

Precision Gas System Isotope Analyzer (PGSISO) Instrument Handbook

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Acronyms and Abbreviations

ARM	Atmospheric Radiation Measurement
ASCII	American Standard Code for Information Interchange
BNF	Bankhead National Forest
CCL	Central Calibration Laboratory
DOE	U.S. Department of Energy
DQR	Data Quality Report
FTIR	Fourier Transform Infrared
HITRAN	high-resolution transmission molecular absorption line parameters database
I/O	input/output
IR	infrared
LPM	liters per minute
MALT	Multiple Atmospheric Layer Transmission
MCT	mercury-cadmium-telluride
NOAA	National Oceanic and Atmospheric Administration
PGSISO	precise gas system for isotopes
PPB	parts per billion
PPM	parts per million
QA	quality assurance (data)
QC	quality control/checks (data)
RMSE	root-mean-square error
SGP	Southern Great Plains
VPDB	Vienna Pee Dee Belemnite
WMP	World Meteorological Organization

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1.0 Instrument Title

Precision gas system isotope analyzer (PGSISO)

2.0 Mentor Contact Information

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3.0 Instrument Design

The PGSISO is a combination of several systems in series; (1) gas processing components that pressurize and prevent liquid water entering the sample stream, and (2) the Spectronus FTIR spectrometer, which measures continuous CO₂, δ¹³C, δ¹⁸O, CH₄, CO, and N₂O. The Spectronus analyzer has been developed by the Centre for Atmospheric Chemistry at the University of Wollongong, Australia (Griffith et al. 2012), and manufactured by Ecotech Pty Ltd (<https://www.ecotech.com/>), headquartered in Melbourne, Australia.

Operating parameters internal to the Spectronus are monitored and logged. There are four tower sample inlet channels (for four tower sample heights) and five calibration cylinders that are sequentially selected via Valco multi-port valve. Data are logged by the native Spectronus software. The Spectronus database file is converted to ascii format and further processed to form the pgsiso.b1 datastream.

3.1 Instrument/Masurement Theory

The Spectronus FTIR trace gas analyzer is used to determine simultaneously the concentrations of several trace gases in air or another gas stream by collecting and analyzing the Fourier Transform Infrared (FTIR) spectrum of the gas sample. In the closed-path trace gas analyzer the air is contained in a sample cell that is multi-passed by the infrared (IR) beam. The analyzer consists of separate subsystems controlled by a single computer program:

- The sample handling subsystem, which carries out all sample handling, inlet sample stream selection, cell evacuation, and flushing procedures. This includes a 12-channel digital input/output (I/O) switching capability for switching 12 (or optionally more) solenoid valves, and also an 8-channel analogue-digital converter for logging environmental variables such as temperatures, pressures, and flows.

- The FTIR spectrometer, which produces and records the interferogram and then performs Fourier transformation in order to obtain the infrared spectrum of sampled air. This spectrometer is a Bruker IR cube fitted with a thermoelectrically cooled MCT (mercury-cadmium-telluride) detector (wavenumber range 1500-7800 cm^{-1}). The IR cube is coupled to a 24-meter multi-pass gas cell that contains the air to be analyzed.
- The spectrum analyzer, which provides quantitative analysis of measured spectra immediately after collection, with real-time display.
- Logging of analyzed concentrations, analysis parameters, and analogue input quantities to database file that are parsed to hourly .csv files for ingest by the U.S. Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) user facility.

Optical techniques such as FTIR spectrometry determine the absolute concentrations of individual trace gas species from the quantitative analysis of selected absorption bands or lines in the measured spectrum. The FTIR spectrometer records a broadband mid-IR spectrum that can be analyzed in selected spectral regions for several trace gases. For CH_4 , CO , N_2O , and CO_2 combination bands near 3600 cm^{-1} , the low-resolution FTIR spectrometer does not resolve individual isotopic species, and the relevant whole absorption bands are fitted assuming that all isotopologues are present in natural abundance.

For these determinations, natural variations in isotopic abundances do not significantly affect the FTIR measurements. In some cases, such as for $^{12}\text{CO}_2$ and $^{13}\text{CO}_2$ analyzed in the ν_3 bands near 2300 cm^{-1} , individual isotopologue concentrations can be determined independently from the spectrum, allowing the calculation of isotopic ratios.

