GASCATENA · PRODUCT FACTSHEET

Gravimetric calibration gas preparation

From recipe and weighing to a traceable certificate with GUM uncertainty: what GasCatena does, how it evaluates the uncertainty, and the standards it is built on.

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What GasCatena does

GasCatena guides laboratories through the gravimetric preparation of calibration gas mixtures according to ISO 6142-1: from the recipe, through every weighing at the balance, to a certificate with the composition, its uncertainty according to the GUM and the gas properties according to ISO 6976. It works alongside the analytical balance you already have, and documents every link of the traceability chain: the calibrated balance, the purity of the base gases from their certificates, the molar masses and the air at the balance.

Catena is Latin for chain. The International Vocabulary of Metrology defines metrological traceability as the property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty (VIM, JCGM 200:2012, 2.41). GasCatena is built to keep that chain complete and on record for every cylinder you prepare.

GasCatena is in development; the release is expected in early 2027.

The workflow in six steps

Step	What happens
1. Recipe	Target composition, the order of addition and any pre-mixtures or dilutions, with the expected uncertainty and gas properties known before you start.
2. Guided weighing	Target pressure and expected balance reading for every addition, with checks on stability and weighing direction, and a cooling wait after large pressure steps. The Aura1 records the air at the balance at every weighing.
3. Composition	Mole fractions with their standard uncertainty and covariance, normalised according to ISO 14912 and evaluated according to the GUM.
4. Verification	Comparison with an independent analysis of the same cylinder, judged with the E_n test (ISO 13528).
5. Scope check	The result is checked against the calibration and measurement capabilities (CMC) of one or more accreditation scopes.

Step	What happens
6. Certificate	A certificate as PDF and as ISO 23219 XML, with the composition, the uncertainty and the ISO 6976 properties.

Planning before you weigh

- A register of recipes for the mixtures you prepare regularly.
- The order of addition follows the vapour pressure of the components; pre-mixtures and dilutions are flagged.
- A pre-estimate of the uncertainty and the ISO 6976 properties of the mixture, before the first weighing.
- A warning when a component could condense at the final filling pressure.

Fewer errors at the balance

- Before the preparation starts: checks on the retest date of the cylinder, the calibration of the balance and the shelf life of the base gases.
- For every addition: the target pressure from the real-gas behaviour of the mixture (ISO 6976 compression factor) and the balance reading to expect.
- Unstable weighings and weighings in the wrong direction are rejected on the spot.
- A configurable cooling wait after large pressure steps, before the cylinder is weighed.
- Every preparation has a unique number, from the first weighing to the certificate.

Uncertainty according to the GUM

Every contribution is expressed as a standard uncertainty, combined according to the GUM (JCGM 100) and reported as an expanded uncertainty $U = k \cdot u$ with $k = 2$, in line with EA-4/02.

One principle: the larger one counts. Where GasCatena has two estimates of the same uncertainty, one specified (a calibration certificate or a data sheet) and one measured (from the measurement itself), it takes the larger of the two. A balance that was quieter than its certificate never leads to a smaller uncertainty than the certificate supports; a balance that was less quiet makes the budget honestly larger.

Included in the certified result:

- **Weighing**: the random part (reading noise, averaged over a series of readings) and the systematic part (scale error from the balance calibration, with the correlation between the weighings before and after an addition).
- **Purity** of each base gas, from its certificate.
- **Molar masses**, from the atomic weights (ISO 6976:2016) with their uncertainty.
- **Dilution**, for preparations with a dilution or blow-off step.
- **Normalisation**: the mole fractions add up to one (ISO 14912), with the resulting correlations propagated.
- **Additional terms** from process studies, such as a conservative term for air buoyancy and a term for the pressurised component after a large pressure step.
- **Stability** over the shelf life, when your scope sets a drift rate (ISO 6142-1): combined in quadrature, with its value and basis noted on the certificate. By default the drift rate is zero.
- **Gas properties**: calorific value, density, Wobbe index and compression factor according to ISO 6976, each with its uncertainty according to Annex B.

The air at the balance: the Aura1

A balance weighs in air, and the air pushes the cylinder up. In a difference weighing only the change in air density between the weighing before and after an addition matters. GasCatena reads the Aura1 next to the balance at every weighing: temperature, humidity and barometric pressure give the air density and the buoyancy effect of that addition. The Aura1 is compact, powered over USB and read directly by GasCatena; it is the recommended companion of every GasCatena installation.

The buoyancy correction is calculated, shown during the preparation and reported on the certificate. By default the certified uncertainty uses a conservative fixed term for air buoyancy. A method setting bases the certified result on the measured correction instead; it is off by default and not yet validated, so it is for use only once you have validated the correction within your own accreditation. The ambient readings are also checked against the limits of your scope or your stricter internal specifications.

Verification with NexChrom

Every prepared mixture can be compared with an independent analysis of the same cylinder and judged with the E_n test. NexChrom, the GC software from the same product line, provides such an analysis: errors-in-variables regression in conformity with ISO 6143 against certified reference gases, with GUM uncertainty on every mole fraction.

Certificates and records

- A certificate per preparation as PDF, with the fields of ISO 6141, and as machine-readable ISO 23219 XML.
- On the certificate: the composition with its expanded uncertainty, the ISO 6976 properties and an ambient snapshot per weighing with in-limit and out-of-limit flags against the scope.
- A register of base gases (pure gases and pre-mixtures, with their declared impurities), cylinders and balances with their calibration history.
- Reminders for expiring certificates, calibrations and shelf lives; a register of limits.
- An append-only change history, four user roles (operator, manager, auditor and administrator) that record who did what, and a one-click Excel export of all laboratory data for back-up and review.

Standards

Built for laboratories and reference material producers working to ISO/IEC 17025 and ISO 17034.

Standard	Role in GasCatena
ISO 6142-1	Gravimetric preparation of calibration gas mixtures: the method
ISO 6976:2016	Molar masses, compression factor and gas properties, with Annex B uncertainty
ISO 14912	Conversion and normalisation of the composition, with covariance
GUM (JCGM 100), EA-4/02	Evaluation and expression of the uncertainty
ISO 6141	Contents of the certificate
ISO 23219	Certificate data as XML
ISO 13528	E_n test for the verification
ISO 6143	Comparison method for the independent analysis (in NexChrom)

Standard	Role in GasCatena
ISO/IEC 17025, ISO 17034	The framework of the laboratories GasCatena is built for

Technical

- A web application that runs as a local service and is used in a web browser, at the bench or from another computer on the laboratory network.
- Fully offline, without a cloud account: preparations and certificates stay in your own laboratory.
- Runs on Windows or Linux.
- Works alongside your existing analytical balance; the balance is not part of GasCatena.
- Ambient conditions from the Aura1 sensor module (temperature, relative humidity and barometric pressure) over USB.

Status and contact

GasCatena is in development, with release expected in early 2027. This factsheet describes the product as it is being developed; details may change before release.

Register your interest or request a preview of a preparation from recipe to certificate: info@qualimetric.nl · nexchrom.nl/gascatena