



Product User Guide and Specification (PUGS) – ANNEX C for product CH4_GOS_SRPR (v2.3.9, 2009-2018)

C3S_312b_Lot2_DLR – Atmosphere

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Contributors

**INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP),
UNIVERSITY OF BREMEN, BREMEN, GERMANY
(IUP)**

M. Buchwitz

**SRON NETHERLANDS INSTITUTE FOR SPACE RESEARCH,
UTRECHT, THE NETHERLANDS
(SRON)**

I. Aben

L. Wu

O. P. Hasekamp



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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.3	20-October-2017	New document for data set CDR1 (2009-2016)	All
2.0	4-October-2018	Update for CDR2 (2009-2017)	All
3.0	12-August-2019	Update for CDR3 (2009-2018)	All
3.1	03-November-2019	Update after review by Assimila: Some typos corrected and references added.	All



Related documents

Reference ID	Document
D1	<p>Main PUGS:</p> <p>Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO₂ & CH₄) data set CDR 3 (2003-2018), project C3S_312b_Lot2_DLR – Atmosphere, 3.1, 2019.</p> <p><i>(this document is an ANNEX to the Main PUGS)</i></p>
D2	<p>TRD GHG, 2017: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1.3, 20-October-2017, pp. 53, 2017.</p>
D3	<p>Related ATBD:</p> <p>Wu, L., et al.: Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH₄_GOS_SRPR (v2.3.9, 2009-2018), C3S project C3S_312b_Lot2_DLR, v3.1, 2019.</p>



Acronyms

Acronym	Definition
ATBD	Algorithm Theoretical Basis Document
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CRG	Climate Research Group
D/B	Data base
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOSAT	Greenhouse Gases Observing Satellite
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
KIT	Karlsruhe Institute of Technology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NetCDF	Network Common Data Format
NIES	National Institute for Environmental Studies
NIR	Near Infra Red



NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PROxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SNR	Signal-to-Noise Ratio
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wave Infra Red
SZA	Solar Zenith Angle
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)



General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO ₂	Column-averaged dry-air mixing ratios (mole fractions) of CO ₂
XCH ₄	Column-averaged dry-air mixing ratios (mole fractions) of CH ₄
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO ₂ and CH ₄ information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO ₂ and CH ₄ information, e.g., 5 deg times 5 deg, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO ₂ and CH ₄



Scope of document

This document is a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) greenhouse gas (GHG) component as covered by project C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO₂) and methane (CH₄) Essential Climate Variable (ECV) data products will be generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The GHG satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO₂ and CH₄, denoted XCO₂ (in parts per million, ppm) and XCH₄ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO₂ (in ppm) and CH₄ (in ppb).

This document describes the C3S product CH₄_GOS_SRPR.

This product is the XCH₄ Level 2 product as retrieved from GOSAT using algorithms developed at SRON, The Netherlands.



Executive summary

This document is the Product User Guide (PUG), which is a deliverable of the C3S project. This document describes the RemoteC XCH₄ PROXY data product (CH4_GOS_SRPR) so that it will be clear for the user how to use the product. The description includes quality flags and metadata, data format, product grid, known limitations, bias correction, and the product (column) averaging kernels and a description how to use them.



1. Product description

The Japanese Greenhouse gases Observing SATellite (GOSAT) was launched on 23rd January 2009 (Yokota *et al.*, 2009) by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column CO₂ and CH₄ from its SWIR bands, Yoshida *et al.*, 2010. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS) as well as a dedicated Cloud and Aerosol Imager (TANSO-CAI).

The TANSO-FTS instrument has four spectral bands with a high spectral resolution 0.3 cm⁻¹, three of which operate in the SWIR at around 0.76, 1.6 and 2.0 μm providing sensitivity to the near-surface absorbers with the fourth channel operating in the thermal infrared between 5.5 and 14.3 μm providing mid-tropospheric sensitivity.