The quantitative analysis of measured IR absorption spectra uses a computational approach to best-fit regions of the measured spectrum with a calculated spectrum based on knowledge of the sample conditions (pressure, temperature, pathlength), the HITRAN database of spectral line parameters (Rothman et al. 2005, 2009) and a model of the FTIR instrument line shape. Trace gas concentrations and instrument parameters are iteratively adjusted in the calculation to achieve best fit. This approach uses the program MALT (Multiple Atmospheric Layer Transmission; Griffith 1996) to calculate spectra and is described in more detail in Griffith et al. 2012 and the MALT user's manual.

From each measured spectrum, MALT retrieves the concentration of each target gas and converts to a mole-fraction scale using the measured total pressure and temperature of the sample. The raw FTIR scale depends on the accuracy of HITRAN parameters, the MALT spectrum model, the optical pathlength, temperature, pressure, and other parameters. It is usually within a few percent of established standard reference scales (Smith 2011).

3.2 Instrument System Functional Diagram

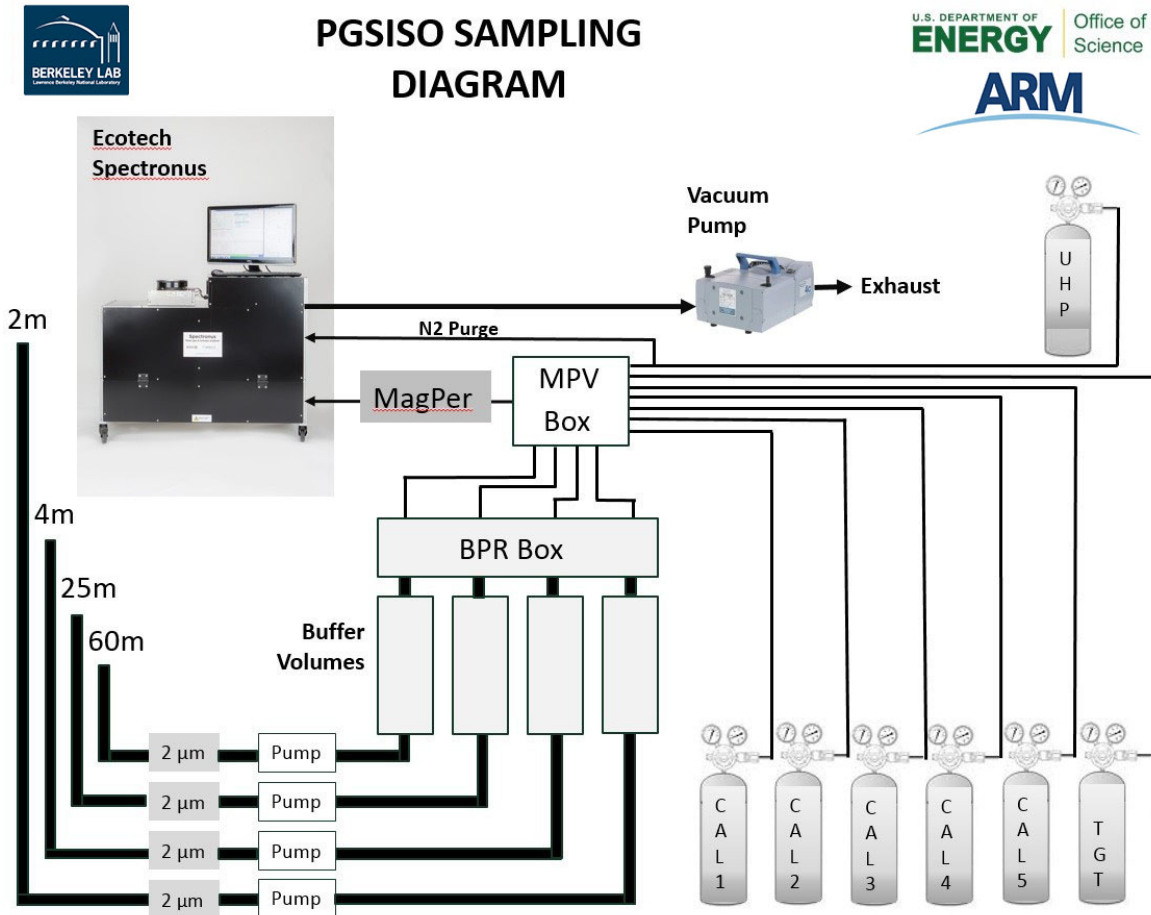


Figure 1. Plumbing diagram for PGSISO.

