RI URBANS
HORIZON 2020
European Commission

Guidance documents for measurements and modelling of novel air quality pollutants

IAGOS profiles of AQ parameters

with the support of:
AXA Research Fund

Authors: Hannah Clark (IAGOS-CNR), Christoph Mahnke (ZJ), Andreas Petzold (FZJ)

Reviewers: Xavier Querol (CSIC), Christoph Gerbig (MPI-BGC)

Cover image created with AI using RECRAFT

Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS (RI-URBANS)

RI-URBANS (http://www.RIURBANS.eu) is supported by the European Commission under the Horizon 2020 – Research and Innovation Framework Programme, H2020-GD-2020, Grant Agreement number: 10103624

Table of Contents

ABBREVIATIONS

ACTRIS	Aerosols, Clouds and Trace gases Research InfraStructure
AQ	Air quality
AQMN	Air quality monitoring network
CAMS	Copernicus Atmosphere Monitoring Service
GAW	Global Atmosphere Watch programme by WMO
EU	European Union
IAGOS	In-service Aircraft for a Global Observing System
IAGOS-CORE	IAGOS system for providing global coverage on a day-to-day basis of key observables
IR	Infrared radiation
RI-URBANS	Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS EU-project
UV	Ultraviolet radiation

CHEMICAL SPECIES

CO	Carbon monoxide
H_2O	Water
NO	Nitrogen monoxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides ($NO+NO_2$)
O_2	Molecular oxygen/dioxygen
O_3	Ozone

1. ABOUT THIS DOCUMENT

This document was prepared as part of the "Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS" (RI-URBANS) EU-project that connects the atmospheric observation expertise from In-service Aircraft for a Global Observing System (IAGOS), as well as the urban air quality observation capacities of the regulatory air quality monitoring networks.

This document is a guide for the service tool "IAGOS profiles of air quality parameters". It describes the available air quality parameters from IAGOS profiling, the data access, examples of the use of IAGOS profiles over RI-URBANS pilot cities, and finally recommendations for this service tool.

This is a RI-URBANS/IAGOS guidance for this specific service tool that is part of the RI-URBANS deliverable D46 (D6.1, containing guidance for all service tools provided in the project) with the support for publication from AXA Research Fund to build up the final dissemination D55 (D7.6). Any dissemination of results must indicate that it reflects only the author's view and that the European Commission is not responsible for any use that may be made of the information it contains.

2. IAGOS PROFILES OF AIR QUALITY PARAMETERS

Using compact and automated in-situ sensors on board of passenger aircraft, the European Research Infrastructure IAGOS (In-service Aircraft for a Global Observing System; see Petzold et al. (2015), Thouret et al. (2022) and www.iagos.org for details) monitors vertical profiles of trace gas concentrations (incl. CO, O_3, NO_x, and H_2O) near airports during take-off and climb-out as well as during descent and landing flight phases between the ground and 10-12 km altitude. These profiles characterise the vertical distribution of trace gases from the free troposphere down to the regional-scale and urban background boundary layer that interacts with the urban pollution layer. In addition, elevated layers of polluted air that are often advected via regional or long-range transport can be identified with the help of IAGOS profiles and are assessed for their impact on urban air quality.

The IAGOS profile data provide valuable information that is otherwise not accessible, and complement the data provided by surface-based Air Quality Monitoring Network (AQMN) stations (Petetin et al., 2018), facilitating the link to high-resolution models and satellite observations particularly in the vertical dimension. Above the planetary boundary layer, the correlation between the IAGOS in-situ and the urban background observations decreases rapidly, while increasingly high correlations with remote Global Atmosphere Watch (GAW) stations like the Jungfraujoch observatory can be found (see Fig. 2). In summary, the representativeness of the IAGOS airborne measurements for the general conditions of the lower troposphere are carefully analysed by Petetin et al. (2018).

In the middle of 2024, IAGOS counts a fleet of 10 aircraft equipped with automatic instruments operated by eight international airlines. Of these, six regularly sample the European troposphere with ozone and CO since 2002 and two of them provide additional NO_x data since 2015 and 2023, respectively. A third one providing NO_x is planned for the end of 2024. Thanks to several equipped aircraft landing or taking off over the same airport, it may be possible to access the diurnal cycle of those parameters, as has been shown for ozone in Petetin et al. (2016).