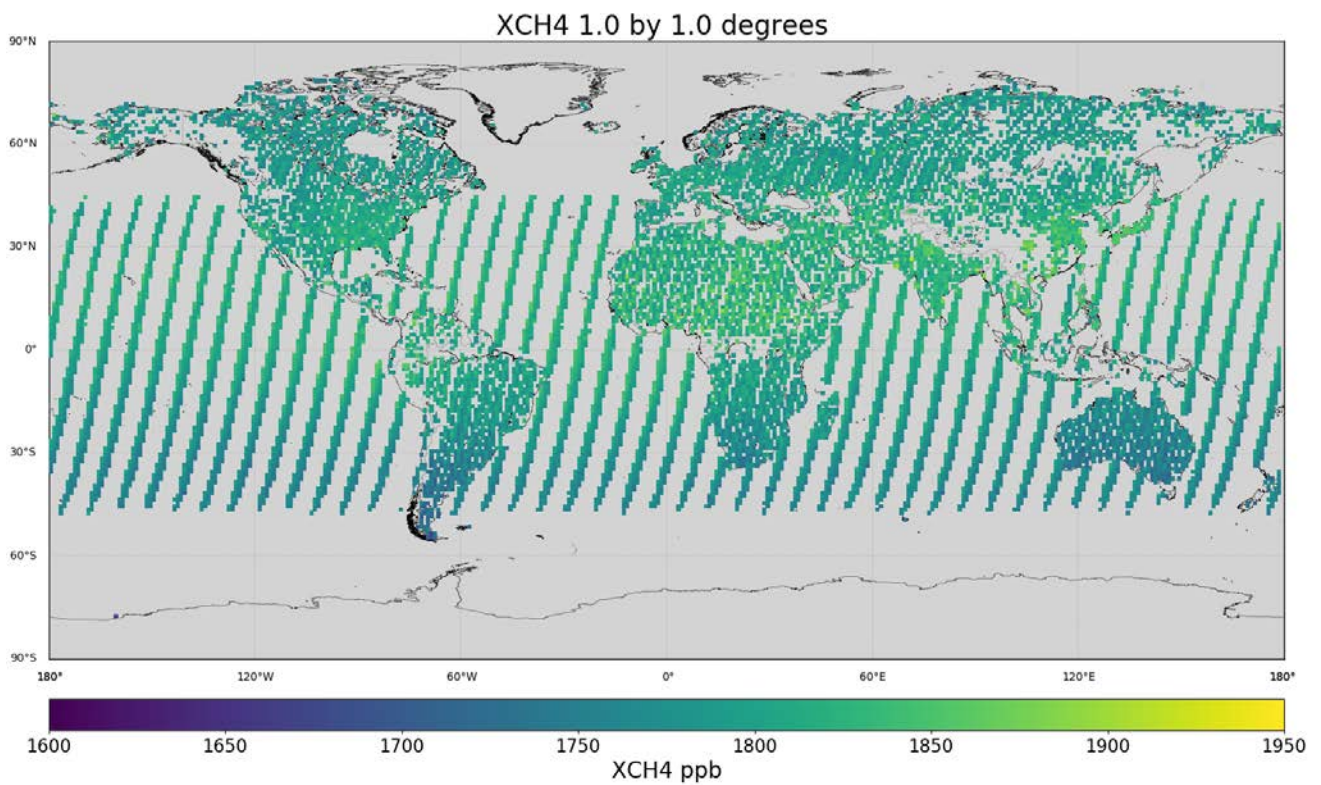
The measurement strategy of TANSO-FTS is optimized for the characterization of continental-scale sources and sinks. TANSO-FTS utilizes a pointing mirror to perform off-nadir measurements at the same location on each 3-day repeat cycle. The pointing mirror allows TANSO-FTS to observe up to ±35° across track and ±20° along-track. These measurements nominally consist of 3 across track points spaced ~100km apart (although measurements are possible with 1, 3, 5, 7 or 9 across track points) with a ground footprint diameter of approximately 10.5 km and a 4 second exposure duration. Whilst the majority of data is limited to measurements over land where the surface reflectance is high, TANSO-FTS also observes in sunglint mode over the ocean within ±20° of the sub-solar latitude.