3.3 Calibration

Measurements of species are calibrated by measuring four span cylinders about every seven days, with measurements of one Target cylinder at the same pace, and another once per day. Linearly interpolated gain and offset coefficients for each species are applied to the sample data that undergo several stages of corrections prior to calibration. Notable regimes for reference calibration are:

- August 2013 deployment to September 2015 – 3-point calibration, linear interpolation.
- September 2015 to April 2023 – 4-point calibration, linear interpolation.
- January 2024 to present – 5-point calibration, quadratic interpolation.

Below are conversions, corrections, and calibration steps included in the a1-level to b1-level ingest processing.

3.3.1 Corrections

H₂O Correction

Water vapor displacement correction must occur for all species measured. The H₂O correction goes as:

$$\chi' = \frac{\chi}{\left(1 - \frac{q}{10^6}\right)}$$

where χ is the concentration of current sample measurement of species ¹²CO₂, ¹³CO₂, ¹⁸O¹²C¹⁶O, CH₄, CO, N₂O. and q is the concentration of H₂O at the coincident to measurement of χ .

Residual Correction

How and whether the residual correction is applied are determined based on measurement modes operated throughout the key time periods pertaining to the ARM Southern Great Plains (SGP) observatory deployment:

- August 2013 deployment to September 2015
 - Tower and Target tank (inlet 1-4, and 10, respectively)
 - $P_{\text{resid}} = P_{\text{evac2}} + 83.2 + 8.3 + 4.0$
where P_{evac2} is the evacuated pressure of previous sample measurement
 - Cal tanks (inlet 5-9)
 - $P_{\text{resid}} = 4.0$
- September 2015 to January 2017
 - Tower (inlet 1-4)
 - $P_{\text{resid}} = P_{\text{evac2}} + 8.3 + 4.0$
 - Target and Cal tanks (inlet 5-9, 10, 16)
 - $P_{\text{resid}} = 4.0$
- January 2017 to present → No residual correction.

Data collected for the upcoming Bankhead National Forest (BNF) deployment in Alabama also do not require a residual correction.

Correction for the presence of residual air sample from previous measurement is required, depending on whether the measurement cell is flushed or not flushed with current sample air prior to measurement of the current sample.

$$\chi' = \frac{(\chi P_{\text{cell}} - \chi_{\text{prev}} P_{\text{resid}})}{(P_{\text{cell}} - P_{\text{resid}})}$$

where χ is the H₂O corrected concentration of sample measurement of species ¹²CO₂, ¹³CO₂, ¹⁸O¹²C¹⁶O, CH₄, CO, N₂O; χ_{prev} is the H₂O corrected concentration from previous adjacent sample measurement; P_{resid} is the residual pressure of sample from previous measurement; P_{cell} is the cell pressure of current sample measurement.

Cross-Sensitivity Correction

This stage is for converting data to standard conditions. To first order, water vapor interference and sample pressure and temperature effects on the spectrum are included in the MALT calculation and spectrum fit. However, due to small inaccuracies and uncertainties in the measured spectrum, HITRAN line parameters, the spectral model, and the measured temperature and pressure, small dependences of apparent (raw) measured mole fractions on these parameters may remain.

$$\chi' = \chi - \frac{d\chi}{dQ}(Q - Q_0) - \frac{d\chi}{dP}(P - P_0) - \frac{d\chi}{dT}(T - T_0) - \frac{d\chi}{dF}(F - F_0) - \frac{d\chi}{dC}(C - C_0)$$

where χ is the H₂O corrected and if applicable, residual corrected concentration of sample measurement of species ¹²CO₂, ¹³CO₂, ¹⁸O¹²C¹⁶O, CH₄, CO, N₂O; $d\chi^*$ is the cross-sensitivity coefficient for the species; Q is the concentration of H₂O and Q₀ = 0 ppm; P is the cell pressure and P₀ = 1100 mbar; T is the cell temperature and T₀ = 35°C; F is the cavity sample flow and F₀ = 1 LPM; C is the concentration of CO₂ and C₀ = 400 ppm.