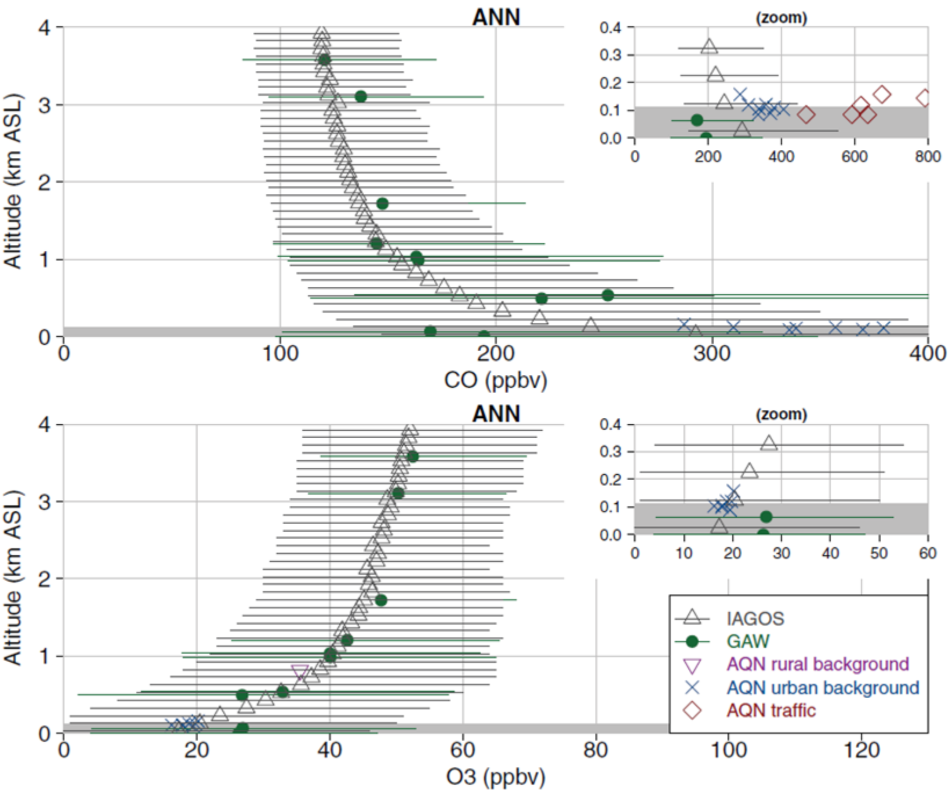
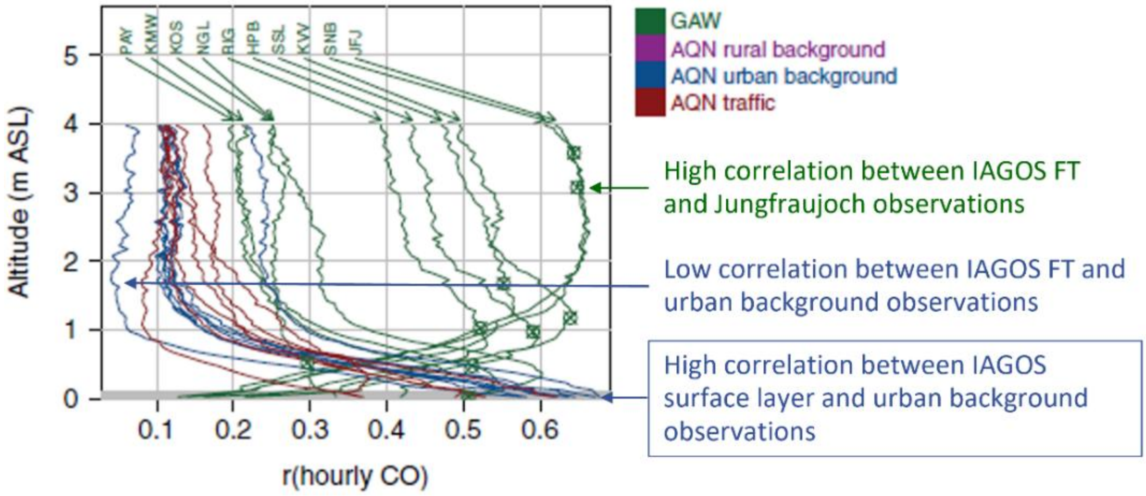


***Figure 1**: IAGOS CO and O3 profiles compared with surface stations (Frankfurt 2002 -2012).*

Source: Fig. 5 from Petetin et al. (2018).