The CH₄_GOS_SRPR product is retrieved from GOSAT TANSO-FTS NIR and SWIR spectra using the RemoTeC algorithm that has been jointly developed at SRON and KIT. The algorithm retrieves simultaneously XCH₄ and XCO₂. For the retrieval, we analyze four spectral regions: the 0.77 μm oxygen band, two CO₂ bands at 1.61 and 2.06 μm, as well as a CH₄ band at 1.64 μm. Within the retrieval procedure the sub-columns of CO₂ and CH₄ in different altitude layers are being retrieved. To obtain the column averaged dry air mixing ratios XCO₂ and XCH₄ the sub-columns are summed up to get the total column which is divided by the dry-air columns obtained from ECMWF model data in combination with a surface elevation data base. As the PROXY retrievals perform a non-scattering retrieval, the retrieved XCH₄ column cannot be used directly, as effects of aerosol scattering modify the light path. To correct for this, in the PROXY approach, the retrieved XCH₄ column is divided by the retrieved XCO₂ column at the 1.61 μm band and then multiplied by a XCO₂ total column obtained from LMD flask-based inversions. As the LMD flask inversions were not yet available at the time of delivery of this product, we extrapolated the 2015 model XCO₂ values by 3 ppm (the growth rate in 2016). The retrieved XCH₄ has been extensively validated with ground based TCCON measurements. To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2014 release of the TCCON data (Wunch *et al.* 2015).



More details on the technical aspects of the retrievals can be found in the ATBD Annex-C (D3).

Figure 1: Global XCH₄ for the 2009-2018 period for the CH₄_GOS_SRPR product on a 1 by 1 degree resolution.





2. Target requirements

Table 1: Target requirements for XCH₄.

Random and systematic error requirements for XCH ₄					
Parameter	Req. type	Random error ("Precision")		Systematic error	Stability
		Single obs.	1000 ² km ² monthly		
XCH ₄	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	< 1 ppb/year (absolute)
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative ^s)	< 2 ppb/year (relative ^s)
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative #)	< 3 ppb/year (relative #)

Table 1 shows the target requirements for XCH₄ (Threshold, Breakthrough and Goal) as derived in the Target Requirements Document (TRD) (D2).



3. Data usage information

3.1 Product Content and Format

The RemoteC XCH4 data product is stored per day in a single NetCDF file. Retrieval results are provided for the individual GOSAT spatial footprints, i.e. no averaging has been applied. The product file contains the key products, i.e. the retrieved column averaged dry air mixing ratio XCH4 with and without bias correction. Information relevant for the use of the data is included in the data file, like the vertical layering and averaging kernels. Also, the parameters that are retrieved simultaneously with XCH4 are included (e.g. surface albedo), as well as retrieval diagnostics like retrieval errors, quality of the fit.

Table 2: Common variables for the CH4_GOS_SRPR product

Name	Type	Dim.	Units	Description
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
time	float	n	seconds	Seconds since 1970-01-01 00:00:00
longitude	float	n	degrees_ east	Center longitude
latitude	float	n	degrees_ north	Center latitude
pressure_levels	float	n, 5	hPa	Pressure levels
pressure_weight	float	n, 4		Layer dependent weights needed to apply the averaging kernels
xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb
xch4_uncertainty	float	n	1e-9	1-sigma uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
xch4_averaging_kernel	float	n, 4		Normalized column averaging kernel
ch4_profile_apriori	float	n, 4	1e-9	A priori dry-air mole fraction profile of atmospheric methane
xch4_quality_flag	int	n		Quality flag for XCH4 retrieval, 0 = good, 1 = bad