Rescale CO₂ Isotope Measurements from HITRAN to VPDB scale

To allow for calculation of $\delta^{13}\text{C}$ on the Vienna Pee Dee Belemnite (VPDB) scale:

$$^{12}\chi_{\text{vpdb}} = ^{12}\chi' \times 1.000150$$

$$^{13}\chi_{\text{vpdb}} = ^{13}\chi' \times 1.005280$$

$$^{18}\chi_{\text{vpdb}} = ^{18}\chi' \times 0.96319$$

where ¹² χ' , ¹³ χ' and ¹⁸ χ' are the H₂O-corrected, residual-corrected, cross-sensitivity-corrected concentration of scaled mole fractions for ¹²CO₂, ¹³CO₂, and ¹⁸O¹²C¹⁶O calculated from the HITRAN scale, respectively.

3.3.2 Reference Calibration

Calibration coefficients are determined by linear or quadratic regression by measuring known values of species for a set of calibration tanks. For linear calibration, gain and offset coefficients are calculated for each species. For quadratic calibration, curve, gain, and offset coefficients are calculated for each species.

The linear calibration for data from Aug 2013 to Apr 2023 goes as:

$$\chi_{\text{corr}} = (\chi' - b) / a$$

where χ' is the measured concentration of each species ¹²CO₂, ¹³CO₂, ¹⁸O¹²C¹⁶O, CH₄, CO, N₂O with relevant corrections from Section 3.3.1 applied, b is the offset coefficient, a is the gain coefficient, and χ_{corr} is the calibrated concentration of each species.

The quadratic calibration for data from Jan 2024 to present goes as:

$$\chi_{\text{corr}} = c \chi'^2 + a \chi' + b$$

where χ' is the measured concentration of each species $^{12}\text{CO}_2$, $^{13}\text{CO}_2$, $^{18}\text{O}^{12}\text{C}^{16}\text{O}$, CH_4 , CO , N_2O with relevant corrections from Section 3.3.1 applied, c is the curve coefficient, b is the offset coefficient, a is the gain coefficient, and χ_{corr} is the calibrated concentration of each species.

CO₂ Isotope Calibration

Known values of calibration cylinders are reported for $\delta^{13}\text{C}$, $\delta^{18}\text{O}$, and CO_2 , while scaled mole-fraction values are reported by the analyzer as χ'_{626} , χ'_{636} , χ'_{628} , for the $^{16}\text{O}^{12}\text{C}^{16}\text{O}$, $^{16}\text{O}^{13}\text{C}^{16}\text{O}$, and $^{18}\text{O}^{12}\text{C}^{16}\text{O}$ isotopologues respectively, and must first be converted. The steps to calculate calibrated CO_2 , $\delta^{13}\text{C}$, and $\delta^{18}\text{O}$ are:

1. Convert the reported known values of CO_2 , $\delta^{13}\text{C}$, and $\delta^{18}\text{O}$ into the scaled mole-fraction values for χ_{626} , χ_{636} and χ_{628} as:

$$\chi_{626} = \frac{y_{\text{co2}}}{R_{\text{sum}}x_{626}}$$

$$\chi_{636} = \frac{(1 + \delta^{13})y_{\text{co2}}}{R_{\text{sum}}x_{626}}$$

$$\chi_{628} = \frac{(1 + \delta^{18})y_{\text{co2}}}{R_{\text{sum}}x_{626}}$$

where y_{co2} is the known value of the mole fraction of CO_2 , δ^{13} is shorthand for the known value of the isotope ratio $\delta^{13}\text{C}/1000$, similarly for δ^{18} as the known value of the isotope ratio $\delta^{18}\text{O}/1000$, R_{sum} is the approximated sum of the dominant CO_2 isotopologues as:

$$R_{\text{sum}} = (1 + {}^{13}r)(1 + {}^{17}r + {}^{18}r)^2$$

where,

$${}^{13}r = {}^{13}r_{\text{ref}}(1 + \delta^{13})$$

$${}^{18}r = {}^{18}r_{\text{ref}}(1 + \delta^{18})$$

$${}^{17}r = {}^{17}r_{\text{ref}}(1 + (0.528 \delta^{18}))$$

and,

$${}^{13}r_{\text{ref}} = 0.111802, \text{ the abundance ratio of } ^{16}\text{O}^{13}\text{C}^{16}\text{O} \text{ to } ^{16}\text{O}^{12}\text{C}^{16}\text{O},$$

$${}^{18}r_{\text{ref}} = 0.00208835, \text{ the abundance ratio of } ^{18}\text{O}^{12}\text{C}^{16}\text{O} \text{ to } ^{16}\text{O}^{12}\text{C}^{16}\text{O},$$

$${}^{17}r_{\text{ref}} = 0.0003931, \text{ the abundance ratio of } ^{17}\text{O}^{12}\text{C}^{16}\text{O} \text{ to } ^{16}\text{O}^{12}\text{C}^{16}\text{O},$$

and,

$$x_{626} = 0.984054, \text{ the abundance of } ^{16}\text{O}^{12}\text{C}^{16}\text{O} \text{ in reference to VPDB}$$

2. Calculate the calibration coefficients independently for χ_{626} , χ_{636} and χ_{628} in the same manner as the other species.
3. Calculate calibrated CO_2 , $\delta^{13}\text{C}$ and $\delta^{18}\text{O}$ using χ_{corr} , the calibrated scale mole-fraction values from each isotopologue:

$$\delta^{13}\text{C} = \left(\frac{\chi'_{636,\text{corr}}}{\chi'_{626,\text{corr}}} - 1 \right) \times 1000\text{‰}$$

$$\delta^{18}O = \left(\frac{\chi'_{628,corr}}{\chi'_{626,corr}} - 1 \right) \times 1000\text{‰}$$

$$y_{co2} = \chi'_{626,corr} R_{sum} x_{626}$$

where, $\chi'_{626,corr}$, $\chi'_{636,corr}$ and $\chi'_{628,corr}$ are the calibrated scaled mole fractions of the isotopologues $^{16}O^{12}C^{16}O$ and $^{16}O^{13}C^{16}O$ and $^{18}O^{12}C^{16}O$ respectively, with relevant corrections from Section 3.3.1 applied, y_{co2} is the calibrated total isotopic mole fraction of CO_2 , and

$$R_{sum} = (1 + {}^{13}r)(1 + {}^{17}r + {}^{18}r)^2$$

where,

$${}^{13}r = {}^{13}r_{ref} (1 + \delta^{13}C/1000)$$

$${}^{18}r = {}^{18}r_{ref} (1 + \delta^{18}O/1000)$$

$${}^{17}r = {}^{17}r_{ref} (1 + (0.528 \delta^{18}/1000))$$

where $\delta^{13}C$ and $\delta^{18}O$ are the calibrated isotope ratios

3.4 Uncertainty

Overall instrument uncertainty is characterized by the variability in the calibration residual from measurements of Target cylinders compared to the known secondary values of each species, across the record from October 2013 to present (as of the date of this handbook).

This allows for the uncertainty to encompass components of uncertainty that are caused by systematic and/or operational errors that may or may not be characterized and that come from the actual operation of the system.

3.4.1 Uncertainty from Calibration Residuals

The Target calibration residual is defined as: Residual = (Calibrated, Measured) – (Known Value).

The table below represents uncertainty metrics used by mentors to assess instrument performance, where columns are defined as:

- MEAN = mean of difference measured and known quantities as $\chi_{resid} = \chi_{meas} - \chi_{known}$

where χ are subscripted as measured calibrated or known values of species CO_2 , $\delta^{13}C$, $\delta^{18}O$, CH_4 , CO , and N_2O

- STDERR = the standard error of the mean of residuals
- RMSE = the root-mean-square error calculated as,

$$\sqrt{(\sum \chi_{resid}^2 / N)}$$

where the summation occurs over the square of residual from of N Target tank measurements used in the assessment.

Table 1. Target calibration residual statistics on N Target calibration tank measurements from the SGP deployment AUG 2013 to APR 2023.