High correlation between IAGOS FT and Jungfraujoch observations

Low correlation between IAGOS FT and urban background observations

High correlation between IAGOS surface layer and urban background observations

***Figure 2**: Correlation (r) profiles for IAGOS observations over Frankfurt (Main) airport (2002 -2012) with observations at surface stations. Source: Adapted from Fig. 7 in Petetin et al. (2018).*

3. AQ PARAMETERS AVAILABLE FROM IAGOS PROFILING

3.1 Ozone

3.1.1 Measurement technique

Ozone (O_3) is measured by UV absorption at a wavelength of 253.7 nm, using the optical block of a Thermo Instruments Model 49 analyser. Ozone-free air is generated by passing the ambient air through a scrubber. In-flight calibration checks are made with a built-in ozone generator.

3.1.2 Measurement performance

Time resolution: 4s

Precision: ±2%

Accuracy: ±2 ppb

A detailed overview of the IAGOS-CORE ozone measurements is given by Nédélec et al. (2015).

3.2 Carbon monoxide

3.2.1 Measurement technique

Carbon monoxide (CO) is measured by infrared absorption using the gas filter correlation technique. To achieve larger sensitivity and time response, the absorption cell is operated at a pressure of 2 bar and at a flow rate of 4 standard litres per minute (SLM). The IR detectors are Peltier cooled for noise reduction. In-flight calibration includes regular measurements of CO-free air generated by passing the dried ambient air over a bed of Sofnocat, a highly active precious metal catalyst for gas cleaning.

3.2.2 Measurement performance

Time resolution: 30s

Precision: ±5%

Accuracy: ±5 ppb

A detailed overview of the IAGOS-CORE carbon monoxide measurements is given by Nédélec et al. (2015).

3.3 Nitrogen Oxides

3.3.1 Measurement technique

The IAGOS Package 2b (P2b) instrument is designed for the autonomous measurement of nitrogen oxides (NO_x). NO_x is defined as the sum of nitrogen monoxide (NO) and nitrogen dioxide (NO_2). The measurement principle is based on chemiluminescence, i.e., the photoelectric detection of the photons of energy hν, produced in a chemical reaction (R1) between atmospheric NO and ozone (O_3). Conversion of NO_2 to NO is achieved by photolytic conversion (R2) using the light of 4 UV-LEDs.

R1: $NO + O_3 \Rightarrow NO_2 + O_2 + h\nu$ ($600 < \lambda < 3000$ nm)

R2: $NO_2 + h\nu + O_2 \Rightarrow NO + O_3$ ($\lambda = 390$ nm)

The instrument measures NO and NO_x sequentially, by switching the LEDs of the converter off and on.

The P2b instrumentation consists of the instrument unit and two pressure cylinders, which provide oxygen and synthetic air for operation and in-flight calibration. The instrument is connected with PFA tubing to the inlet (Rosemount TAT housing) at the fuselage. The communication for data transmission between P2b and P1 is implemented via Ethernet connection.

3.3.2 Measurement performance

Time resolution: 4s (not all intervals contain data; sequential measurement of NO and NO_x)

Precision: NO: ±5% or ±25 ppt (4s, 1 sigma); NO_x: ±5% or ±35 ppt (4s, 1 sigma)

Accuracy: NO: ±7% or ±25 ppt (1 sigma); NO_x: ±15% or ±40 ppt (1 sigma)

Further details on the characterisation of the P2b NO_x instrument are described by Berkes et al. (2018).