Table 3: Product specific (additional) variables for the CH4_GOS_SRPR product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunglint	int	n		0 = no sunglint, 1 = sunglint
gain	char	n		gain setting of sensor, H = gain H, M = gain M
exposure_id	int	n		Exposure identification number of the sounding
l1b_name	char	n, 44		Name of the Level 1B file of the sounding
signal_to_noise_window	float	n, 4, 2		Signal to noise ratio per retrieval window and for both polarization directions
dry_airmass_layer	float	n, 4	m-2	Dry airmass per layer
altitude	float	n	m	Vertical altitude above the surface
air_temperature	float	n, 5	K	The bulk temperature of the air at each level
surface_altitude_stdv	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 5	m s-1	Eastward wind velocity
y_wind	float	n, 5	m s-1	Northward wind velocity
chi2	float	n		Chi-squared value of the sounding
optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol	float	n, 4		Scattering optical thickness per retrieval window
raw_xch4_err	float	n	1e-9	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
h2o_column_1593	float	n	m-2	Retrieved total water column at 1593 nm
h2o_column_1629	float	n	m-2	Retrieved total water column at 1629 nm
h2o_column_2042	float	n	m-2	Retrieved total water column at 2042 nm
surface_albedo_758	float	n		The retrieved albedo at 758 nm
surface_albedo_1593	float	n		The retrieved albedo at 1593 nm
surface_albedo_1629	float	n		The retrieved albedo at 1629 nm
surface_albedo_2042	float	n		The retrieved albedo at 2042 nm
intensity_offset_o2a	float	n	W cm-2	The retrieved intensity offset in the O2A band
raw_xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before scattering correction
xch4_no_bias_correction	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction
raw_xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before scattering correction
xco2_apriori	float	n	1e-6	A priori dry-air mole fraction of atmospheric carbon dioxide
co2_profile_apriori	float	n, 4	1e-6	A priori dry-air mole fraction profile of atmospheric carbon dioxide
xco2_averaging_kernel	float	n, 4		Normalized column averaging kernel for carbon dioxide
raw_xco2_err	float	n	1e-6	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide



3.2 Quality Flags and Metadata

There is a quality flag "xch4_quality_flag" included in the data file. The quality flag can have 2 values:

- 0: retrievals for **H-gain**, **M-gain** or **sunlint** data, quality has been checked
- 1: data should not be used (e.g. bad fit to data, residual cloud contamination)

For a GOSAT ground pixel to be processed by the RemoTeC PROXY algorithm it has to fulfill the following criteria: GOSAT nominal quality flags should be good and the standard deviation of the elevation in the pixel should be less than 1000 meters (to filter out the most extreme terrain).

After the retrieval the data that fulfill the following criteria are flagged as '0':

- Number of iteration steps in retrieval < 10.
- χ^2 of fit < 7.
- SNR > 50.
- Standard deviation of surface elevation within GOSAT ground pixel should be < 150 m
- SZA < 75°.
- $0.98 < \text{CO}_2$ (1.6 micron) / CO_2 (2.0 micron) < 1.15
- $0.88 < \text{O}_2$ (retrieved) / O_2 (prior) < 1.035
- $0.9 < \text{H}_2\text{O}$ (1.6 micron) / H_2O (2.0 micron) < 1.5

3.3 Bias Correction

From comparison with TCCON it was found that the error in XCH4 correlates with the retrieved albedo α at 1.6 um in band 2. Based on this correlation the following bias correction has been developed for XCH4:

$$XCH4_{corr} = XCH4 * (a + b * \alpha)$$

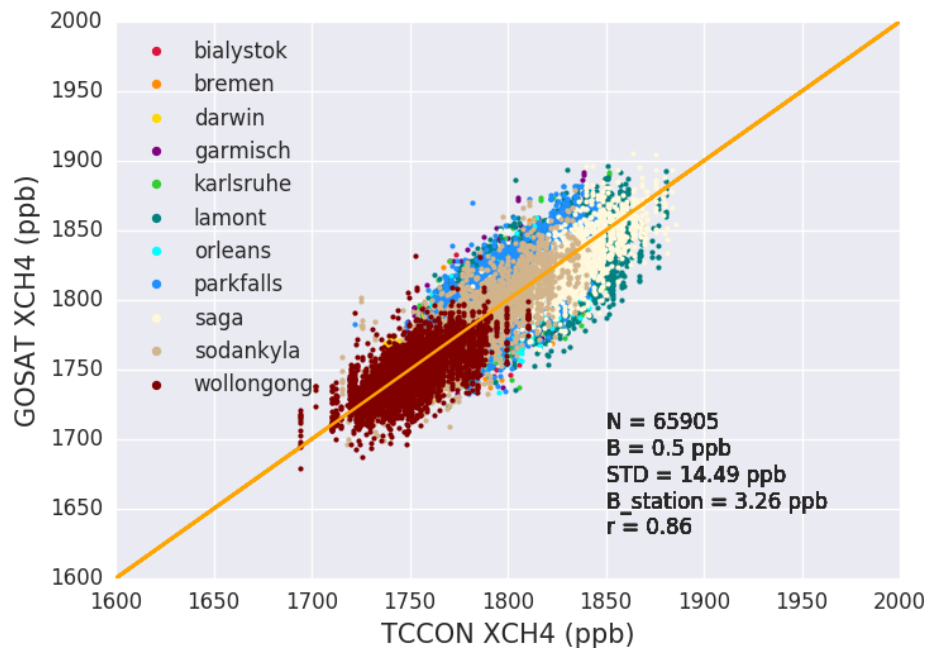
with $a = 0.9869$, $b = 0.01788$ for **H-gain** data and $a=0.98446$, $b = 0.01892$ for **M-gain** data. The bias correction parameters are obtained from fits to the GOSAT-TCCON differences. For **sunlint** observations we apply a global offset as a bias correction:

$$XCH4_{corr} = XCH4 * a$$

With $a = 0.992557$.



Figure 2: Co-located GOSAT-TCCON XCH4 measurements for gain H measurements.





3.4 Recommended data usage

It is strongly recommended to only use the bias-corrected data in: "xch4" except if users explicitly correct for biases themselves (e.g. in an inverse modeling framework). Here, it should be noted that the bias correction has been developed independently for the different GOSAT-FTS instrument settings (**H-gain**, **M-gain**, **sunlint**).

Also, use only data over land (land_type=0) except for sunlint cases.

If the data are to be compared with other XCO₂ and/or XCH₄ data for which vertical profile information is available (e.g. inverse modeling, comparison to models, comparison to measured profiles), the column averaging kernels should be used. Here it should be noted that **the column averaging kernels are to be applied to layer sub-columns (m-2)**, as these are the quantities directly retrieved in the RemoTeC algorithm. For model comparisons the retrieved XCO₂ should be compared to $[VCO_2]_{model}'/[VAIR]_{model}$ where $[VAIR]_{model}$ is the total dry air column provided by the model and $[VCO_2]_{model}'$ is the model total CO₂ column after applying the column averaging kernel, viz.:

$$[VCO_2]_{model}' = [VCO_2]_{prior} + \mathbf{a}^T (\mathbf{x}_{model} - \mathbf{x}_{prior})$$

where $[VCO_2]_{prior}$ is the prior CO₂ total column used in the retrieval, \mathbf{x}_{model} is the vertical CO₂ profile from the model (as sub-columns) and \mathbf{x}_{prior} is the prior vertical profile from the retrieval. For application of the column averaging kernel the model vertical profile should be re-calculated on the vertical grid of the retrieval (preferred) or the averaging kernel has to be interpolated to the vertical grid of the model.

3.4 Tools for Reading the Data

The data are stored in Netcdf format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc).

3.5 Known Limitations and Issues

- The data retrieved for the H-gain instrument settings are considered highest quality and are well validated. In the "raw" retrievals (i.e. before bias correction) there is a bias between **H-gain** and **sunlint** and **M-gain** retrievals, respectively. Although these biases have been corrected in the bias-corrected products, there may still be a small residual bias left, especially due to the limited number of validation sites for **sunlint** and **M-gain** retrievals.
- The 2nd half of December 2014 and the whole of January 2015 have no data due to the GOSAT satellite being in calibration mode after switching to the backup pointing system.



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