	MEAN	STDERR	RMSE	N
CO ₂ (ppm)	-0.1	0.0	0.2	1313
δ ¹³ C (‰)	0.1	0.0	0.2	1350
δ ¹⁸ O (‰)	-0.1	0.0	0.5	1404
CH ₄ (ppb)	-0.1	0.0	0.3	1329
CO (ppb)	1.3	0.0	1.6	1325
N ₂ O (ppb)	0.1	0.0	0.2	712

3.4.2 Culling Data for Residuals Statistics

Not all Target cylinder measurements are used in the assessment of instrument uncertainty. In addition to the diagnostic QC tests the measurements undergo (Section 4.2), specified periods of measurements of the Target tank are excluded from statistics using machine-readable documentation describing possible or confirmed periods of instrument instability coincident with those measurements. This machine-readable documentation is a mentor-compiled .csv file of all of the Data Quality Reports (DQRs) associated with the datastream and is used as a configuration file in the data ingest process. Examples of criteria for manually identified periods of instrument instability include:

- If H₂O measurements are abnormally high or variable
- Calibration coefficient outliers or periods of systematic deviation from expected values; significant outliers suggest the instrument was not in optimal condition and may be coincident with the previous criteria.

For the case of coefficients, when data is being reprocessed and coefficients are recalculated, the QC state of coefficients corresponding to the DQR entries are overwritten as “missing value” to then be excluded from linear interpolation of coefficients.

4.0 Definitions and Relevant Information

The b1-level datastreams are:

sgppgisisoC1.b1
bnfpgisisoS10.b1

Auxiliary and input datastreams associated with b1-level datastreams;

- for SGP:
 - sgppgisisoC1.a1
 - sgppgisisoC1.b0
 - sgppgisisocoeffC1.b1
- for BNF:
 - bnfpgisisoS10.a1
 - bnfpgisisoS10.b0
 - bnfpgisisocoeffS10.b1

4.1 Primary Variables

At b1-level, primary variable names are:

- CO2_AVG_CORR
- CH4_AVG_CORR
- CO_AVG_CORR
- N2O_AVG_CORR
- DELTA13C
- DELTA18O

Associated QC variables:

- CO2_AVG_CORR_QC
- CH4_AVG_CORR_QC
- CO_AVG_CORR_QC
- N2O_AVG_CORR_QC
- DELTA13C_QC
- DELTA18O_QC

Note:

- The “best data” are those with *_QC values of 0 for tower sample or Target measurements
- Tower sample data correspond to VALCOPOSITION variable equal to integers 1, 2, 3, or 4, for the four tower sample heights respectively.

4.2 QC Bit Definitions

flag_method = "bit" ;
bit_1_description = "Value is equal to missing_value -9999."; 1
bit_2_description = "Value is less than the valid_min."; 2
bit_3_description = "Value is greater than the valid_max."; 4
bit_4_description = "Value for *_slope is missing value"; 8
bit_5_description = "Value for *_slope_err is missing value"; 16
bit_6_description = "Value for *_slope is below valid_min."; 32
bit_7_description = "Value for *_slope is above valid_max."; 64
bit_8_description = "Value for *_slope is significant with respect to a slope of zero, where (abs(co2_slope-co2_slope_err) > 0)"; 128
bit_9_description = "QC state for at least one of the mentor-defined auxiliary variables is not equal to 0"; 256
bit_10_description = "Measurement follows a tank for which residual correction is not a sufficient correction"; 512
bit_11_description = "Measurement of N2 Purge Tank"; 1024

4.3 Calibration Database

Calibration tank values are transcribed to a machine-readable configuration file used in ARM ingest processing. The file is updated by the mentor each time the calibration tanks are changed out – about once

every five years. The values are provided by the World Meteorological Organization (WMO)'s Central Calibration Laboratory (CCL) at the U.S. National Oceanic and Atmospheric Administration (NOAA)'s Earth System Research Laboratory. The calibration scales used for each of the species for current installed calibration cylinders (July 2018) are given below in Table 2.

Table 2. WMO CCL scale spans for each species.

	Calibration Scale
CO ₂	WMO-CO ₂ -X2019
CH ₄	WMO-CH ₄ -X2004A
CO	WMO-CO-X2014A
N ₂ O	WMO-N ₂ O-X2006A

Contact the mentor for access to calibration certificates of each species.

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