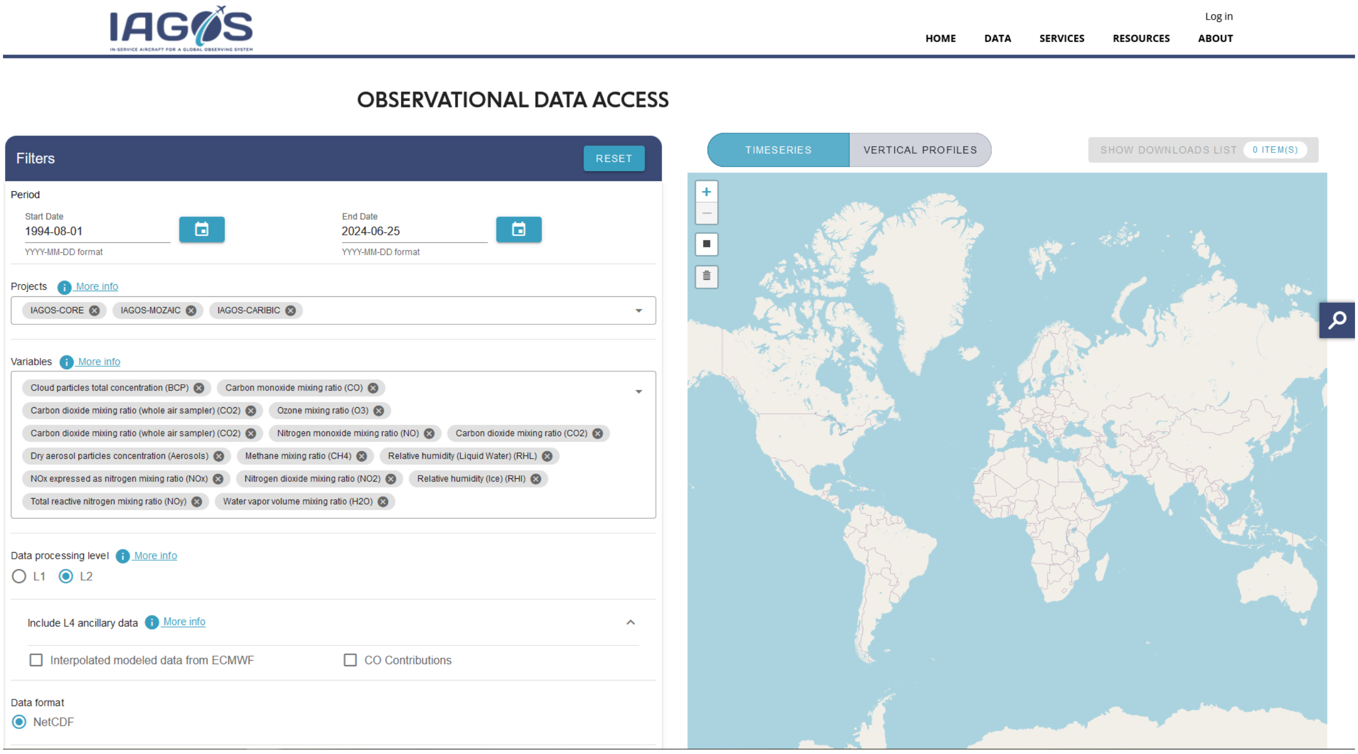
4. DATA ACCESS

The IAGOS data is available from www.iagos.org and can be selected using the “IAGOS data portal”. Registration is necessary and an account can easily be created via a personal ORCID.

4.1 Where to find and download the profile data

For RI-URBANS IAGOS’ vertical profiles data can be accessed at: https://www.iagos.org/products/

IAGOS data can be downloaded via the portal using the selection tool (see Fig. 3).



OBSERVATIONAL DATA ACCESS

Period

Start Date: 1994-08-01 (YYYY-MM-DD format)

End Date: 2024-06-25 (YYYY-MM-DD format)

Projects: IAGOS-CORE, IAGOS-MOZAIC, IAGOS-CARIBIC

Variables: Cloud particles total concentration (BCP), Carbon monoxide mixing ratio (CO), Carbon dioxide mixing ratio (whole air sampler) (CO2), Ozone mixing ratio (O3), Carbon dioxide mixing ratio (whole air sampler) (CO2), Nitrogen monoxide mixing ratio (NO), Carbon dioxide mixing ratio (CO2), Dry aerosol particles concentration (Aerosols), Methane mixing ratio (CH4), Relative humidity (Liquid Water) (RHL), NOx expressed as nitrogen mixing ratio (NOx), Nitrogen dioxide mixing ratio (NO2), Relative humidity (Ice) (RHI), Total reactive nitrogen mixing ratio (NOy), Water vapor volume mixing ratio (H2O)

Data processing level: ○ L1 ● L2

Include L4 ancillary data

☐ Interpolated modeled data from ECMWF ☐ CO Contributions

Data format: ● NetCDF

***Figure 3**. Screenshot of the IAGOS observational data selection tool.*

4.2 File Format

The datafiles on the IAGOS data portal are provided in netcdf format.

