHCs (aromatics and alkenes) can also be measured without preconcentration, using specific detection such as proton transfer reaction–mass spectrometry (e.g., PTR-MS).



# Measurement Guidelines

Standardised procedures for measurement, data evaluation, quality assurance, quality control, and data reporting of ACTRIS variables.

Currently updated for GC-FID/MS techniques  
To be released for PTR-MS in 2022



*NO<sub>x</sub>/VOC QA workshop 2023; Online – April, 17<sup>th</sup> -*

WORLD METEOROLOGICAL ORGANIZATION

GLOBAL ATMOSPHERE WATCH



GLOBAL  
ATMOSPHERE  
WATCH

GUIDELINE

FOR MEASUREMENTS OF

NON-METHANE HYDROCARBONS (NMHCs)

IN THE TROPOSPHERE

Contributing authors in alphabetical order:

E. C. Apel, A. Baldan, A. Claude, J. Englert, A.-M. Fjaeraa, M. Guillevic, D. Helmig, C. C. Hoerger, J. Hopkins, A. C. Lewis, C. Plass-Duelmer, S. Reimann, S. Sauvage, I. J. Simpson, R. Steinbrecher, D. Worton

# Data quality objectives for NMHCs measured by GC

Table 3 Data quality objectives (DQOs) for the measurements of NMHCs in whole air compressed test gases (inter-laboratory compatibility) expressed as the expanded combined uncertainty ( $k=2$ ) and the repeatability ( $k=1$ ; standard deviation). The basic station performance requirements correspond to the former and weaker DQOs of GAW Report 171 (2006).

	GAW basic performance expanded combined uncertainty	GAW basic performance repeatability	<b>ACTRIS</b> target performance expanded combined uncertainty	<b>ACTRIS</b> target performance repeatability
Alkanes	10%	5%	5%	2%
alkenes incl. isoprene	20%	10%	5%	2%
Alkynes	15%	5%	5%	2%
Aromatics	15%	10%	5%	2%
mole fraction <sup>(1)</sup>	10/15/20			
<100 pmol/mol	pmol/mol	5/10 pmol/mol	5 pmol/mol	2 pmol/mol

<sup>(1)</sup>For mole fractions below 100 pmol/mol, the DQO are expressed in pmol/mol, reference is the above stated relative value at 100pmol/mol e.g. for alkanes basic performance 10 pmol/mol.



# NMHC-Gas Standard Requirements

The Central Calibration Laboratory (CCL) maintains the primary standard that defines the calibration scale. → NPL (UK)

Standard requirements for ACTRIS-NFs:

1. (secondary) **Laboratory standard:** multi-component standard (synthetic mixture), produced and certified by the CCL.
2. (tertiary) **Working standards:** Cover most (ideally all) components measured and are used for regular calibration. WS can be other-certified or custom-made synthetic mixtures, or compressed whole air, calibrated by CiGas.
3. A **target gas mixture:** Compressed whole air / synthetic mixture calibrated by CiGas.

The target gas is used to check the assigned values of the calibration mixtures and the calibration process itself, and is treated as an air sample with unknown amount fraction. Monitoring the target gas concentrations yields information about the performance of the instrument, drifts of the laboratory standard, and potential instrument problems.

*Recommended frequencies for standard, blank and target gas measurements*

System	Lab. Standard	Working Standard	Blank	Target gas	Stand. Addition
GC-FID	2/year*	2/month*	1/week	1/month*	1/year*
GC-MS	2/year*	Every 2-4 samples	1/week	1/month*	1/year*

\*) 3-5 replicates



## Certificate of Calibration

NPL PRIMARY REFERENCE MATERIAL

Cylinder Number: D933529

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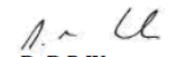
**CUSTOMER:** Forschungszentrum Jülich GmbH  
**ADDRESS:** Institut IEK-8: Troposphäre, Wilhelm-Johnen-Strasse, 52425 Jülich, Germany  
**CALIBRATION DATE:** 08 December 2020  
**AMOUNT FRACTIONS:**