5. EXAMPLES: PROFILES OF OZONE AND CARBON MONOXIDE OVER RI-URBANS PILOT CITIES

A visualisation service is available at www.iagos.org/products. This service displays the most recent profiles at worldwide airports as compared with the Copernicus Atmosphere Monitoring Service's models on both global and regional scales. A subset of profiles over the RI-URBANS pilot cities is accessible under the category RI-URBANS (see Figure 4). Currently, the pilot cities available are Amsterdam, Barcelona, Milano, Paris, and Zurich. In the first instance, they are compared with the CAMS global models, but will soon include the CAMS European AQ models on the regional scale. Profiles currently available are for O_3 and carbon monoxide and a similar service is under development for NO_x.

Figure 4 further illustrates the vertical profile of O_3 as observed over Barcelona during the morning profile (a) with around 15 ppb of ozone at the surface and the second profile b) with and around 55 ppb by noon.

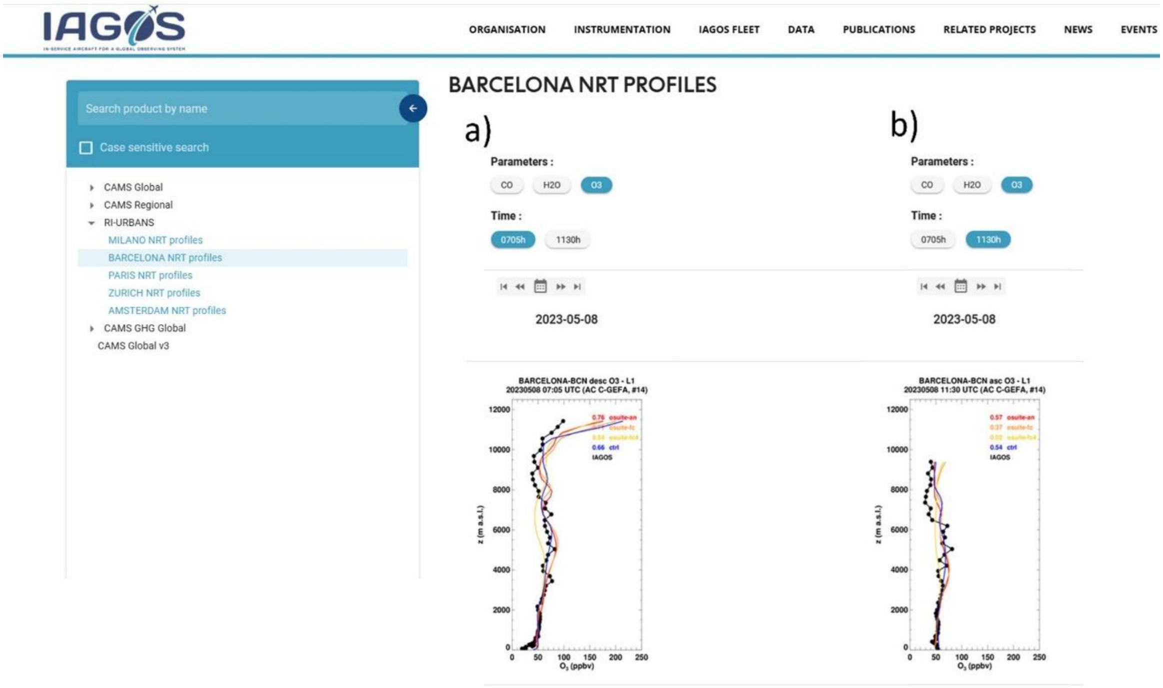


***Figure 4**. Combined screenshots of the visualisation service for profiles (available at www.iagos.org/products) over Barcelona. The diurnal O_3 profile as observed during the morning (a) and around noon (b).*

6. RECOMMENDATIONS

The IAGOS (In-service Aircraft for a Global Observing System; Petzold et al., 2015 and Thouret et al., 2022) vertical profiles of trace gas concentrations (incl. CO, O_3, and NO_x) near airports are measured in-situ during take-off and landing between the ground and 10-12 km altitude. These profiles characterise the vertical distribution of trace gases in the background atmosphere that interacts with the urban boundary layer. In addition, elevated layers that are often advected via regional or long-range transport are assessed for their pollution concentrations. We recommend using the valuable information provided by the IAGOS profile data complementary to the surface-based AQMN stations.

Furthermore, it is recommended to use the data with additional services, such as those developed in the context of the Research Infrastructure. To further interpret and assess the origin of polluted air masses, IAGOS provides the so-called added-value products and services to facilitate the analysis of vertical profiles.

For example, an application has been developed to provide the origin of the observed anomalies of CO along the vertical profiles. The SOFT-IO model (Sauvage et al., 2017) gives for every single vertical profile of CO recorded by IAGOS the origin of the emission in terms of type of source (either Anthropogenic or Biomass Burning) and in terms of geographical area. The visualisation tool has been developed in the frame of the ATMO-ACCESS project is available vi this link: https://www.atmo-access.eu/virtual-access/#/footprint-services

The possibilities to perform a timeseries analysis at different levels in the troposphere, with basic statistics and metrics are also available via https://www.atmo-access.eu/virtual-access/#/

7. REFERENCES

Berkes, F., Houben, N., Bundke, U., Franke, H., Pätz, H. W., Rohrer, F., Wahner, A., and Petzold, A., 2018. The IAGOS NOx instrument – design, operation and first results from deployment aboard passenger aircraft, Atmos. Meas. Tech., 11, 6, 3737-3757; https://doi.org/10.5194/amt-11-3737-2018.

Nédélec, P., Blot, R., Boulanger, D., Athier, G., Cousin, J.-M., Gautron, B., Volz-Thomas, A., Petzold, A., and Thouret, V., 2015. Instrumentation on commercial aircraft for monitoring the atmospheric composition on a global scale: The IAGOS system, technical overview of ozone and carbon monoxide measurements, Tellus B, 67, 27791; https://doi.org/10.3402/tellusb.v67.27791.

Petetin, H., Thouret, V., Athier, G., Blot, R., Boulanger, D., Cousin, J.-M., Gaudel, A., Nédélec, P., and Cooper, O., 2016. Diurnal cycle of ozone throughout the troposphere over Frankfurt as measured by MOZAIC-IAGOS commercial aircraft, Elem. Sci. Anth., 4:000129; https://doi.org/10.12952/journal.elementa.000129.

Petetin, H., Jeoffrion, M., Sauvage, B., Athier, G., Blot, R., Boulanger, D., Clark, H., Cousin, J.-M., Gheusi, F., Nedelec, P., Steinbacher, M., and Thouret, V., 2018. Representativeness of the IAGOS airborne measurements in the lower troposphere, Elem. Sci. Anth., 6, 23; https://doi.org/10.1525/elementa.280.

Petzold, A., Thouret, V., Gerbig, C., Zahn, A., Brenninkmeijer, C. A. M., Gallagher, M., Hermann, M., Pontaud, M., Ziereis, H., Boulanger, D., Marshall, J., Nédélec, P., Smit, H. G. J., Frieß, U., Flaud, J.-M., Wahner, A., Cammas, J.-P., Volz-Thomas, A., and IAGOS-Team, 2015. Global-Scale Atmosphere Monitoring by In-Service Aircraft – Current Achievements and Future Prospects of the European Research Infrastructure IAGOS, Tellus B, 67, 28452; https://doi.org/10.3402/tellusb.v67.28452.

Sauvage, B., Fontaine, A., Eckhardt, S., Auby, A., Boulanger, D., Petetin, H., Paugam, R., Athier, G., Cousin, J.-M., Darras, S., Nédélec, P., Stohl, A., Turquety, S., Cammas, J.-P., and Thouret, V., 2017. Source attribution using FLEXPART and carbon monoxide emission inventories: SOFT-IO version 1.0, Atmos. Chem. Phys., 17, 15271–15292; https://doi.org/10.5194/acp-17-15271-2017.

Thouret, V., Clark, H., Petzold, A., Nédélec, P., and Zahn, A., 2022. IAGOS: Monitoring Atmospheric Composition for Air Quality and Climate by Passenger Aircraft, in: Handbook of Air Quality and Climate Change, edited by: Akimoto, H., and Tanimoto, H., Springer Nature Singapore, Singapore, 1-14, ISBN 978-981-15-2527-8; https://doi.org/10.1007/978-981-15-2527-8_57-1.