Component	Amount fraction / (nmol/mol)	Component	Amount fraction / (nmol/mol)
Ethane	4.24 ± 0.13	2-methylpentane	4.39 ± 0.09
Ethene	4.15 ± 0.09	n-hexane	4.39 ± 0.09
Propane	4.18 ± 0.09	Isoprene	4.37 ± 0.09
Propene	4.15 ± 0.09	n-heptane	4.40 ± 0.09
2-methylpropane	4.26 ± 0.11	Benzene	3.72 ± 0.08
n-butane	4.22 ± 0.09	2,2,4-trimethylpentane	4.13 ± 0.09
Ethyne	4.37 ± 0.22	n-octane	4.14 ± 0.09
trans-but-2-ene	4.23 ± 0.09	Toluene	3.61 ± 0.10
But-1-ene	4.21 ± 0.09	Ethylbenzene	3.91 ± 0.10
cis-but-2-ene	4.22 ± 0.09	m-xylene + p-xylene	7.60 ± 0.20
2-methylbutane	4.16 ± 0.09	o-xylene	3.74 ± 0.10
n-pentane	4.18 ± 0.09	1,3,5-trimethylbenzene	3.80 ± 0.10
1,3-butadiene	4.27 ± 0.09	1,2,4-trimethylbenzene	3.83 ± 0.10
trans-pent-2-ene	4.20 ± 0.09	1,2,3-trimethylbenzene	3.80 ± 0.10
Pent-1-ene	4.27 ± 0.09	Nitrogen	Balance

The reported expanded uncertainties are based on standard uncertainties multiplied by a coverage factor  $k=2$ , providing a coverage probability of approximately 95 %. The uncertainty evaluation has been carried out in accordance with UKAS requirements.

**METHODS:** Preparation: gravimetry; Analysis: gas chromatography (FID)  
**TRACEABILITY:** The values on this certificate are traceable to NPL Primary Standards  
**EXPIRY:** Certificate valid for 5 years from the date of issue  
**PRESSURE:** Fill pressure: 100 bar; Minimum utilisation pressure: 10 bar  
**STORAGE:** No special precautions are required  
**HANDLING:** Refer to ISO 16664  
**OUTLET:** DIN 477 No. 1 valve  
**INTENDED USE:** Calibration standard

**Reference:** 2021030009-1 **Date of issue:** 22 March 2021

**Signed:**  (Authorised Signatory)

**Name:** Dr D R Worton (on behalf of NPLML)

**Checked by:** 

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## Certificate of Calibration

NPL PRIMARY REFERENCE MATERIAL

Cylinder Number: D933592

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**CUSTOMER:** Forschungszentrum Jülich GmbH  
**ADDRESS:** Institut IEK-8: Troposphäre, Wilhelm-Johnen-Strasse, 52425 Jülich, Germany  
**CALIBRATION DATE:** 05 May 2021  
**AMOUNT FRACTIONS:**

Component	Amount fraction / (nmol/mol)
Toluene	3.93 ± 0.12
(+/-)- $\alpha$ -pinene	4.17 ± 0.21
(+)-3-carene	3.93 ± 0.20
R-(+)-limonene	3.81 ± 0.12
1,8-cineole	4.08 ± 0.21
Nitrogen	Balance

The reported expanded uncertainties are based on standard uncertainties multiplied by a coverage factor  $k=2$ , providing a coverage probability of approximately 95 %. The uncertainty evaluation has been carried out in accordance with UKAS requirements.

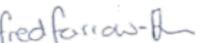
**METHODS:** Preparation: gravimetry; Analysis: gas chromatography (FID)  
**TRACEABILITY:** The values on this certificate are traceable to NPL Primary Standards  
**EXPIRY:** Certificate valid for 1 year from the date of issue  
**PRESSURE:** Fill pressure: 100 bar; Minimum utilisation pressure: 10 bar  
**STORAGE:** No special precautions are required  
**HANDLING:** Refer to ISO 16664  
**OUTLET:** DIN 477 No. 1 valve  
**INTENDED USE:** Calibration standard

**Reference:** 2021030009-2

**Date of issue:** 07 May 2021

**Signed:**  (Authorised Signatory)

**Name:** Dr P J Brewer (on behalf of NPLML)

**Checked by:** 

Page 1 of 1